# Contents

# Plenary Talks

# Artificial Time Integration

*Author(s):*

U. Ascher

University of British Columbia, Vancouver, Canada

Many recent algorithmic approaches involve the construction of a differential equation model for computational purposes, typically by introducing an artificial time variable. The actual computational model involves a discretization of the now time-dependent differential system, usually employing forward Euler. The resulting dynamics of such an algorithm is then a discrete dynamics, and it is expected to be "close enough" to the dynamics of the continuous system (which is typically easier to analyze) provided that small – hence many – time steps, or iterations, are taken. Indeed, recent papers in inverse problems and image processing routinely report results requiring thousands of iterations to converge. This makes one wonder if and how the computational modeling process can be improved to better reflect the actual properties sought.

In this talk we elaborate on several problem instances that illustrate the above observations. Algorithms may often lend themselves to a dual interpretation, in terms of a simply discretized differential equation with artificial time and in terms of a simple optimization algorithm; such a dual interpretation can be advantageous. We show how a broader computational modeling approach may possibly lead to algorithms with improved efficiency.

# Approximations of Differential Forms

*Author(s):*

A. Buffa

Istituto di Matematica Applicata e Tecnologie Informatiche del CNR, Via Ferrata 1, 27100 Pavia, Italy

In a large class of applications, the partial differential equations underlying the physical models have a geometric interpretation and their unknowns can be thought as object from differential geometry such as differential forms. When we approach the problem of discretizing those equations, we have at least two choices: to use only the point of view of analysis, which involves construction of interior or exterior finite dimensional approximations of Banach spaces; to try to preserve the geometric structure of the continuous equations at the discrete level which will imply, e.g., discrete local conservation of physical quantities.

If we decide to pursue the second idea, we have to construct discrete analogues of differential forms, and of the structures they bring with themselves as exterior products, inner products, Hodge-$\star$ operators.

In the literature, there is a number of attempts to provide discretizations of differential forms in the context of finite differences, finite volumes and co-volumes methods, and finite element techniques. We refer, e.g., to [5], to [2] and to [4]. Recently, there has been the effort to construct a complete formalism for discrete exterior calculus and the results can be found in the important review paper [1] (similar ideas but possibly different purposes and terminology can be found in [6]).

After revising the existent techniques which have inspired the present work, I will propose a new framework which provides discretizations of differential forms on very general decompositions (polyhedral meshes) of the computational domain. I will set up the minimal conditions which are necessary to guarantee approximation properties in natural norms and I will also investigate the stability for the discretizations of two model problems: the Darcy flow equations and magnetostatics.

The methods and discretizations I propose are at the same time generalizations of finite differences and of finite elements, providing, in a suitable sense, a link between these two well known strategies in numerical analysis. If suitably designed, they will enjoy features from both techniques: low computational cost from finite differences, high flexibility and optimality from finite elements.

The topic of this talk is object of on going research and will be the content of a joint paper with F. Brezzi [3]. At the end of my talk, I will formulate a number of open questions.

## References

[1] D. N. Arnold, R. S. Falk, and R. Winther. Finite element exterior calculus, homological techniques, and applications. *Acta Numerica*, vol. 15, 1–155, 2006.

[2] P. B. Bochev and J. M. Hyman. Principles of mimetic discretizations of differential operators. In *Compatible spatial discretizations*, volume 142 of *IMA Vol. Math. Appl.*, pp 89–119. Springer, New York, 2006.

[3] F. Brezzi and A. Buffa. Scalar products of discrete differential forms. Technical report, IMATI-CNR, 2007. In preparation.

[4] R. Hiptmair. Finite elements in computational electromagnetism. *Acta Numerica*, vol 11, 237–339, 2002.

[5] J. M. Hyman and M. Shashkov. Natural discretizations for the divergence, gradient, and curl on logically rectangular grids. *Comput. Math. Appl.*, vol. 33(4), 81–104, 1997.

[6] L. Melvin. *Foundations of Computational Geometric Mechanics*. PhD thesis, California Institute of Technology, 2004.

# Near optimal recovery of arbitrary signals from uncomplete measurements

*Author(s):*

A. Cohen

Université Pierre et Marie Curie, Paris, France

Compressed sensing is a recent concept in signal and image processing where one seeks to minimize the number of measurements to be taken from signals or images while still retaining the information necessary to approximate them well. The ideas have their origins in certain abstract results from functional analysis and approximation theory but were recently brought into the forefront by the work of Candes-Romberg-Tao, and Donoho who constructed concrete algorithms and showed their promise in application. There remain several fundamental questions on both the theoretical and practical side of compressed sensing. This talk is primarily concerned about one of these issues revolving around just how well compressed sensing can approximate a given signal from a given budget of fixed linear measurements, as compared to adaptive linear measurements. More precisely, we consider discrete $N$-dimensional signals $x$ with $N \gg 1$, allocate $n \ll N$ linear measurements of $x$, and we describe the range of $k$ for which these measurements encode enough information to recover $x$ to the accuracy of best $k$-term approximation. We also consider the problem of having such accuracy only with high probability.

# Molecular modelling and differential equations: three examples

*Author(s):*

C. Le Bris

CERMICS, École Nationale des Ponts et Chaussées, 6 & 8, avenue Blaise Pascal, 77455 Marne-La-Vallée Cedex 2, and INRIA Rocquencourt, MICMAC project, Domaine de Voluceau, B.P. 105, 78153 Le Chesnay Cedex, France. Email :lebris@cermics.enpc.fr

Molecular modelling is a rich field of investigation for applied mathematics. This is also a rapidly developing field, where a mathematical perspective can definitely bring a lot. The talk will begin with a general presentation of the context and of the challenges of the field. See the monographs [4, 5] or the review articles [6, 7] for more details and also [8] for examples of ongoing works by various groups of researchers worldwide.

We will then present three examples of differential equations arising in the context of molecular modelling: a *partial* differential equation -related to electronic structure calculations-, an *ordinary* differential equation -arising in classical molecular dynamics-, and a *stochastic* differential equation -useful for free energy calculations.

For each of the above equation, we will give some elements of modelling, then see the mathematical and numerical questions raised.

All correspond to ongoing works with various collaborators.

The *partial* differential equation is an approximation of the Schrödinger equation. It yields a linear algebraïc system that is of large a size and is to be solved in linear time. In a series of works [1, 2, 3] in collaboration with M. Barrault, G. Bencteux (both at Electricité de France), E. Cancès (ENPC), and W. Hager (University of Florida), we introduced, developed and studied a domain decomposition algorithm well adapted to the electronic structure calculation context.

The *ordinary* differential equation is a highly oscillatory Hamiltonian system prototypical of those actually arising in molecular dynamics simulations. With F. Legoll (ENPC), we introduced in [9, 10] a systematic way to construct symplectic integrators for such oscillatory systems using the Hamilton-Jacobi form of the equations of motion and a two-scale convergence strategy.

The *stochastic* differential equation, useful for free energy calculations, which are of crucial interest for ensemble averaging techniques, is a *constrained* stochastic differential equation. The state of the art as regards numerical analysis for constrained SDEs is not at the level of that for constrained ODEs. A work in progress [11] with T. Lelièvre (ENPC) aims to introduce new, rigorously based integrators for such equations.

The talk will conclude with some tracks for further research.

## References

[1] M. Barrault, E. Cancès, C. Le Bris, W. Hager, *Multilevel domain decomposition for electronic structure calculations*, Journal of Computational Physics, Volume 222, Issue 1, 1 March 2007, pp 86-109

[2] M. Barrault, G. Bencteux, E. Cancès, C. Le Bris, W. Hager, *Domain decomposition and electronic structure computations: a promising approach*, to appear in Springer Series in scientific computation.

[3] G. Bencteux, E. Cancès, C. Le Bris, W. Hager, *Analysis of a quadratic programming decomposition algorithm*, preprint.

[4] E. Cancès, C. Le Bris, Y. Maday, & G. Turinici, **Mathematical Foundations of Molecular Modelling**, to appear, Oxford University Press.

[5] C. Le Bris, Editor, **Handbook of Numerical Analysis, special volume : computational chemistry**, North Holland, 2003.

[6] C. Le Bris,*Computational chemistry from the perspective of numerical analysis*, **Acta Numerica**, volume 14, 2005, pp 363-444.

[7] C. Le Bris, *Mathematical and numerical analysis for molecular simulation: accomplishments and challenges*, Proceedings of the International Congress of Mathematicians Madrid 2006, EMS, pp 1507-1522.

[8] C. Le Bris, A.T. Patera, Editors, **ESAIM-M2AN, Special volume on Molecular Modelling**, 2007, issue 2, in press.

[9] C. Le Bris, F. Legoll, *Dérivation de schémas numériques symplectiques pour des systèmes hamiltoniens hautement oscillants*, Note aux Comptes Rendus de l'Académie des Sciences, t. 344, Série 1, p 277-282, 2007.

[10] C. Le Bris, F. Legoll, *Symplectic integrators for highly oscillatory Hamiltonian systems.*, preprint.

[11] C. Le Bris, T. Lelièvre, *Consistency of different schemes for constrained SDEs*, in preparation.

# Lie Group and Homogeneous Variational Integrators and their Applications to Geometric Optimal Control Theory

*Author(s):*

M. Leok

Department of Mathematics Purdue University

The geometric approach to mechanics serves as the theoretical underpinning of innovative control methodologies in geometric control theory. These techniques allow the attitude of satellites to be controlled using changes in its shape, as opposed to chemical propulsion, and are the basis for understanding the ability of a falling cat to always land on its feet, even when released in an inverted orientation.

We will discuss the application of geometric structure-preserving numerical schemes to the optimal control of mechanical systems. In particular, we consider Lie group variational integrators, which are based on a discretization of Hamilton's principle that preserves the Lie group structure of the configuration space. In contrast to traditional Lie group integrators, issues of equivariance and order- of-accuracy are independent of the choice of retraction in the variational formulation. The importance of simultaneously preserving the symplectic and Lie group properties is also demonstrated.

In addition, we will introduce a numerically robust shooting based optimization algorithm that relies on the conservation properties of geometric integrators to accurately compute sensitivity derivatives, thereby yielding an optimization algorithm for the control of mechanical systems that is exceptionally efficient. The role of geometric phases in these control algorithms will also be addressed.

Recent extensions to homogeneous spaces yield intrinsic methods for Hamiltonian flows on the sphere, and have potential applications to the simulation of geometric exact rods, structures and mechanisms.

We will place recent work in the context of progress towards a coherent theory of computational geometric mechanics and computational geometric control theory, which is concerned with developing a self-consistent discrete theory of differential geometry, mechanics, and control.

The research has been supported in part by NSF grant DMS-0726263 and DMS-0504747.

# Variational approximations in quantum molecular dynamics

*Author(s):*

C. Lubich

Mathematisches Institut, Universität Tübingen, Auf der Morgenstelle, D-72076 Tübingen, Germany

The talk discusses computationally tractable approximations to the multi-particle time-dependent Schrödinger equation. These approximations are obtained from the Dirac-Frenkel time-dependent variational principle, which yields equations of motion on an approximation manifold. These nonlinear (partial or ordinary) differential equations form a non-canonical Hamiltonian system and hence preserve a symplectic two-form and the total energy. They yield approximations that are close to the best approximation to the wave function on the manifold, at least over short time intervals. Important examples of this variational approach are given by the multi-configuration time-dependent Hartree (MCTDH) method and variational Gaussian wavepacket propagation. Structure-preserving time integrators can be obtained by "variational splitting". To exemplify techniques, results and considerations from the field of geometric numerical integration of ODEs, the variational splitting integration scheme for Gaussian wavepackets and its remarkable properties are considered in some detail.

# Geometric integration of ODEs and PDEs

*Author(s):*

R. McLachlan

Massey University, Palmerston North, New Zealand

Numerical analysis as a whole is moving in the direction of special methods for special problems, so it is natural to ask what kinds of special problems there are. For ODEs, a systematic attack can be made on this question by classifying differential equations as Hamiltonian, symmetric, and so on. I will give an overview of geometric integration from this point of view: for each class, one should understand the members of the class, their generic dynamics and characteristic features, and be able to develop good numerical methods relevant to each class. For PDEs, no such approach is known; "every PDE is different." Known ODE classes can be generalized to PDEs, but the generalization is typically not unique. Symplectic integrators have been strikingly successful for Hamiltonian ODEs; does this carry over to multi-Hamiltonian PDEs? Many so-called multisymplectic integrators are now known; I will survey their features and the prospects they raise for numerical PDEs.

# Pricing financial derivatives in markets with jumps : a risk indifference approach

*Author(s):*

A. Sulem

INRIA Paris-Rocquencourt, B.P. 105, F–78153 Le Chesnay Cedex, France

B. Øksendal

CMA, University of Oslo, Box 1053 Blindern, N–0316 Oslo and Norwegian School of Economics and Business Administration, Helleveien 30, N–5045 Bergen, Norway

Stochastic processes with discontinuous paths are being increasingly considered as relevant alternatives to the log-normal Black-Scholes model for financial assets prices modelling. In this talk, we address the question of pricing derivatives in markets driven by Markov processes with jumps. These markets are generally incomplete : perfect hedge of contingent claims is not possible and the pricing rule depends on the preferences of the agent, which are traditionally expressed in the form of an utility function.

We introduce here the risk indifference pricing principle in incomplete markets: The *risk indifference price* is defined as the initial payment that makes the *risk* involved for the seller of a contract equal to the risk involved if the contract is not sold, with no initial payment The risk is measured here with convex risk measures. We use stochastic control theory to compute this risk indifference price, by studying an associated stochastic differential game problem and its Hamilton-Jacobi-Bellman-Isaacs partial integro-differential equation.

## References

[1] H. Föllmer and A. Schied: Convex measures of risk and trading constraints. *Finance Stochast.* 2: 429–447, 2002.

[2] S. Klöppel and M. Schweizer: Dynamic indifference valuation via convex risk measures *Mathematical Finance*, to appear

[3] B. Øksendal and A. Sulem: Applied Stochastic Control of Jump Diffusions. Second Edition. Springer, 2007.

# Conformal and Optimal Mass Transport Mappings for Surface Warping and Image Registration

*Author(s):*

A. Tannenbaum

Georgia Institute of Technology and Technion Department of Electrical and Computer Engineering

In this talk, we will outline some recent work using conformal and area-preserving mappings for problems in surface warping and image registration.

First, we consider a novel 3D visualization technique based on surface flattening for virtual colonoscopy. Such visualization methods could be important in virtual colonoscopy since they have the potential for non-invasively determining the presence of polyps and other pathologies. Further, we demonstrate a method which presents a surface scan of the entire colon as a cine, and affords viewer the opportunity to examine each point on the surface without distortion. We use certain angle-preserving mappings from differential geometry in order to derive an explicit method for flattening surfaces obtained from 3D colon CT imagery. Indeed, we describe a general method based on a discretization of the Laplace-Beltrami operator for flattening a surface onto the plane in a manner which preserves the local geometry. From a triangulated surface representation of the colon, we indicate how the procedure may be implemented using a finite element technique, which takes into account special boundary conditions. We also provide simple formulas which may be used in a real time cine to correct for distortion. This conformal flattening method will also be employed for flattening the brain on the sphere for visualization in functional MR.

Next, it is well known that a surface of non-zero Gaussian curvature can not be flattened by any means without some distortion. The conformal mapping is an attempt to preserve the appearance of the surface through the preservation of angles. However, in some applications it is desirable to be able to preserve areas instead of angles, so that the sizes of surface structures are accurately represented in the plane. This leads us to the theory of optimal mass transport.

The mass transport problem was first formulated by Gaspar Monge in 1781, and concerned finding the optimal way, in the sense of minimal transportation cost, of moving a pile of soil from one site to another. This problem was given a modern formulation in the work of Kantorovich, and is now known as the "Monge–Kantorovich problem." The registration problem is one of the great challenges that must be addressed in order to make image-guided surgery a practical reality. Registration is the process of establishing a common geometric reference frame between two or more data sets obtained by possibly different imaging modalities. In the context of medical imaging, this is an essential technique for improving preoperative and intraoperative information for diagnosis and image-guided therapy. Registration has a substantial recent literature devoted to it, with numerous approaches effective in varying situations, and ranging from optical flow to computational fluid dynamics to various types of warping methodologies.

The method we discuss in this talk is designed for elastic registration, and is based on an optimization problem built around the L2 Monge–Kantorovich distance taken as a similarity measure. The constraint that we put on the transformations considered is that they obey a mass preservation property. Thus, we are matching "mass densities" in this method, which may be thought of as weighted areas in 2D or weighted volumes in 3D. We will assume that a rigid (non-elastic) registration process has already been applied before applying our scheme.

Our method has a number of distinguishing characteristics. It is parameter free. It utilizes all of the gray-scale data in both images, and places the two images on equal footing. It is thus symmetrical, the optimal mapping from image A to image B being the inverse of the optimal mapping from B to A. It does not require that landmarks be specified. The minimizer of the distance functional involved is unique; there are no other local minimizers. Finally, it is specifically designed to take into account changes in density that result from changes in area or volume.

We believe that this type of elastic warping methodology is quite natural in the medical context where density can be a key measure of similarity, e.g., when registering the proton density based imagery provided by MR. It also occurs in functional imaging, where one may want to compare the degree of activity in various features

deforming over time, and obtain a corresponding elastic registration map. A special case of this problem occurs in any application where volume or area preserving mappings are considered.

This is joint work with Sigurd Angenent of the University of Wisconsin and Steven Haker of the Brigham and Women's Hospital.

# Minisymposium
# Applications to chemistry

Organised by
E. Cancès

## Tackling the Chemical Master Equation Directly by Adaptive Discrete Galerkin Methods

*Author(s):*

W. Huisinga

Hamilton Institute, Maynooth, Ireland

In mathematical biology, the stochastic description of biochemical reaction kinetics is increasingly being employed to model gene regulatory networks and signalling pathways. Mathematically speaking, such models require the numerical solution of the underlying evolution equation, also known as the chemical master equation (CME). Up to now, the CME has almost exclusively been solved by Monte-Carlo techniques, the most prominent of which is the simulation algorithm suggested by Gillespie in 1976. In this talk we present an alternative approach that is based directly on the CME as an evolution equation for the probability distribution. It focuses on the discrete partial differential equation (PDE) structure of the CME and thus allows to adopt ideas from adaptive discrete Galerkin methods. We present the mathematical background, the numerical approach and analyse two rather challenging illustrative model problems. This is joint work with P. Deuflhard, T. Jahnke and M. Wulkow.

## Mathematical and numerical analysis of some QMC methods

*Author(s):*

T. Lelièvre

CERMICS, Marne-La,Vallée, France

Quantum Monte Carlo (QMC) methods are Monte Carlo methods used to compute the ground state of Schrödinger operators. We present some mathematical and numerical results obtained on some QMC methods : - A new algorithm for Variational Monte Carlo computations based on a Langevin dynamics (in phase space) rather than on the classical biassed random walk. - A mathematical analysis of the fixed node approximation for Diffusion Monte Carlo computations. - A numerical analysis of various selection techniques to keep fixed the number of walkers in Diffusion Monte Carlo computations.

## References

[1] E. Cancès, B. Jourdain and T. Lelièvre, Quantum Monte Carlo simulations of fermions. A mathematical analysis of the fixed-node approximation, Mathematical Models and Methods in Applied Sciences, 16(9), 1403-1440, (2006).

[2] M. El Makrini, B. Jourdain and T. Lelièvre, Diffusion Monte Carlo method: numerical analysis in a simple case, To appear in Mathematical Modelling and Numerical Analysis.

[3] A. Scemama, T. Lelièvre, G. Stoltz, E. Cancès and M. Caffarel, An efficient sampling algorithm for Variational Monte Carlo, Journal of Chemical Physics, 125, 114105 (2006).

## A nonlinear model for the description of quantum electrons in a crystal with a defect

*Author(s):*

M. Lewin

Université de Cergy-Pontoise, France

I will present a recent work which was done in collaboration with Eric Cancès and Amélie Deleurence. We have introduced a new nonlinear variational model which allows to describe the behavior of quantum electrons in a crystal with a defect. This was done by comparison with another model of relativistic electrons studied by Hainzl, Séré, Solovej and myself. I will also explain a possible discretization of the model for the crystal, and show some preliminary computational results.

## Effective dynamics for constrained quantum systems

*Author(s):*

S. Teufel

Mathematishes Institut, Tübingen, Germany

We consider the Schroedinger equation on a Riemannian manifold with the assumption that the potential localizes finite-energy states close to a certain submanifold. This situation typically occurs in quantum molecular dynamics and for quantum wave guides. Mathematically the limit of strong localization is modeled by scaling the potential like $\epsilon^{-1}$ in the direction normal to the submanifold for $\epsilon \ll 1$. States with bounded energy are effectively confined to a $\epsilon$-tube around the submanifold by such a potential. We show that the dynamics of such states can be described by an effective Schroedinger equation on the submanifold and derive an asymptotic expansion of the corresponding effective Hamiltonian. This is joint work with Jakob Wachsmuth.

# Minisymposium
# B-series and Butcher trees

Organised by
A. Murua, H. Munthe-Kaas

# A Simplified Approach to the Order Conditions of Integration Methods

*Author(s):*

T.M.H. Chan

Department of Accounting, National Taichung Institute of Technology, Taichung, Taiwan

R.P.K.Chan

Department of Mathematics, the University of Auckland, New Zealand

We present an approach to the numerical integration of ordinary differential equations based on the algebraic theory of Butcher[2] and the $B$-series theory of Hairer and Wanner[9]. By interpreting the elementary weight function as a mapping from input values to output values and introducing some special mappings, we are able to derive the order conditions of several types of integration methods in a straight-forward way. The simplicity of the derivation is illustrated by linear multistep methods that use the second derivative as an input value, Runge-Kutta type methods that use the second as well as first derivatives, and general two-step Runge-Kutta methods.

*Keywords: Rooted trees, real-valued functions on trees, the elementary weight function, $B$-series, two-step Runge-Kutta methods, two-derivative Runge-Kutta methods, linear multi-step methods.*

## References

[1] Albrecht, P.: A new theoretical approach to Runge-Kutta methods. SIAM J. Numer. Anal. 24, 391-406(1987).

[2] Butcher, J.C.: An algebraic theory of integration methods. Math. Comp. 26, 79-106(1972).

[3] Butcher, J.C.: The numerical analysis of ordinary differential equations: Runge-Kutta and general linear methods. Chichester: John Wiley & Sons 1987.

[4] Butcher, J.C., Chan, T.M.H.: A new approach to the algebraic structures for integration methods. BIT 42, 477-489(2002).

[5] Butcher, J.C., Tracogna, S.: Order conditions for two-step Runge-Kutta methods. Appl. Numer. Math. 24, 351-364(1997).

[6] Chan, R.P.K.: Symmetric and symplectic Runge-Kutta-Nyström methods. Internal publication, Auckland 2002.

[7] Chan, R.P.K., Tsai, A.Y.J.: Two-derivative Runge-Kutta methods. Internal publication, Auckland 2003.

[8] Hairer, E., Nørsett, S.P., Wanner, G.: Solving ordinary differential equations I. Nonstiff problems. Second edition. Springer Series in Computational Mathematics 8. Berlin: Springer-Verlag 1993.

[9] Hairer, E., Wanner, G.: On the Butcher group and general multi-value methods. Computing 13, 1-15(1974).

[10] Hairer, E., Wanner, G.: Solving ordinary differential equations II. Stiff and differential-algebraic problems. Springer Series in Computational Mathematics 14. Berlin: Springer-Verlag 1991.

[11] Hairer, E., Wanner, G.: Order conditions for general two-step Runge-Kutta methods. SIAM J. Numer. Anal. 34, 2087-2089(1997).

[12] Hojjati, G., Rahimi Ardabili, M.Y., Hosseini, S.M.: New second derivative multistep methods for stiff systems. To appear.

[13] Kastlunger, K.H., Wanner, G.: Runge-Kutta processes with multiple nodes. Computing 9, 9-24(1972).

[14] Kastlunger, K.H., Wanner, G.: On Turan type implicit Runge-Kutta methods. Computing 9, 317-325(1972).

## On backward error analysis and symplecticity of Lie-Butcher series

*Author(s):*

H.Z. Munthe-Kaas

University of Bergen

LS series (Lie–Butcher series) is the generalization of B-series and S-series to analyze Lie group integrators. We will in this talk present new developments in the understanding of these series.

In the first part of the talk, we will discuss the characterization of backward error analysis, which algebraically is given as the (formal) logarithm with respect to the Grossman–Larson product. An algebraic understanding of this logarithm is obtained by considering the logarithm of the identity endomorphism in the underlying Hopf algebra, with respect to the convolution product. This trick is known in Feynman integrals of renormalization theory. There are also interesting connections between backward error analysis and Solomon descent algebras, which is a dual formulation of the logarithm.

In the second part of the talk we will present new developments in the understanding of symplecticity of Lie group integrators. Much of the established techniques for analyzing symplecticity of classical B-series, which are characterizing commutative group actions on hamiltonian systems with the canonical constant bracket on $\mathbb{R}^{2n}$, carries over to the much more general situation of general Hamiltonian actions on general symplectic– and Poisson–manifolds.

This is still work in progress, but we are now seeing the contours of a general theory of symplectic Lie group methods, with potentially many applications in computational mechanics.

## Preserving first integrals in LS-series integrators

*Author(s):*

B. Owren

The Norwegian University of Science and Technology

It has been known for some time that standard Runge-Kutta methods preserve all linear first integrals, a certain subclass of implicit schemes preserve quadratic first integrals, but no RK-scheme preserves all polynomial first integrals of higher degree than two. Furthermore, Runge-Kutta methods can not be volume preserving. Recently, Chartier, Faou and Murua have discussed similar issues for arbitrary maps which possess a $B$-series expansion. Also Iserles, Quispel and Tse have been doing such work for volume-preserving integrators. In this talk we shall consider how the results mentioned above can be extended to the setting of LS-series associated to for instance Lie group integrators. We shall see that some of the theory developed for standard integrators can be generalised directly, however other aspects may not make sense in the setting of general noncommutative Lie series expansions. The results are of a preliminary kind, but there is hope that this work may lead to a more complete understanding of the potential geometric properties of Lie group integrators.

## References

[1] P. Chartier, E. Faou, A. Murua, *An algebraic approach to invariant preserving integrators: The case of quadratic and Hamiltonian invariants*, Numer. Math. 103 (2006) 575–590.

[2] A. Iserles, G.R.W. Quispel, P.S.P. Tse, *B-series cannot be volume preserving*, BIT 2007 (to appear)

## Modified differential equations and B-series

*Author(s):*

P. Chartier

INRIA Rennes

E. Hairer

University of Geneva

G. Vilmart

INRIA Rennes and University of Geneva

Inspired by the theory of modified equations (backward error analysis), a new approach to high-order, structure-preserving numerical integrators for ordinary differential equations is developed [2, 3]. The idea is to apply a numerical integrator to a modified differential equation so that arbitrarily high-order can be obtained.

Special focus is paid to B-series for which a new composition law, called substitution law, is introduced [1, 2]. It is obtained by substituting a B-series into the vector field appearing in another B-series. We derive explicit formulas for the computation of this law and study its algebraic properties. It is shown that it allows a convenient derivation of the modified equations.

This is illustrated with the implicit midpoint rule applied to the full dynamics of the free rigid body [2] (see also [4]). Recently, this approach was also used in [5] to develop a new integrator for the Kepler problem, based on the implicit midpoint rule. It relies on the Kustaanheimo-Stiefel transformation, which links the three-dimensional Kepler problem to the four-dimensional harmonic oscillator.

# References

[1] P. Chartier, E. Hairer, and G. Vilmart. A substitution law for B-series vector fields. *INRIA Report*, No. 5498, 2005.

[2] P. Chartier, E. Hairer, and G. Vilmart. Numerical integrators based on modified differential equations. *Math. Comput.*, at press, 2007.

[3] P. Chartier, E. Hairer, and G. Vilmart. Modified differential equations. *ESAIM: Proc.*, to appear, 2007.

[4] E. Hairer and G. Vilmart. Preprocessed discrete Moser-Veselov algorithm for the full dynamics of the rigid body. *J. Phys. A: Math. Gen.* **39**, 13225-35, 2006.

[5] R. Kozlov. Conservative discretizations of the Kepler motion. *J. Phys. A: Math. Theor.* **40**, 4529-4539, 2007.

# Minisymposium
# Computation of invariant objects in dynamical systems

Organised by
C. Simo

## Classification of homoclinic connections in the planar circular restricted three-body problem

*Author(s):*

M. Gidea

Northeastern Illinois University, Chicago, U.S.A.

J. J. Masdemont

Universitat Politècnica de Catalunya, Barcelona, Spain

We consider the planar circular restricted three-body problem with primaries of equal masses; we let $L_1, L_2, L_3$ denote the collinear libration points, with $L_1$ being the point located between the primaries. For energy levels between those of $L_1$ and $L_2$, we compute the stable and and unstable invariant manifolds associated with Lyapunov orbits about the libration point $L_1$. The intersections of the invariant manifolds with the Poincaré plane of section $y = 0$, before a homoclinic connection occurs, consist of topological circles; after the homoclinic connection, the circles are destroyed and symbolic dynamics is created. We classify the homoclinic orbits according to the number of turns about the primaries. Details can be found in [2].

The intersections of the stable and unstable manifolds with the Poincaré section are charted out by a Cantor-type set shaped like a 'fish'; this region is similar to the 'maple leaf' stochastic region described for Hill's problem in [3].

Similar geometric structures are present for other mass ratios as well. We discuss potential applications of these geometric mechanisms of instability to space mission design and dynamical astronomy (see [1]).

## References

[1] E. Canalias and J.J. Masdemont, *Homoclinic and Heteroclinic Transfer Trajectories Between Planar Lyapunov Orbits in the Sun-Earth and Earth-Moon Systems*, Discrete and Continuous Dynamical Systems **14**, 2006, 261–279.

[2] M. Gidea and J.J. Masdemont, *Geometry of homoclinic connections in a planar circular restricted three-body problem*, International Journal of Bifurcation and Chaos, 2007, in press.

[3] C. Simó and T.J. Stuchi, *Central stable/unstable manifolds and the destruction of KAM tori in the planar Hill problem*, Phys. D **140**, 2000, 1–32.

## Technical aspects about the computation of the central and hyperbolic manifolds

*Author(s):*

G. Gómez

Dept. Matemàtica Aplicada i Anàlisi, Universitat de Barcelona, Barcelona, Spain

In this lecture we will present present and compare some methods that have been used for the description of the phase space around the collinear libration points, of either the RTBP and Hill's problem. The procedures are of three kinds: purely numerical, based on the Lindstedt-Poincare method and in normal forms computations.

## On the parallel computation of invariant tori

*Author(s):*

A. Jorba

University of Barcelona

E. Castellà
University of Barcelona

E. Olmedo
Deimos Space

The numerical approximation of invariant tori of flows (or maps) is a computationally intensive task, specially when the tori are of dimension strictly larger than 2 (or 1 for maps). In this talk we will discuss several ways of taking advantage of the parallel capacities offered by a cluster of computers. We will use examples coming from problems of Astrodynamics, that require the computation of 3-D and 4-D invariant tori.

## Symbolic dynamics and heteroclinic transitions for the Rossler system

*Author(s):*

P. Zgliczynski
Jagiellonian University,
Institute of Computer Science, Krakow, Poland

The Rössler system is given by

$$\begin{aligned} \dot{x} &= -(y+z) \\ \dot{y} &= x + by \\ \dot{z} &= b + z(x-a) \end{aligned} \tag{1}$$

where $a, b \in \mathbb{R}$ are fixed parameters. We chose $a = 5.7, b = 0.2$, these are parameters values originally considered by Rössler.

For the Rössler system we give a computer assisted proof of the existence of symbolic dynamics and heteroclinic chains joining period one and period two orbits. The period is meant in terms of the Poincaré map on section $x = 0$.

# Minisymposium
# Computation of orbits and n-body problems

Organised by
C. Simo

## Polynomial series methods in orbit determination

*Author(s):*

R. Barrio

Dpto. Matemática Aplicada, University of Zaragoza, E-50009 Zaragoza, Spain. Email: rbarrio@unizar.es

This talk will address some polynomial series methods developed (in fact some of them are variations of classical ones) to help in the orbit determination of particular problems in Dynamical Systems and Celestial Mechanics:

- When we face to the qualitative analysis of a dynamical system a carefully done numerical simulation is of great value. Some important objets are the periodic orbits and the study of the chaoticity [1] of the system. To reach this goal we need to solve the system itself and the variational equations (up to first or second order) with very high precision in some regions. A numerical method suitable for these problems is the *Taylor Series* method. This method is very classical but scarcely used by the numerical analysis community, although currently it is the preferred method of several Dynamical Systems groups. We present the modified Taylor Series method [2] to solve the system and the variational equations for ODEs/DAEs and we show several results for the RING problem, a particular case of the $N$-body problem.
- A classical test problem in numerical ODE methods is the two body problem, but this is a highly simplified model. When we face with a real Earth artificial satellite some demands are required. By instance, an useful task is to provide the output in a highly compressed way to send to an user all the relevant information or a high precision for short periods. We show, for some real Earth artificial satellites, the application of a *Chebyshev Series* method that provides a *compressed dense output* or very high precision using in the integration process a specially designed formulation of the variation of parameters formula [3].

## References

[1] R. Barrio, Sensitivity tools vs. Poincaré sections. *Chaos Solitons Fractals*, 25:711–726, 2005.

[2] R. Barrio, Sensitivity analysis of ODEs/DAEs using the Taylor series method. *SIAM J. Sci. Comput.*, 27:1929–1947, 2006.

[3] R. Barrio, S. Serrano, Modifications of the method of variation of parameters. *Comput. Math. Appl.*, 51:451–466, 2006.

## Multiple Solutions in Preliminary Orbit Determination

*Author(s):*

G.F. Gronchi

Dipartimento di Matematica, Università di Pisa

A. Milani, D. Farnocchia

Dipartimento di Matematica, Università di Pisa

In view of the next generation asteroid surveys, like Pan-STARRS, the interest in orbit determination methods has been greatly renewed in the last years. The huge amount of data expected to be produced by the new surveys requires both the creation of new methods, e.g. to deal with very short arcs of observations [2], and to improve the knowledge of the classical methods.

We shall focus on the problem of defining a preliminary orbit, to be used as a starting guess for the differential corrections [1]. The ODEs of the two-body problem are used in Gauss' and Laplace's methods to obtain an

algebraic equation with degree eight in the heliocentric distance of the observed celestial body (assumed on a Keplerian orbit around the Sun). The solution to this equation may be not unique: Charlier's theory [4] gives a complete geometric description of the occurrence of multiple solutions of the degree eight equation for the preliminary orbits in case of geocentric observations.

At the present days solving such algebraic equations is not a problem at all from the computational point of view, but on the other hand a deeper understanding of the geometry of the problem is useful when dealing with a very large set of different data.

We shall present the changes occurring in Charlier's theory when we take into account the position of the observer on the surface of the rotating Earth [3]. The introduction of this topocentric correction, needed to improve the reliability of the model, produces significant changes in the results: we can find additional preliminary orbits that may help in some cases to search for a nominal solution.

## References


[1] J. M. A. Danby: 1962, 'Fundamentals of Celestial Mechanics', The Macmillan Company, New York

[2] A. Milani, G. F. Gronchi, M. de' Michieli Vitturi, Z. Knežević, 2004. Orbit Determination with Very Short Arcs. I Admissible Regions. CMDA 90, 59–87.

[3] A. Milani et al.: 2007, 'Preliminary Orbits with Topocentric Corrections', in preparation

[4] H. C. Plummer: 1918, 'An introductory treatise on Dynamical Astronomy', Cambridge University press, reprinted by Dover publications, New York., 1960


# Stability of the Eight solution


*Author(s):*

T. Kapela
Jagiellonian University, Kraków, Poland

Carles Simó
Univ. de Barcelona, Spain


We will present a method of computer assisted proofs of choreographies existence. It provides not only existence results but also as a byproduct it returns rigorous estimations for the initial configuration and for the monodromy matrix of the choreography. These data are used to show linear stability of the Eight solution restricted to the plane and zero angular momentum motions.

We will also report on our work in progress to prove stability of the Eight solution in the sense of the KAM theorem.

# On the use of Taylor methods for long time integrations: efficiency, propagation of errors and examples


*Author(s):*

C. Simó
Dept. Matemàtica Aplicada i Anàlisi, Universitat de Barcelona, Barcelona, Spain


First a quick description of Taylor method will be presented, including details on implementation. The suitability for analytic non stiff equations will be discussed. Relevant points are the study of efficiency and propagation of round off errors. Several examples, ranging from toy models in low dimension, either Hamiltonian or not, to $N$-body problems, will be shown with both regular and chaotic orbits.

# Minisymposium
# Computational Systems Biology

Organised by
Y. Cao, L. Petzold

# The Adaptive Explicit-Implicit Tau-Leaping Method for Chemically Reacting Systems

*Author(s):*

Y. Cao

Department of Computer Science, Virginia Tech, Blacksburg, VA 24061

Dan Gillespie

Dan T. Gillespie Consulting, 30504 Cordoba Place, Castaic, CA 9138

Linda Petzold

Department of Computer Science, University of California, Santa Barbara, Santa Barbara, CA 93106

In recent years, concerns over stochastic effects resulting from the small numbers of certain reactant molecules in microscopic systems have called for accurate and efficient stochastic simulation methods. The fundamental simulation method is Gillespie's Stochastic Simulation Algorithm (SSA)[1]. As an exact procedure that simulates every reaction, it is necessarily inefficient for most realistic problems. The tau-leaping method [2] has been proposed to improve the efficiency. Further improvements of tau-leaping method, particularly the implicit and trapezoidal tau-leaping methods and the corresponding implementation strategies, have been proposed [3, 4].

A tau-selection strategy, based on the stochastic partial equilibrium assumption and the slow-scale SSA method [5], is presented here for the implicit tau-leaping method, allowing for longer steps when the system is stiff. Further, an adaptive strategy is proposed that identifies stiffness and automatically chooses between the explicit and the (new) implicit tau-selection methods to achieve better efficiency. Numerical testing demonstrates the advantages of the adaptive method for stiff systems.

## References

[1] D. Gillespie. A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. *J. Comput. Phys.*, 22:403–434, 1976.

[2] D. Gillespie. Approximate accelerated stochastic simulation of chemically reacting systems. *J. Chem. Phys.*, 115:1716, 2001.

[3] M. Rathinam, L. Petzold, Y. Cao, D. Gillespie. Stiffness in stochastic chemically reacting systems: the implicit tau-leaping method. *J. Chem. Phys.*, 119:12784–94, 2003.

[4] Y. Cao, D. Gillespie and L. Petzold. Efficient Stepsize Selection for the Tau-Leaping Method. *J. Chem. Phys.*, 124:044109, 2006.

[5] Y. Cao, D. Gillespie and L. Petzold. The slow-scale stochastic simulation algorithm. *J. Chem. Phys.*, 122:014116, 2005.

# Solving multi-dimensional chemical master equations by a semi-dynamical low-rank approximation

*Author(s):*

T. Jahnke

Freie Universität Berlin
Fachbereich Mathematik und Informatik
Berlin, Germany

and

DFG Research Center Matheon
Berlin, Germany

jahnke@math.fu-berlin.de

Biochemical reaction systems are traditionally modelled by ordinary differential equations (ODE's) representing the concentrations of the species. The reaction-rate approach, however, is insufficient if some of the species are present in a very low number of copies and small-scale stochastic fluctuations can have large-scale effects. In this situation, the appropriate description is provided by the solution of the chemical master equation, a time-dependent probability distribution on a multi-dimensional discrete state space.

Although the chemical master equation can be reformulated as a system of ODEs, computing its solution is a challenging problem. The numerical difficulties are due to the large number of degrees of freedom, which originates from the fact that each single state of the state space is represented by one ODE. Even a rather small system of, e.g., three species with copy numbers varying between 0 and 99 contains $100^3$ states, and hence 1000000 ODEs have to be solved in order to determine its probability distribution! As a consequence, multi-dimensional master equations cannot be treated with traditional ODE methods unless the state space is extremely small.

The semi-dynamical low-rank approximation presented in this talk allows to reduce the large number of degrees of freedom considerably and thereby turns the chemical master equation into a computationally feasible set of equations. The underlying idea is to find a low-rank approximation of the solution by a Galerkin-type method where some of the basis functions are kept fixed while others are moving along with the solution. This semi-dynamical framework conserves the mass of the solution and avoids the problem of over-approximation by changing the number of dynamic basis functions adaptively. Equations of motion for the new variables are derived by projecting the master equation onto the tangent space of the manifold according to the Dirac-Frenkel-McLachlan variational principle. The efficiency of this method will be illustrated by means of a model problem with bimodal solution density.

## Multiscale Discrete Stochastic Simulation of Biochemical Systems

*Author(s):*

L. Petzold
Department of Computer Science, University of California Santa Barbara, Santa Barbara, CA 93106, USA

H. Li
Department of Computer Science, University of California Santa Barbara, Santa Barbara, CA 93106, USA

S. Lampoudi
Department of Computer Science, University of California Santa Barbara, Santa Barbara, CA 93106, USA

Y. Cao
Department of Computer Science, Virginia Tech, Blacksburg, VA 24061, USA

D. Gillespie
Dan T. Gillespie Consulting, 30504 Cordoba Place, Castaic, CA 91384, USA

Traditional deterministic approaches for simulation of chemically reacting systems fail to capture the randomness inherent in such systems at scales common in intracellular biochemical processes. In this lecture we briefly review recent work in discrete stochastic and multiscale algorithms for simulation of biochemical systems and we present the StochKit software toolkit.

## Title to be announced

*Author(s):*

C. Schütte
Freie Universität Berlin, Berlin, Germany

# Minisymposium
# DAEs in Applications

Organised by
L. Jay, R. März

## Orthogonal complement based divide and conquer algorithm for the modelling of constrained multibody systems

*Author(s):*

K. S. Anderson

Computational Dynamics Laboratory Department of Mechanical Aerospace and Nuclear Engineering. Rensselaer Polytechnic Institute 110 8th Street. Troy NY 12180 USA e-mail: anderk5@rpi.edu

An Orthogonal complement Based Divide-and-Conquer Algorithm (O-DCA), is presented for calculating the forward dynamics of constrained bodies including multi-rigid-topologies involving single or coupled kinematic closed loops. The algorithm is exact and noniterative. The constraints are imposed at the acceleration level by utilizing a kinematic relation between the joint motion subspace (or partial velocities) and its orthogonal complement. Sample test cases indicate excellent constraint satisfaction and robust handling of singular configurations. Since the present algorithm does not use either a reduction or augmentation approach in the traditional sense for imposing the constraints, it does not suffer from the associated problems for systems passing through singular configurations. The computational complexity of the algorithm is expected to be O(n + m) and O(log(n + m)) for serial and parallel implementation, respectively, where n is the number of generalized coordinates and m is the number of independent algebraic constraints.

## Direct Transcription Methods for Optimal Control Problems and DAEs

*Author(s):*

S.L.V. Campbell

North Carolina State University, Raleigh, USA

Optimal control problems naturally lead to DAEs in a number of different ways so it is to be expected that theory and numerical methods for DAEs play a roll in the numerical solution of optimal control problems. In some cases this application is straightforward, but in others the existing theory or methods need modification. This talk will include some general comments about DAEs and optimal control but will then focus on some of the ways that DAE theory needs reinterpretation.

## Coupled simulation in nanoelectronics - the COMSON approach

*Author(s):*

M. Günther

Bergische Universität Wuppertal, Fachbereich Mathematik und Naturwissenschaften, Lehrstuhl für Angewandte Mathematik/Numerische Analysis

Performing the step from micro- to nanoelectronics, one is faced with heterogeneous multiscale models which couple DAE and PDE descriptions. To meet the new scientific and training challenges, the Marie-Curie Research Training Network COMSON is currently developing a demonstrator platform: on the one hand, to test mathematical methods and approaches, so as to assess whether they are capable of adressing the industry's problems: on the other hand, to adequately educate young researchers by obtaining immediate hands-on experience for state-of-the-art problems.

This talk will discuss the idea behind the demonstrator platform, report on first results and provide an outlook on future work.

## DAEs and Instationary Saddle Point Problems in Computational Mechanics

*Author(s):*

B. Simeon

Zentrum Mathematik TU Munich Germany

Computational mechanics and its various applications in vehicle analysis, aerospace engineering, robotics, and materials sciences have experienced a significant development over the last decades. In many cases, a dynamic saddle point problem is at the core of the mathematical model, and it can be viewed as an infinite-dimensional DAE or a PDAE system. By discretization in space, we obtain a semi-explicit DAE of index three if the constraints have full rank. In this context, the inf-sup condition plays a crucial role.

The talk concentrates on this relationship between DAE's and PDE models in saddle point formulation and discusses flexible multibody systems, domain decomposition approaches, incompressibility constraints, and dynamic contact. It turns out that all these fields can be cast in basically the same abstract framework. Simulation results based on the method of lines with Finite Elements in space and DAE-solvers in time illustrate the problem class.

# Minisymposium
# Delay-differential equations

Organised by
A. Bellen, N. Guglielmi, M. Zennaro

## Non-Fickian delay reaction-diffusion equations-theoretical and numerical study

*Author(s):*

J.A. Ferreira

Departamento de Matematica, Universidade de Coimbra, Coimbra, Portugal

P.M. da Silva

Departamento de Fisica e Matematica, ISEC, Coimbra, Portugal

In this talk we study continuous and discrete models to describe reaction transport systems with memory. In these models the memory effect is described by a reaction term with a delay and a flux of non-Brownian type. Numerical results illustrating the behavior of the solution of discrete models are also presented.

## Numerical solution of threshold problems in epidemics and population dynamics

*Author(s):*

Z. Jackiewicz

Department of Mathematics, Arizona State University, Tempe (AZ), USA

B. Zubik-Kowal

Department of Mathematics, Boise State University, Boise (ID), USA

A new algorithm is proposed for the numerical solution of threshold problems in epidemics and population dynamics. These problems are modelled by the delay-differential equations, where the delay function is unknown and has to be determined from the threshold conditions. The new algorithm is based on embedded pair of continuous Runge Kutta method of order $p = 4$ and discrete Runge-Kutta method of order $q = 3$ which is used for the estimation of local discretization errors, combined with the bisection method for the resolution of the threshold condition. Error bounds are derived for the algorithm based on continuous one-step methods for the delay-differential equations and arbitrary iteration process for the threshold conditions. Numerical examples are presented which illustrate the effectiveness of this algorithm.

## Time transformations for delay differential equations

*Author(s):*

S. Maset

Dipartimento di Matematica e Informatica, Università di Trieste, Trieste, Italy

H. Brunner

Department of Mathematics and Statistics, Memorial University of Newfoundland, St. John's (NL), Canada

This talk deals with changes of variable, called time transformations, which reduce a Delay Differential Equation (DDE) with variable delay (possibly state dependent) to another DDE with a simpler delay, e.g. a constant delay.
By using this reduction, we can easily:

- obtain a superconvergent integration of the original equation even in case of a non-strictly-increasing lag function,
- study the type of decay to zero of solutions of asymptotically stable linear equations,

- compute the breaking points in the state-dependent case.

# Numerical approximation of characteristic values of Partial Retarded Functional Differential Equations

*Author(s):*

R. Vermiglio

Dipartimento di Matematica e Informatica - Università degli Studi di Udine

D. Breda

Dipartimento di Matematica e Informatica - Università degli Studi di Udine

S. Maset

Dipartimento di Matematica e Informatica - Università degli Studi di Trieste

We consider semi-linear Partial Retarded Functional Differential Equations (PRFDEs) restated as abstract semi-linear retarded functional differential equations.

The stability analysis of equilibrium points plays a main role in the study of PRFDEs and it requires to determine the position in the complex plane of the characteristic values of the linearization of PRFDEs around the equilibrium, which yields to an abstract fully-linear retarded functional differential equation (see [4]).

Recently, numerical approaches have been proposed to approximate the characteristic values of linear Retarded Functional Differential Equations (RFDEs) (see [1], [2], [3]). They are based on the discretization of the infinitesimal generator (IG) into a finite dimensional linear operator whose eigenvalues provide approximations of the characteristic values .

The aim of this work is to apply the IG-approach to approximate the characteristic values of abstract fully-linear retarded functional differential equations. We propose to join together pseudospectral and spectral techniques for the discretization. The convergence of the computed characteristic values is of infinite order with respect to the pseudospectral discretization and of finite order with respect to the spectral one. We present some numerical experiments and we conclude with a deeper convergence analysis to explain, in case of one dimensional reaction diffusion equations with delay, the behaviour of the numerical results, which turns out to be much better than the general convergence theorem predicts.

## References

[1] D. Breda, S. Maset and R. Vermiglio. Computing the characteristic roots for delay differential equations *IMA J. Numer. Anal.* 1–19, 2004 .

[2] D. Breda, S. Maset and R. Vermiglio. Pseudospectral differencing methods for characteristic roots of delay differential equations *SIAM J. Sci. Comput.*, 482–495, 2005.

[3] D. Breda, S. Maset and R. Vermiglio. Pseudospectral approximation of eigenvalues of derivative operators with non-local boundary conditions *Appl. Numer. Math.*, 318–331, 2006.

[4] J. Wu. Theory and applications of partial functional differential equations. *AMS series n.119*, Springer-Verlag, 1996.

# Minisymposium
# Exponential fitting

Organised by
M. Van Daele, G. Vanden Berghe

# Title to be announced

*Author(s):*

M. Calvo

Departamento Matematica Aplicada Universidad de Zaragoza. 50009-Zaragoza, Spain. email: calvo@unizar.es

In this paper the existence and construction of variable coefficients symplectic $(2s)$-stages variable coefficients Runge-Kutta (RK) methods that integrate exactly ODEs whose solution is a trigonometrical polynomial of order $s$ with a given frequency $\omega$ is considered. The resulting methods are fully implicit, symmetric and symplectic RK methods with variable nodes and coefficients that are even functions of $\nu = \omega h$ ($h$ is the step size) and for $\omega \to 0$ tend to the conventional RK Gauss methods and extend previous results on symplectic exponentially fitted integrators of H. Van de Vyver (Comput. Phys. Comm. 174 (2006), 217-239), and the author together with J.M. Franco, J.I. Montijano and L. Randez ( J. Comput. Appl. Math., to be published). Furthermore, it is shown that these methods can be considered as collocation methods with respect to a trigonometrical polynomial with order $s$ at suitable variable nodes. Finally, by using some results by K. Ozawa ( Japan J. Indust. Appl. Math., 18, (2001), 107-130) the order of the proposed $2s$-stage method is shown to be $4s$ like conventional RK methods.

This work was supported by project DGIMTM2004-06466-C02-01

# Short survey on the exponential fitting

*Author(s):*

L. Gr. Ixaru

"Horia Hulubei" National Institute of Physics and Nuclear Engineering, Department of Theoretical Physics, P.O.Box MG-6, Bucharest, Romania, e-mail: ixaru@theory.nipne.ro

A short review is made on the development of the ideas which lead to what is now known as the exponential fitting procedure. It is shown how the ideas behind the classical approach, based on approximations to smooth functions, had to be generalized and adapted to work on oscillatory functions and/or on functions with an exponential behaviour. We explain that one of the main advantages with the exponential fitting technique is that it covers a large variety of shapes for the functions and a large number of numerical operations on them: numerical differentiation, quadrature, interpolation, solving differential equations etc. Another important advantage is that most of the theoretical aspects are nowadays well understood. We also mention some problems in natural sciences to be successfully approached by this technique, report on the existing software, and formulate some interesting directions for further development.

# Functionally Fitted Linear Multistep Methods

*Author(s):*

K. Ozawa

Akita Prefectural University, Faculty of Systems Science and Technology, Yuri-Honjyo, Akita, Japan

Consider the $k$-step linear multistep method with variable coefficients

$$\begin{aligned} & y_{n+k} + \alpha_{k-1}\, y_{n+k-1} + \cdots + \alpha_0\, y_n \\ & \quad = h\left(\beta_k\,(t_n,\, h)\, f_{n+k} + \beta_{k-1}\,(t_n,\, h)\, f_{n+k-1} + \cdots + \beta_0\,(t_n,\, h)\, f_n\right), \\ & \qquad f_j = f(t_j,\, y_j), \quad t_j = t_0 + jh, \quad j = 0, 1, \ldots, \end{aligned} \tag{2}$$

for solving the initial value problem

$$y'(t) = f(t,\, y), \qquad t \in (t_0,\, T], \qquad y(t_0) = y_0. \tag{3}$$

We assume that the coefficients $\alpha$'s of the method are the constants satisfying the stability and consistency conditions, i.e., the characteristic polynomial given by

$$\rho(\zeta) = \zeta^k + \alpha_{k-1}\,\zeta^{k-1} + \cdots + \alpha_0 \tag{4}$$

has root $\zeta_1 = 1$ and all the other ones satisfy the condition

$$|\zeta_i| \le 1, \qquad i = 2, \ldots, k.$$

We determine the coefficients $\beta$'s so as to make the method (2) exact, when the ODE (3) has the solution $y(t)$ which satisfies $y(t) \in \operatorname{span}\{\Phi_1(t), \ldots, \Phi_{k+1}(t)\}$ for given functions $\{\Phi_m\}_{m=1}^{k+1}$. More specifically, we determine $\beta$'s by the simultaneous equation

$$\begin{aligned}&\Phi_m(t+kh) + \alpha_{k-1}\,\Phi_m\left(t+(k-1)h\right) + \cdots + \alpha_0\,\Phi_m(t)\\ &\quad = h\left(\beta_k\,\varphi_m(t+kh) + \beta_{k-1}\,\varphi_m(t+(k-1)h) + \cdots + \beta_0\,\varphi_m(t)\right), \quad m = 1, 2, \ldots, k+1,\end{aligned}$$

where $\varphi_m(t) = \Phi'_m(t)\,(m = 1, 2, \ldots, k+1)$. The method is a variant of the functionally fitted Runge–Kutta method given by Ozawa [1]. We will investigate the algebraic order of the method when applied to general ODEs.

## References


[1] K. Ozawa, A Functional Fitting Runge-Kutta Method with Variable Coefficients, Japan Journal of Industrial and Applied Mathematics **18** (2001), pp.105–128.


# P-stable exponentially-fitted Obrechkoff methods


*Author(s):*

M. Van Daele

Ghent University, Belgium

G. Vanden Berghe

Ghent University, Belgium


We consider Obrechkoff methods for solving $y'' = f(x, y)$, $y(a) = \alpha$, $y'(a) = \beta$ of the form

$$y_{n+1} - 2y_n + y_{n-1} = \sum_{j=1}^{m} h^{2j}\left[\beta_{j0}\,y_{n+1}^{(2j)} + 2\beta_{j1}\,y_n^{(2j)} + \beta_{j0}\,y_{n-1}^{(2j)}\right].$$

Such methods have been studied in the past by several authors. One of them, Ananthakrishnaiah [1], constructed P-stable methods of this type of order $2\,m$ for $m = 3$ and $m = 4$. Recently, we were able [2] to generalise this approach, making use of the theory of Padé approximants, such that for any given $m$ a P-stable method of order $2\,m$ can be constructed.

On the other hand, we also considered the construction of exponentially fitted Obrechkoff methods [3], following the ideas of Ixaru and Vanden Berghe [4]. Instead of fitting the method only to polynomials, we also fitted to functions related to $\sin\omega\,x$ and $\cos\omega\,x$ (or in the imaginary case to $\exp(\pm\mu\,x)$). In this way, methods are obtained where the coefficients depend upon the product $\omega\,h$.

In the present talk, we will show how the idea of the Padé approximants can be generalised towards exponential fitting, such that P-stable exponentially fitted methods can be generated for any $m$.

# References


[1] U. Ananthakrishnaiah, P-stable Obrechkoff Methods with Minimal Phase-Lag for Periodic Initial Value Problems. *Math. Comput.* **49** (1987), 553-559.

[2] G. Vanden Berghe and M. Van Daele, Exponentially-fitted Obrechkoff methods for second-order differential equations, APNUM, Proceedings of Numdiff11 (accepted for publication).

[3] M. Van Daele and G. Vanden Berghe, P-stable Obrechkoff methods of arbitrary order for second-order differential equations, Numerical Algorithms (accepted for publication).

[4] L. Gr. Ixaru and G. Vanden Berghe, Exponential Fitting, Mathematics and Its Application **568** (Kluwer Academic Publications, 2004).

# Minisymposium
# Exponential integrators

Organised by
M. Hochbruck, A. Ostermann

## Efficient implementation of exponential Rosenbrock-type methods

*Author(s):*

M. Caliari

Department of Pure and Applied Mathematics, University of Padua (Italy) and Department of Mathematics, University of Innsbruck (Austria)

A. Ostermann

Department of Mathematics, University of Innsbruck (Austria)

We present a variable step size implementation of exponential Rosenbrock-type methods. These integrators require the evaluation of exponential and related functions of the Jacobian matrix. To this aim, the Real Leja Points Method is used. We solve semilinear parabolic PDEs in one and two space dimensions and we compare our method with others from literature. We find a great potential of our method for parabolic problems with large advection in combination with moderate diffusion and mildly stiff reactions. Finally, we present an adaptive "meshfree" exponential integrator for a bidimensional pure advection problem.

## References

[1] M. Caliari and A. Ostermann. Implementation of exponential Rosenbrock-type methods. *Appl. Numer. Math.*, accepted for publication, 2007.

[2] M. Caliari, M. Vianello, and L. Bergamaschi. Interpolating discrete advection-diffusion propagators at Leja sequences. *J. Comput. Appl. Math.*, 172(1):79–99, 2004.

[3] M. Hochbruck and A. Ostermann. Exponential integrators of Rosenbrock-type. *Oberwolfach Reports*, 3:1107–1110, 2006.

[4] M. Hochbruck, A. Ostermann, and J. Schweitzer. Exponential Rosenbrock-type methods. *In preparation*, 2007.

## Exponential integrators for advection and wave equations

*Author(s):*

A. Ostermann

Department of Mathematics, University of Innsbruck, Austria

M. Caliari

Department of Pure and Applied Mathematics, University of Padua, Italy, and Department of Mathematics, University of Innsbruck, Austria

In this talk, we present exponential integrators for linear advection and wave equations with variable coefficients

$$\frac{\partial u}{\partial t} \;=\; \frac{\partial}{\partial x}\Big(a(x)u\Big), \qquad\qquad \frac{\partial^2 u}{\partial t^2} \;=\; \frac{\partial}{\partial x}\Big(a(x)\frac{\partial u}{\partial x}\Big) \tag{5}$$

in one, two and three space dimensions. For the spatial discretisation of (5), we employ symmetric *Mehrstellen* formulas of high order. The resulting semi-discretisations are integrated in time by exponential integrators.

As we are dealing with variable coefficients, a straightforward implementation of exponential integrators using *fast Fourier transform* techniques is not feasible. We propose instead to approximate the matrix exponentials by Newton interpolation, based on symmetrised complex Leja points. This method requires matrix-vector multiplications only and combines well with FFT techniques for solving the linear equations that arise in *Mehrstellen* formulas.

We present numerical experiments for periodic as well as for outflow boundary conditions. For a full analysis and more details, we refer to our forthcoming paper [1].

## References

[1] M. Caliari, A. Ostermann: Exponential integrators for linear advection and wave equations. In preparation, 2007.

# Solving stiff reaction–diffusion equations with exponential integrators

*Author(s):*

T. Schmelzer

Oxford University Computing Laboratory, UK

L. N. Trefethen

Oxford University Computing Laboratory, UK

Among the fastest methods for solving stiff PDE are exponential integrators, which require the evaluation of $f(A)$, where $A$ is a negative semidefinite matrix and $f$ is the exponential function or one of the related "$\varphi$ functions" such as $\varphi_1(z) = (e^z - 1)/z$. Building on previous work by Trefethen and Gutknecht, Minchev, and Lu, we propose two methods for the fast evaluation of $f(A)$ that are especially useful when shifted systems $(A + zI)x = b$ can be solved efficiently, e.g. by a sparse direct solver. The first method is based on best rational approximations to $f$ on the negative real axis computed via the Carathéodory-Fejér procedure. Three matrix solves suffice to evaluate $f(A)$ to approximately six digits of accuracy. The second method is an application of the trapezoid rule on a Talbot-type contour.

We address the efficient implementation of exponential integrators in the context of this methods and apply them to various reaction–diffusion equations.

Details can be found in [1].

## References

[1] Evaluating matrix functions for exponential integrators via Carathéodory-Fejér approximation and contour integrals. *ETNA*, submitted.

# Numerical simulation of relativistic laser plasma dynamics

*Author(s):*

J. Schweitzer

Heinrich-Heine-University, Düsseldorf, Germany

M. Hochbruck

Heinrich-Heine-University, Düsseldorf, Germany

A mathematical model of the interaction of relativistically intense electromagnetic waves with a plasma leads to a system of coupled nonlinear Klein-Gordon equations. The quantities of interest are the vector potential of the laser pulse and the electron density of the plasma. Numerical difficulties of this problem arise because of the oscillatory nature of the solution both in time and space and because of the interest in long-time simulations.

In this talk we discuss some recent advances in the construction of numerical methods for simulations in two space dimensions.

# Minisymposium
# Geometric and symplectic integration

Organised by
J.L. Hong, R. Quispel

## Propagation of Uncertainty in Rigid Body Attitude Flows

*Author(s):*

M. Leok

Department of Mathematics, Purdue University, West Lafayette, USA

Motivated by attitude control and attitude estimation problems for a rigid body, computational methods are proposed to propagate uncertainties in the angular velocity and the attitude. The nonlinear attitude flow is determined by Euler-Poincare equations that describe the rotational dynamics of the rigid body acting under the influence of an attitude dependent potential and by a reconstruction equation that describes the kinematics expressed in terms of an orthogonal matrix representing the rigid body attitude. Uncertainties in the angular velocity and attitude are described in terms of ellipsoidal sets that are propagated through this highly nonlinear attitude flow.

Computational methods are proposed, one method based on a local linearization of the attitude flow and two methods based on propagation of a small (unscented) sample selected from the initial uncertainty ellipsoid. Each of these computational methods is constructed using the Lie group variational integrator algorithm, viewed as a discretization of the attitude flow dynamics. Computational results are obtained that indicate (1) the strongly nonlinear attitude flow characteristics and (2) the limitations of each of these methods, and indeed any method, in providing effective global bounds on the nonlinear attitude flow.

Joint work with Taeyoung Lee, Nalin A. Chaturvedi, Amit Sanyal, and N. Harris McClamroch. The research has been supported in part by NSF grant DMS-0726263 and DMS-0504747.

## Preservation of Periodic Orbits for Hamiltonian Systems

*Author(s):*

D. O'Neale

I.F.S., Massey University, Palmerston North, New Zealand

When a numerical integrator is applied to a system of ordinary differential equations some of the dynamics are preserved exactly while others are only approximated (or are even destroyed). It is well known that for Hamiltonian systems with $d$ degrees of freedom, non-resonant invariant tori, of dimension $d$ survive small perturbations — a result of KAM theory [1]. It has been shown that an equivalent result holds when one replaces the flow of the Hamiltonian system with a symplectic map, that is, most of these tori are also preserved when the system is discretised with a symplectic integrator [2]. Recent results show that invariant tori of dimension $l \leq d$ also survive quasi-periodic perturbations[3]. When $l = 1$ these correspond to periodic orbits. We conjecture that these results can be extended to symplectic maps by using a non-autonomous modified vector field (MVF) to interpolate the points of the map (e.g. [4]) and then working with the flow of the MVF.

## References

[1] V.I. Arnold. Mathematical Methods of Classical Mechanics. Springer-Verlag, New York, 1989.

[2] Z. Shang. KAM theorem of symplectic algorithms for Hamiltonian systems. *Numer. Math.* 83:477–496, 1999.

[3] Á. Jorba and J. Villanueva. On the persistence of lower dimensional invariant tori under quasi-periodic perturbations. *J. Nonlinear Sci.* 7:427–473, 1997.

[4] P.C. Moan. On modified equations for discretizations of ODEs. *J. Phys. A*, 19:5545–5561, 2006.

# Dynamics of transition to turbulence

*Author(s):*

D. Viswanath

University of Michigan, Ann Arbor, USA

Fluids undergo transition to turbulence when slight perturbations cause the laminar solution to become turbulent. Historically, efforts to understand transition to turbulence have focused on a small neighborhood of the laminar solution. This talk will describe a more geometric approach based on steady solutions and traveling waves that act as intermediaries between the laminar solution and turbulence.

# Minisymposium
# Geometric integration of PDEs

Organised by
E. Faou, C. Lubich

## Geometric integration methods for PDEs with symmetries and conservation laws

*Author(s):*

C. Budd

University of Bath

Geometric integration methods are now well developed for ODE problems but have received much less attention in the study of PDES. One reason for this is that PDEs have many possible qualitative structures that we might want a numerical method to preserve. These include: conservation laws, many different symmetries, and ordering principles. In general it is impossible to preserve all qualitative structures and it is not always a-priori evident which structure a numerical method should preserve. In this talk I will look at the application of geometric based methods (both adaptive and non-adaptive) to a variety of nonlinear partial differential equations, including equations which develop singularities in a finite time, and will compare the effects of preserving conservation laws and symmetries. oussinesq equations.

## Long-time behaviour of numerical discretizations for nonlinear wave equations

*Author(s):*

E. Hairer

University of Geneva

D. Cohen

Department of Mathematical Sciences NTNU, Trondheim

C. Lubich

University of Tübingen

For numerical discretizations of nonlinearly perturbed wave equations the long-time near-conservation of energy, momentum, and harmonic actions is studied. The time step is not assumed to be small compared to the inverse of the largest frequency in the space-discretized system, so that classical backward error analysis cannot be applied.

The proofs of the statements on the long-time conservation properties are based on the technique of modulated Fourier expansions.

## Numerics of harmonic map heat flow and wave maps to the sphere

*Author(s):*

A. Prohl

University of Tuebingen, Germany

J. Barrett

Imperial College, London

S. Bartels

Humboldt University, Berlin

X. Feng

University of Knoxville

C. Lubich

University of Tuebingen

.

The harmonic map heat flow to the sphere is a prototype evolution problem, with many applications e.g., in materials science (Landau-Lifshitz equation, Ericksen-Leslie equation, ..). The key difficulty of space-time discretizations is to conserve the sphere constraint, to eventually construct weak solutions with practical (e.g., finite element based) schemes when discretization parameters tend to zero.

In the talk, I discuss (i) discretizations of reformulations of the problem, and (ii) formulations which use discrete Lagrange multipliers. Both cases employ lowest order conforming finite elements, and I show convergence to weak solutions for mesh-parameters tending to zero. The results are then extended to p-harmonic map heat flow, Landau-Lifshitz Gilbert with variants, and wave maps to the sphere.

## Explicit multisymplectic integrators

*Author(s):*

B.N. Ryland

Massey University, Palmerston North, New Zealand

Many of the important equations that describe wave-like phenomena can be written as a multi-Hamiltonian PDE in the form

$$\mathbf{K}\mathbf{z}_t + \mathbf{L}\mathbf{z}_x = \nabla_{\mathbf{z}} S(\mathbf{z}), \tag{6}$$

where $\mathbf{z} \in \mathbb{R}^n$, $\mathbf{K}$ and $\mathbf{L}$ are skew-symmetric matrices and $S(\mathbf{z})$ is a smooth function. Such PDEs possess a multisymplectic conservation law,

$$\omega_t + \kappa_x = 0, \tag{7}$$

where $\omega = \frac{1}{2}\mathbf{K}\mathrm{d}\mathbf{z} \wedge \mathrm{d}\mathbf{z}$ and $\kappa = \frac{1}{2}\mathbf{L}\mathrm{d}\mathbf{z} \wedge \mathrm{d}\mathbf{z}$ are 2-forms evaluated on solutions to the first variation of the PDE.

Previously, it has been shown that two-part partitioned Runge-Kutta discretisations of Eq. (6) in time and space, with the same partitioning of the variables ($z^{(1)} \in \mathbb{R}^{n_1}$ and $z^{(2)} \in \mathbb{R}^{n_2}$ such that $n_1 + n_2 = n$), formally satisfy a discrete version of Eq. (7), however generally it is not desirable for the variables to share this partitioning. In the first part of my talk I will demonstrate that a PRK discretisation of Eq. (6) with an arbitrary number of partitions ($z^{(\gamma)} \in \mathbb{R}^{n_\gamma}$ such that $\sum_\gamma n_\gamma = n$) and independent partitioning in time and space formally satisfies a multisymplectic conservation law when the coefficients of the spatial PRK method satisfy

$$\begin{aligned} b_j^{(\gamma)} &= b_j, \\ -a_{kj}^{(\gamma)} b_k^{(\beta)} - b_j^{(\gamma)} a_{jk}^{(\beta)} + b_j^{(\gamma)} b_k^{(\beta)} &= 0, \end{aligned} \tag{8}$$

for all $j$, $k$ and pairs $(\beta, \gamma)$ such that $\mathbf{L}_{\beta\gamma} \neq 0$ and similarly for the temporal PRK method.

Formally satisfying a multisymplectic conservation law, however, is only part of constructing a multisymplectic integrator. The system of discretised equations must also form a well-defined numerical integrator in order to be useful. Generally, if the discretisation gives rise to a numerical integrator that is explicit, then that integrator will be well-defined. In the second part of my talk I will show that subject to certain conditions on $\mathbf{K}$, $\mathbf{L}$ and $S(\mathbf{z})$, a discretisation of Eq. (6) belonging to the Lobatto IIIA–IIIB class of PRK methods leads to a system of explicit ODEs in time. An explicit PRK discretisation in time may then be applied to these ODEs to form a high-order, explicit, multisymplectic integrator. Examples of PDEs for which explicit multisymplectic integrators may be constructed include the nonlinear wave, nonlinear Schrödinger and Boussinesq equations.

# Minisymposium
# Highly oscillatory problems

Organised by
A. Iserles, S.P. Norsett

## Spectral Methods and modified Fourier Series

*Author(s):*

B. Adcock

DAMTP, University of Cambridge, Cambridge, UK

In this talk we present a new spectral method for linear PDEs with non-periodic boundary conditions. The trial functions come from the *modified Fourier basis*, which, unlike the conventional Fourier basis, converges uniformly for non-periodic functions on the unit interval. We will first consider constant-coefficient linear problems with Neumann boundary conditions. We then look at techniques firstly to increase the convergence rate and secondly to deal with other boundary conditions. These methods are in fact Petrov-Galerkin methods with suitable trial and test spaces, and hence can be analysed in the standard way. We will also consider problems in the unit square, and again look at techniques to accelerate convergence.

## Oscillatory Integrals and Integral Operators in High Frequency Scattering

*Author(s):*

S. Chandler-Wilde

University of Reading

In this paper we review recent developments in the solution of high frequency time harmonic scattering problems by boundary integral equation methods. For simplicity (and because much recent work has considered this simplest problem) we focus on acoustic scattering by a sound soft surface, so that the solution $u$ satisfies the Helmholtz equation $\Delta u + k^2 u = 0$ in the domain exterior to the scatterer and $u = 0$ on its boundary. Our focus is a novel class of methods which have a hybrid asymptotic-numeric flavour, in that they attempt to obtain efficiency by using basis functions which incorporate explicitly the highly oscillatory behaviour of the solution in the limit $k \to \infty$, as known e.g. from the geometric theory of diffraction. In contrast to conventional discretisation methods, for which the number of degrees of freedom increases at least in proportion to $k$ in 2D, to $k^2$ in 3D, the aim is to achieve algorithms for which the number of degrees of freedom remains fixed or increase only mildly (e.g. proportional to $\log k$) as $k \to \infty$. Necessarily this last constraint implies that, while the linear system to solved remains manageable, the entries in the matrix are highly oscillatory integrals in the limit $k \to \infty$.

## References

[1] S. Arden, S. Langdon and S.N. Chandler-Wilde, A collocation method for high frequency scattering by convex polygons *J. Comp. Appl. Math.*, published online, 2006.

[2] O.P. Bruno and C.A. Geuzaine, An $O(1)$ integration scheme for three-dimensional surface scattering problems, *J. Comp. Appl. Math.*, published online, 2006.

[3] S. N. Chandler-Wilde and S. Langdon, A Galerkin boundary element method for high frequency scattering by convex polygons, *SIAM J. Numer. Anal.*, 45:610–640, 2007.

[4] V. Domínguez, I. G. Graham and V. P. Smyshlyaev, A hybrid numerical-asymptotic boundary integral method for high-frequency acoustic scattering, *Numer. Math.*, 106:471–510, 2007.

[5] M. Ganesh, S. Langdon, and I.H. Sloan, Efficient evaluation of highly oscillatory acoustic scattering integrals, *J. Comp. Appl. Math.*, published online, 2006.

[6] D. Huybrechs and S. Vandewalle, On the evaluation of highly oscillatory integrals by analytic continuation, *SIAM J. Numer. Anal.*, 44:1026–1048, 2006.

## Asymptotic least squares approximation for highly oscillatory differential equations

*Author(s):*

S. Olver
University of Cambridge

We present a new approach for approximating highly oscillatory ordinary differential equations. By using the asymptotic expansion in a least squares system, we are able to obtain a result that preserves the asymptotic accuracy of the expansion, while converging rapidly to the exact solution. We are thus able to accurately approximate such differential equations by solving a very small linear system. We apply this method to the computation of highly oscillatory integrals, as well as second order oscillatory differential equations.

## References

[1] S. Olver, Moment-free numerical integration of highly oscillatory functions, *IMA J. Num. Anal.*, 26:213–227, 2006.

[2] S. Olver, On the quadrature of multivariate highly oscillatory integrals over non-polytope domains, *Numer. Math.*, 103:643–665, 2006.

[3] S. Olver, Moment-free numerical approximation of highly oscillatory integrals with stationary points, *Euro. J. Appl. Maths*, to appear, 2007.

[4] S. Olver, Numerical approximation of vector-valued highly oscillatory integrals, *BIT*, to appear, 2007.

## Fast Phase Space Methods for Computing Creeping Rays

*Author(s):*

O. Runborg
Department of Numerical Analysis, KTH, Stockholm, Sweden

M. Motamed
Department of Numerical Analysis, KTH

Creeping rays can give an important contribution to the solution of medium to high frequency scattering problems. They are generated at the shadowlines of the illuminated scatterer and propagate along geodesics on the scatterer surface, continuously shedding diffracted rays in their tangential direction. We show how the ray propagation problem can be formulated as a partial differential equation (PDE) in a three-dimensional phase space using a technique from [1]. The PDE solution give information about all possible creeping rays. Computationally the cost of solving the PDE is less than tracing all rays individually. We show numerical results and an application to monostatic radar cross section problems where creeping rays from all illumination angles must be computed. Details can be found in [2, 3].

## References

[1] S. Fomel and J. A. Sethian. Fast phase space computation of multiple arrivals. *Proc. Natl. Acad. Sci. USA*, 99(11):7329–7334 (electronic), 2002.

[2] M. Motamed and O. Runborg. A fast phase space method for computing creeping rays. *J. Comput. Phys.*, 219:276–295, 2006.

[3] M. Motamed and O. Runborg. A multiple-patch phase space method for computing trajectories on manifolds with applications to wave propagation problems. Accepted in *Comm. Math. Sci.*, 2007.

# Minisymposium
# Implementation of multivalue-multistage methods

Organised by
J. Butcher, Z. Jackiewicz

## Comparison between different types of continuous extensions to stiffly accurate TSRK methods of order three

*Author(s):*

Z. Bartoszewski

Department of Mathematics, Gdańsk University of Technology, Poland

In the talk there will be described three types of interpolation formulas applied to the newly constructed stiffly accurate two-step Runge-Kutta methods in order to obtain their continuous extensions: Hermite interpolation, cubic spline interpolation and an interpolation that for A-stable methods guarantees that their continuous extensions are P-stable. The performance of the obtained continuous two step Runge-Kutta methods will be demonstrated by comparing the results of the tests conducted on a number of well known stiff delay differential equations.

## Error propagation of general linear methods

*Author(s):*

Z. Jackiewicz

Department of Mathematics, Arizona State University, Tempe, USA

J.C. Butcher

Department of Mathematics, University of Auckland, New Zealand

W.M. Wright

Department of Mathematics, La Trobe University, Melbourne, Australia

We will discuss error propagation for general linear methods for ordinary differential equations up to the terms of order $p + 2$, where $p$ is the order of the method. These results are then applied to the estimation of local discretization errors of method of order $p$ and of adjacent order $p + 1$. The results of numerical experiments confirm the reliability of these estimates. This research has applications to the design of robust stepsize and order changing strategies for algorithms based on general linear methods.

## Searching for practical general linear methods

*Author(s):*

H. Podhaisky

Department of Mathematics, University of Halle, Germany

General linear methods can have favourable properties, in particular the unique combination of A-stability, high stage order, and a diagonally implicit scheme is possible. However, it seems to be difficult to construct methods which behave robustly enough in a variable stepsize implementation to supersede Runge-Kutta and multistep methods in real applications. A crucial question is how to find and identify good practical methods. The main aim of the talk is to describe computational and analytical techniques to built an atlas of diagonally implicit methods of low order suitable for stiff systems. Numerical results for problems taken from the CWI/Bari IVP-testset are presented.

## Adaptivity and Computational Cost in the Numerical Solution of ODEs

*Author(s):*

G. Söderlind

Numerical Analysis, Lund University, Sweden

S. Ilie

We analyze the problem of adaptivity for numerical methods for solving ODEs, both IVPs and BVPs, with a view to generating optimal grids for local error control. The grids are generated by introducing an auxiliary independent variable $\tau$ and finding a grid deformation map, $t = \Theta(\tau)$, that maps an equidistant grid $\{\tau_j\}$ to a non-equidistant grid in the original independent variable, $\{t_j\}$. The optimal deformation $\Theta$ is determined by a variational approach. Finally, we investigate the cost of the solution procedure and compare it to the cost of using equidistant grids. We show that the efficiency gain due to adaptivity can be arbitrarily high.

# Minisymposium
# Methods for DAEs

Organised by
L. Jay, R. März

# A second order extension of the generalized-$\alpha$ method for constrained systems in mechanics.

*Author(s):*

L. Jay

Department of Mathematics, 14 MacLean Hall, The University of Iowa, Iowa City, IA 52242-1419, USA.
ljay@math.uiowa.edu

We present a new second order extension of the generalized-$\alpha$ method of Chung and Hulbert for systems in mechanics with a nonconstant mass matrix, holonomic constraints, and nonholonomic constraints. A new variable stepsizes formula preserving the second order of the method is also proposed.

# Adjoint DAEs and Feedback Construction for Optimal Control Problems with DAE Constraints

*Author(s):*

R. März

Humboldt University Berlin, Institute of Mathematics, maerz@mathematik.hu-berlin.de

K. Balla (1947-2005) In Memoriam

This talk reports and continues joint research results with Katalin Balla and Galina A. Kurina. We concentrate on two closely related aspects, the structure of adjoint DAEs and the solution of linear-quadratic optimal control problems via feedback construction.

Feedback construction by means of the Riccati matrix differential equation is one of the best-known and approved standard methods to solve linear-quadratic optimal control problems with constraints described by explicit ODEs.

If the constraint of an optimal control problem is no longer given by an explicit ODE but by a general linear DAE, things are much more difficult. In particular, then, though an appropriate Hamiltonian DAE system is given [1], the standard approach to obtain the Riccati equation from the corresponding Hamiltonian system yields a Riccati type DAE that strongly suffers from impracticable solvability conditions (cf.[2]). Under mild conditions, an actually useful Riccati DAE having reasonable solvability properties can be directly derived from the minimization problem [2], and, moreover, the resulting closed loop system represents a regular DAE with tractability index one.

Adjoint equations play an important role within the optimal control framework but also in further areas. We end up by considering the related structures of general regular DAEs and their adjoints. By this, results known already for index one and two DAEs [3] are generalized to the case of arbitrary index.

## References

[1] Katalin Balla, Galina A.Kurina and Roswitha März. Index criteria for differential algebraic equations arising from linear-quadratic optimal control problems. *Journal of Dynamical and Control Systems*, Vol.12, Nr.3, 289-311, 2006.

[2] Galina A.Kurina and Roswitha März. Feedback solutions of optimal control problems with DAE constraints. *SIAM J. Control Optim.* , to appear 2007.

[3] Katalin Balla and Roswitha März. A unified approach to linear differential algebraic equations and their adjoints. *Journal for Analysis and its Application*, Vol.21, Nr.3, 783-802, 2002.

# A local reduction framework for the analysis of singular nonlinear DAEs

*Author(s):*

R. Riaza

Departamento de Matemática Aplicada a las Tecnologías de la Información, ETSI Telecomunicación, Universidad Politécnica de Madrid, Spain. E-mail: rrr@mat.upm.es

We discuss in this talk geometric reduction methods for the analysis of quasilinear autonomous differential-algebraic equations (DAEs) of the form

$$A(x)x' = f(x), \tag{9}$$

with $A \in C^k(W_0, \mathbb{R}^{n\times n})$, $f \in C^k(W_0, \mathbb{R}^n)$, $k \geq 1$ and $W_0$ open in $\mathbb{R}^n$. The matrix mapping $A(x)$ is typically assumed to be rank-deficient in the whole of $W_0$. The framework of Rabier and Rheinboldt [1], based on the subimmersion theorem, relies on global algebraic conditions which allow one to reduce (9) to an explicit ODE on a lower-dimensional submanifold of $W_0$. This framework accommodates "last-step" singularities, not affecting the validity of the reduction procedure.

A local restatement of this approach makes it possible to define in an invariant manner the notion of a singular point of (9), reflecting the failure of the above-mentioned algebraic conditions at any reduction step. The working conditions can be relaxed in a way such that the reduction is still feasible and drives the analysis to a quasilinear ODE setting, the reduced problem having the form

$$A_\nu(u)u' = f_\nu(u), \tag{10}$$

where $A_\nu$ is non-singular on a dense subset of the "reduced" state-space. This way, the dynamical phenomena displayed by quasilinear ODEs (which include impasse points but also so-called $K$, $I$ and $IK$ singularities [3]) can be addressed for quasilinear DAEs with arbitrary index.

A detailed discussion can be found in the forthcoming title [2].

*Supported by Research Project MTM2004-5316 of Ministerio de Educación y Ciencia, Spain.*

## References

[1] P. J. Rabier and W. C. Rheinboldt, Theoretical and numerical analysis of differential-algebraic equations, *Handbook of Numerical Analysis,* Vol. VIII, 183-540, North-Holland (2002).

[2] R. Riaza, *Analytical Aspects and Circuit Applications of Differential-Algebraic Systems,* World Scientific, to appear, 2008.

[3] J. Sotomayor and M. Zhitomirskii, Impasse singularities of differential systems of the form $A(x)x' = F(x)$, *J. Differential Equations* **169** (2001) 567-587.

# Stability Issues of Numerical Methods for DAEs

*Author(s):*

C. Tischendorf

University of Cologne, Math. Institute

Our considerations are motivated by the basic question *When numerical methods do provide solutions that reflect the asymptotic behaviour of differential-algebraic equations (DAEs) properly?* We discuss whether stability concepts as A-, B- or G-stability for ordinary differential equations (ODEs) are also appropriate for the classification of methods for DAEs. We will see that an answer to this question is far from being trivial and answered in the general case. We are confronted with the problem that the asymptotical solution behaviour of a DAE is not only influenced by that one of the inherent ODE but also by the behaviour of the solution manifold, in particular when time-dependent constraints are involved in the DAE. We analyze the reasons why A-stable methods for ODEs may lead to stepsize restrictions when applied to DAEs. Additionally, we show that the kind of formulation of methods for DAEs may strongly influence the numerical solution behaviour.

## General Linear Methods in Electrical Circuit Simulation

*Author(s):*

S. Voigtmann

Qimonda AG, Munich, Germany

Electrical Circuit Simulation relies on an efficient and robust solution of the differential algebraic equations (DAEs) arising from the modified nodal analysis (MNA). Classical methods for the transient analysis of electrical circuits are known to have certain shortcomings. Linear multistep methods suffer from poor stability properties while Runge-Kutta methods are usually too expensive.

General linear methods (GLMs) are suggested as a means to overcome these difficulties. John Butcher introduced GLMs in order to combine advantages of both linear multistep and Runge-Kutta schemes. Hence GLMs are designed for efficiency (similar to LMMs) and stability (similar to RK methods).

Starting from a structural analysis of the charge oriented MNA equations, order conditions and practical methods are derived. These developments led to a test implementation within Qimonda's in-house circuit simulator Titan.

Several case studies for industrial applications illustrate the potential of general linear methods for electrical circuit simulation. Some problems and open questions will be discussed as well.

## References

[1] J.C. Butcher *Numerical methods for ordinary differential equations* John Wiley & Sons, 2003.

[2] S. Voigtmann *General linear methods for integrated circuit design* Logos Verlag Berlin, 2006.

## Convergence of Collocation Schemes for BVPs in DAEs with Singularities

*Author(s):*

E. Weinmüller

Vienna University of Technology, Vienna, Austria

O. Koch,

Vienna University of Technology, Vienna, Austria

R. März,

Humboldt University Berlin, Berlin, Germany

and D. Praetorius

Vienna University of Technology, Vienna, Austria

We investigate the convergence of collocation for index-1 DAEs, where the *inherent ODE* may have a singularity of the first kind. We analyze the error of collocation methods applied to a linear system of DAEs given in the following form:

$$A(t)(D(t)x(t))' + B(t)x(t) = g(t), \quad t \in (0,1], \tag{11}$$

where $A(t) \in \mathbb{R}^{m\times n},\ D(t) \in \mathbb{R}^{n\times m},\ B(t) \in \mathbb{R}^{m\times m},\ g(t),\ x(t) \in \mathbb{R}^m$, with $n \leq m$. Here, we focus on DAEs with so-called *properly stated leading term*. In order to describe the boundary conditions which are necessary and sufficient for (11) to be well-posed, we use the decoupling technique developed in [1].

For the numerical solution of (11) we apply polynomial collocation to the enlarged system,

$$A(t)u'(t) + B(t)x(t) = g(t), \tag{12}$$
$$D(t)x(t) - u(t) = 0, \quad t \in (0,1]. \tag{13}$$

We give a proof for the convergence order of the scheme and illustrate the convergence behavior by means of experiments for model problems exhibiting different difficulties. In the proof we again utilize the above decoupling technique and use convergence results for the collocation applied to solve singular ODEs, developed in [2]. It turns out that the collocation method retains the stage order in case of sufficiently smooth problem data and shows order reductions otherwise. Superconvergence cannot be expected to hold in general.

# References


[1] K. Balla, and R. März, *A Unified Approach to Linear Differential Algebraic Equations and their Adjoint Equations*, J. Anal. Appl. **21**(2002), pp. 783–802.

[2] W. Auzinger, O. Koch, and E. Weinmüller, *Analysis of a New Error Estimate for Collocation Methods Applied to Singular Boundary Value Problems*, SIAM J. Numer. Anal. **42**(2005), pp. 2366–2386.

# Minisymposium
# Molecular dynamics

Organised by
E. Darve, F. Legoll

## Transition Path Sampling of Complex Activated Processes

*Author(s):*

P. Bolhuis

Department of Chemistry, University of Amsterdam

Designed for studying activated processes in complex environment, the transition path sampling (TPS) technique harvests a collection of dynamical trajectories that connect the reactant with the product states. This ensemble of true dynamical paths allows detailed understanding of the kinetics and mechanism of the activated process. The main advantage is that the method does not need prior knowledge of the reaction coordinate. In addition, TPS can be applied to identify mechanisms and determine rate constants.

The TPS technique has matured to a universal tool for the study of rare events in the decade since its development. In this presentation I will give a brief overview of the method, and describe current progress, with an emphasis on rate constant calculation and the analysis of reaction coordinates. As an example I will discuss an application on protein folding.

## Optimal Prediction in Classical Molecular Dynamics

*Author(s):*

C. Hartmann

Freie University of Berlin, Institute of Mathematics II

Basic issue in molecular dynamics is the sound causal explanation of observable macroscopic properties in terms of the dynamics of a single molecule and in terms of dimension-reduced models. This talk addresses model reduction for mechanical molecular models from the viewpoint of projection operator techniques and optimal prediction. Given a suitable reaction coordinate, we derive a simple expression for the optimal prediction Hamiltonian, which is non-separable and contains an effective potential which is, surprisingly, not the standard free energy. The effective Hamiltonian allows for a lucid physical interpretation as a mechanical system with a curved configuration space.

We illustrate that optimal prediction performs remarkably well, when it is applied to molecular dynamics problems that are intrinsically non-deterministic (e.g., conformation dynamics). It turns out that the intrinsic geometry of the reaction coordinate can have significant dynamical effects on the conformation dynamics that compete with the effects induced by the potential energy.

## Temperature regulated microcanonical dynamics

*Author(s):*

B. Leimkuhler

Maxwell Institute and School of Mathematics, University of Edinburgh

Molecular dynamics simulations typically incorporate devices to facilitate canonical sampling (or sampling with respect to some other prescribed density of states). However, many systems possess sufficiently ergodic internal dynamics so that thecanonical averages are well approximated by microcanonical trajectories. We have developed a simple adaptive dynamical technique for automatic equilibration of molecular dynamics. In our new method, temperature is moderated by a control law and an additional variable, as in Nosé dynamics, but whose influence on the system adaptively diminishes as the system approaches equilibrium. This drives the system towards a microcanonical state consistent with a given target temperature. This talk describes joint work with F. Legoll and E. Noorizadeh.

# A Multiscale Method for Stiff Ordinary Differential Equations with Resonance

*Author(s):*

Y. Tsai

Department of Mathematics and ICES, The University of Texas at Austin

G. Ariel

Department of Mathematics and ICES, The University of Texas at Austin

B. Engquist

Department of Mathematics and ICES, The University of Texas at Austin

A multiscale method for computing the effective behavior of a class of stiff and highly oscillatory ordinary differential equations (ODEs) is presented. The oscillations may be in resonance with one another and thereby generate a hidden slow dynamics. The method relies on correctly tracking a set of slow variables whose dynamics is closed up to $\epsilon$ perturbation, and is sufficient to approximate any variable and functional that are slow under the dynamics of the ODE. This set of variables is found by our numerical methods. Error and complexity estimates are obtained. The advantages of the method is demonstrated with a few examples that include a commonly studied problem of Fermi, Pasta, and Ulam.

# Minisymposium
# Multiscale and adaptive methods

Organised by
A. Cohen

## Multilevel preconditioners for DG methods

*Author(s):*

M. Campos Pinto

IRMA, CNRS and ULP Strasbourg, Strasbourg, France

In this talk we present multilevel preconditioners for interior penalty discontinuous Galerkin discretizations of second order elliptic boundary value problems that gives rise to uniformly bounded condition numbers. The underlying triangulation is only assumed to be shape regular and locally quasi-uniform and no extra regularity assumptions on the solution are needed.

This is a joint work with Wolfgang Dahmen and Kolja Brix.

## Exponential parametrization for solution of Kohn Sham Equations (DFT)

*Author(s):*

R. Schneider

Institute for Computer Science, Kiel, Germany

Electronic structure calculation plays an increasing role in the nuemrical simulation of molecular phenomena. Density functional theory povides an effective one particle model for the computation of the groundstate energy of a quantum mechanical system of $N$ electrons moving in a Coulombic field given by fixed nuclei. Instead of the high dimensional Schrödinger equation one has to solve nonquadratic optimzation problem in three space dimensions.

Since the exchange correlation potential is not known yet there remains a modelling error. The ground-state energy is the minimum of the Kohn-Sham engergy functional depending on $N$ pairwise orthogonal orbital functions. This is a minimization problem on a prescribed Stiefel resp. Grassman manifold. This problem can be treaten either as a constraint optimization problem, or by local parametrization of the manifold. The analysis of gradient type minmization procedure in both cases will be considered, and the connection of both approaches will be highlighted.

For insulating materials it is known, that the subspace generated by the orbital functions can be spanned, approximatively, by local functions, e.g. Wannier orbital. Linear scaling with respect to the number of atoms of the computational costs can be achieved by enforcing the locality of the iterates in each iteration step. For this purpose, local, or better multi-scale high order basis functions in conjunction with smooth, nonlocal, pseudo-potentials can provide an efficient alternative to either plane wave basis sets or Gaussian functions. This approach has been integrated in the BigDFT electronic structure program. In this code the discretization is based on Daubechies scaling function and wavelets.

This is a joint EU project with T. Deutsch, S. Goedecker, X. Gonze.

## Sparse Second Moment Analysis of Elliptic Problems in Stochastic Domains

*Author(s):*

C. Schwab

ETH Zurich, Zurich, Switzerland

We consider the numerical solution of Elliptic problems in domains with a class random boundary perturbations. Assuming perturbations with small amplitude and known mean field and two-point correlation function, we derive, using a second order shape calculus, deterministic equations for the mean field and the two-point correlation function of the random solution for the Dirichlet problem in the stochastic domain.

Using a variational boundary integral equation formulation on the unperturbed, 'mean' boundary and a wavelet discretization, we present and analyze an algorithm to approximate the random solution's two-point correlation function at essentially optimal order in essentially $\mathcal{O}(N)$ work and memory, where $N$ denotes the number of unknowns required for consistent discretization of the boundary of the domain.

This is a joint work with Reinhold Schneider and Helmut Harbrecht.

## An adaptive wavelet method for solving high-dimensional elliptic PDEs

*Author(s):*

R. Stevenson

Utrecht University, Utrecht, The Netherlands

When solving elliptic PDEs of say second order in $n$ space dimensions, using (adaptive) wavelet or finite element methods of order $d$, the best possible rate in energy norm is $\mathcal{O}(N^{-d/n})$, with $N$ being the number of degrees of freedom. When applying hyperbolic cross approximation (sparse grids), the curse of dimensionality can be avoided in the sense that a rate $\mathcal{O}(N^{-d})$ can be realized. This, however, requires $L_2$ boundedness of certain mixed derivatives of the solution, which is satisfied actually in exceptional cases only. In [Nit06], it was shown that best $N$-term approximations in tensor product wavelet bases realize this rate $\mathcal{O}(N^{-d})$ under very mild regularity conditions.

The rate of best $N$-term approximation can be realized computationally with adaptive wavelet methods, as introduced by Cohen, Dahmen and DeVore, *assuming* that the operator in wavelet coordinates, i.e., the (infinite) stiffness matrix is sufficiently close to a computable sparse matrix. Due to the higher rates of $N$-term approximations, for tensor product wavelets the requirements concerning near-sparsity are much stronger. Nevertheless, we were able to show that these requirements are satisfied for general partial differential operators with sufficiently smooth coefficients (cf. [SS07]).

A point of concern is the behaviour of the "hidden constant" in front of the rate. Without taking special care, one easily ends up with a constant that grows exponentially with $n$, making the method unpractical except for small $n$. Restricting ourselves to operators with constant coefficients, we present an adaptive wavelet method that produces approximations of length $N$ that up to some absolute constant are as good as best $N$-term approximations, at the cost of $CnN$ operations, with C being another absolute constant.

This is a joint work with Christoph Schwab.

## References

[DSS07] T J. Dijkema, Ch. Schwab, and R.P. Stevenson. An adaptive wavelet method for solving high-dimensional elliptic PDEs. Technical report, 2007. In preparation.

[Nit06] P.-A. Nitsche. Best $N$-term approximation spaces for tensor product wavelet bases. *Constr. Approx.*, 41(1):49–70, 2006.

[SS07] Ch. Schwab and R.P. Stevenson. Adaptive wavelet algorithms for elliptic PDEs on product domains. *Math. Comp.*, 2007. To appear.

# Minisymposium
# Nonlinear evolution equations

Organised by
M. Thalhammer

## Time discretisation of evolution equations by the backward differentiation formula

*Author(s):*

E. Emmrich

Technische Universität Berlin, Germany

We consider the time discretisation of first-order evolution equations governed by time-dependent monotone operators with strongly continuous perturbations. For the two-step backward differentiation formula (BDF) on a uniform grid, the questions of a priori estimates, convergence of piecewise polynomial prolongations, stability, and smooth-data error estimates are addressed. A main tool is an algebraic relation that reflects the G-stability of the two-step BDF with constant time steps. Moreover, the difficulties in the analysis that arise when studying variable time steps are discussed.

## On the computation of trigonometric operator-valued functions in the Gautschi-type exponential integrator

*Author(s):*

V. Grimm

Heinrich-Heine-University, Düsseldorf, Germany

M. Hochbruck

Heinrich-Heine-University, Düsseldorf, Germany

The Gautschi-type exponential integrator is favourable to numerically solve second-order wave equations since, in this integration scheme, the step size is independent of the space discretisation in sharp contrast to standard integrators. For its application, certain trigonometric operator-valued functions have to be computed. This is a challenging task whenever finite-elements in general domains are used. A Krylov procedure is proposed that renders a rational approximation even in the continuous abstract second-order problem which ensures that the approximation is again independent of the space discretisation. Or, to put it another way, the proposed procedure can be used to approximate a trigonometric matrix function times a vector independent of the norm of the matrix.

## Full discretizations of porous medium type equations

*Author(s):*

E. Hansen

University of Innsbruck, Austria

A. Ostermann

University of Innsbruck, Austria

We analyze the convergence properties of full discretizations of a class of generalized porous medium equations. For the spatial and time discretizations, we use continuous piecewise linear finite elements and algebraically stable Runge-Kutta methods, respectively. We prove an optimal convergence result for solutions that are sufficiently smooth in time, without any assumption on the spatial regularity. We will illustrate the convergence results with a few numerical experiments.

## Time-splitting spectral methods for the Gross–Pitaevskii equation

*Author(s):*

M. Thalhammer

University of Innsbruck, Austria

M. Caliari
University of Padua, Italy

We are concerned with the numerical discretisation of the Gross–Pitaevskii equation (GPE) by pseudospectral methods in space and high-order exponential operator splitting methods in time. The considered numerical methods are favourable in view of accuracy and efficiency; moreover, geometric properties of the equation are well captured.

For the spatial discretisation of the GPE, we analyse two approaches. On the one hand, in the unbounded domain, we employ a spectral decomposition into Hermite basis functions; this decomposition also facilitates to compute the ground state as well as excited states of the GPE. On the other hand, restricting the equation to a sufficiently large bounded domain, Fourier techniques are applicable. For the time integration of the GPE, we study exponential operator splitting methods of convergence orders two, four, and six.

Our main objective is to provide a thorough accuracy and efficiency comparison of time-splitting Fourier and Hermite pseudospectral methods for the time evolution of the GPE. Furthermore, we illustrate the effectiveness of higher-order exponential operator splitting methods in long-term computations.

# Minisymposium
# ODE's and optimization

Organised by
U. Ascher

## Title to be announced

*Author(s):*

H.G. Bock

IWR, Heidelberg, Germany

## Fast Denoising of Surface Meshes with Intrinsic Texture

*Author(s):*

H. Huang

University of British Columbia, Vancouver, Canada

We describe a fast, dynamic, multiscale iterative method that is designed to smooth, but not oversmooth, noisy triangle meshes. Our method not only preserves sharp features but also retains visually meaningful fine scale components or details, referred to as intrinsic texture. An anisotropic Laplacian (AL) operator is first developed. It is then embedded in an iteration that gradually and adaptively increases the importance of data fidelity, yielding a highly efficient multiscale algorithm (MSAL) that is capable of handling both intrinsic texture and mesh sampling irregularity without any significant cost increase.

## Robust optimization issues in parameterestimation and optimum experimental design for DAE models

*Author(s):*

E. A. Kostina

Faculty of Mathematics and Computer Science, University of Marburg

Estimating model parameters from experimental data is crucial to reliably simulate dynamic processes.

The identification problem can be described as follows. Let the dynamics of the model be described by a system of differential algebraic equations where the right-hand side depends on an unknown vector of parameters. It is assumed that there is a possibility to measure a signal of an output device that writes at given time points the output signal of the dynamic system with some errors. According to the common approach, in order to determine the unknown parameters the optimization problem is solved in which the special functional is minimized under constraints that describe the specifics of the model. Any norm of the measurement errors may be used as the functional in the optimization problem. The choice of an adequate norm depends on the statistical properties of the measurement errors. The traditional choice is weighted $l_2$ norm. In practical applications, however, it often appears that the data contains outliers. Thus, a reliable parameter estimation procedure (e.g. based on $l_1$ norm) is necessary that deliver parameter estimates less sensitive (robust) to errors in measurements.

Another difficulty that occurs in practical applications is that the experiments performed to obtain necessary measurements are expensive, but nevertheless do not guarantee sufficient identifiability. The optimization of one or more dynamic experiments in order to maximize the accuracy of the results of a parameter estimation subject to cost and other technical inequality constraints leads to very complex non-standard optimal control problems. One of the difficulties is that the objective function is a function of a covariance matrix and therefore already depends on a generalized inverse of the Jacobian of the underlying parameter estimation problem. Another difficulty is that the optimization results depend strongly on the assumed values of parameters which are only known to lie in a - possibly large - confidence region. Hence, robust optimal experiments are required that solve worst-case (min-max) optimization problems

The talk presents new effective algorithms for robust parameter estimation and design of robust optimal experiments in dynamic systems. Numerical results for real-life applications from chemistry and chemical engineering will be presented.

This talk is based on joint work with H. G. Bock, S. Körkel and J. P. Schlöder.

# Discrete Mechanics and Optimal Control

*Author(s):*

S. Ober-Blöbaum

Faculty of Computer Science, Electrical Engineering and Mathematics, University of Paderborn, D-33095 Paderborn, Germany

In this talk, we will propose a new approach to the solution of optimal control problems for mechanical systems ([2]). It is based on a direct discretization of the Lagrange-d'Alembert principle for the system (as opposed to using, for example, collocation or multiple shooting to enforce the equations of motion as constraints). The resulting forced discrete Euler-Lagrange equations then serve as constraints for the optimization of a given cost functional which leads to a finite dimensional optimization problem with structure preserving equality constraints.

This approach is extended to the optimal control of multi-body systems formulated as a constrained mechanical system. We reduce the discretized model using the discrete null space method ([1]), eliminating the constraint forces and leading to a discrete model of minimal dimension.

We illustrate the method by problems in space mission design and biomechancis, i.e. the optimal reconfiguration of a group of formation flying spacecraft as motivated by the Darwin (ESA) and TPF (NASA) space missions ([3]) and optimally controlled motion sequences, i.e. of an athlete's body.

This is joint work with Michael Dellnitz (University of Paderborn), Oliver Junge (TU Munich), Sigrid Leyendecker (Caltech) and Jerry Marsden (Caltech).

## References

[1] Betsch, P., and Leyendecker, S., "The discrete null space method for the energy consistent integration of constrained mechanical systems. Part II: Multibody dynamics", *Int. J. Numer. Meth. Engng.,* **67**(4), pp. 499–552, (2006).

[2] Junge, O., Marsden, J., and Ober-Blöbaum, S., "Discrete mechanics and optimal control", *In Proceedings of the 16th IFAC World Congress*, (2005).

[3] Junge, O., and Ober-Blöbaum, S., "Optimal Reconfiguration of Formation Flying Satellites", *In Proceedings of the IEEE Conference on Decision and Control and European Control Conference ECC, Seville, Spain*, (2005).

# Minisymposium
# Optimal control

Organised by
F. Bonnans, W. Hager

# Second-order optimality conditions for optimal control problems with state constraints

*Author(s):*

J.F. Bonnans
CMAP and INRIA-Futurs

A. Hermant
CMAP and INRIA-Futurs

The talk will review some recent progress in the study of second-order optimality conditions for optimal control problems of ordinary differential equations with state constraints and its relation to shooting algorithms.

Mre precisely, we deal with optimal control problem of an ordinary differential equation with several pure state constraints, of arbitrary orders, as well as mixed control-state constraints. We assume (i) the Hamiltonian to be strongly convex and the mixed constraints to be convex w.r.t. the control variable, and (ii) a linear independence condition of the active constraints at their respective order to hold. We give a complete analysis of the smoothness and junction conditions of the control and of the constraints multipliers. This allow us to obtain, when there are finitely many nontangential junction points, a theory of no-gap second-order optimality conditions and a characterization of the well-posedness of the shooting algorithm. These results generalize those obtained in the case of a scalar-valued state constraint and a scalar-valued control.

## References

[1] J.F. Bonnans, A. Hermant Well-Posedness of the Shooting Algorithm for State Constrained Optimal Control Problems with a Single Constraint and Control. Rapport de Recherche INRIA RR-5889 (2006). *SIAM J. Control Optimization*, to appear.

[2] J.F. Bonnans, A. Hermant: No-gap Second-order Optimality Conditions for Optimal Control Problems with a Single State Constraint and Control. Rapport de Recherche INRIA 5837 (2006). *Mathematical Programming Series B*, to appear.

[3] J.F. Bonnans, A. Hermant: Second-order Analysis for Optimal Control Problems with Pure and Mixed State Constraints. Rapport de Recherche INRIA RR-6199, 2007.

[4] J.F. Bonnans, A. Hermant Stability and Sensitivity Analysis for Optimal Control Problems with a First-order State Constraint. Rapport de Recherche INRIA RR-5889, 2006..

# Jacobi Type Conditions for Singular Extremals

*Author(s):*

A. Dmitruk
Russian Academy of Sciences, Central Economics & Mathematics Institute; email: vraimax@mail.ru

Consider the following optimal control problem on a fixed time interval $[t_0, t_1]$:

$$\begin{cases} \dot{x} = f_0(t,x) + F(t,x)\,u, \qquad u \in U(t), \\ \eta_j(x(t_0), x(t_1)) = 0, \quad j = 1, \dots, \mu, \\ J = \ \varphi_0(x(t_0), x(t_1)) \to \min, \end{cases}$$

where $x \in \mathbf{R}^n$, $u \in \mathbf{R}^r$, and study a singular extremal $(x^0, u^0)$ with $u^0(t) \in int\, U(t)$, assuming that the Lagrange multipliers are unique. Then the "second" order optimality conditions [1] have the form of sign definiteness of the second variation of Lagrange function

$$\Omega(\bar{x}, \bar{u}) \;=\; (l''\bar{p}, \bar{p}) - \int_{t_0}^{t_1} \left((H_{xx}\,\bar{x}, \bar{x}) + 2(\bar{x}, H_{xu}\bar{u})\right)\, dt\,,$$

where $H = \psi\,(f_0(t,x) + F(t,x)\,u)$, $l(p) = \varphi_0(p) + \sum \beta_j\,\eta_j(p)$, $p = (x(t_0), x(t_1)) \in \mathbf{R}^{2n}$, with respect to the quadratic order

$$\gamma(\bar{x}, \bar{u}) = \; |\bar{x}(t_0)|^2 + |\bar{y}(t_1)|^2 + \int_{t_0}^{t_1} |\bar{y}(t)|^2\, dt, \qquad \dot{\bar{y}} = \; \bar{u}\,, \quad \bar{y}(t_0) = 0,$$

on the subspace of critical variations:

$$\dot{\bar{x}} = f'_{0x}(t, x^0)\,\bar{x} + F'_x(t, x^0)\,\bar{x}\,u^0 + F(t, x^0)\,\bar{u},$$

$$\eta'_j(p^0)\,\bar{p} \;=\; 0, \quad j = 1, \ldots, \mu,$$

The functional $\Omega$ does not contain the main, Legendre term with $\bar{u}^2$, which immediately puts us out of the framework of the classical Jacobi theory on conjugate points. However, using the so-called Goh transformation, we can convert $\Omega$ into a new quadratic functional having almost a classical form (involving an additional parameter), that possibly satisfies the strengthened Legendre condition. Then, by applying the Hestenes approach, we determine its sign definiteness in terms of a conjugate point, which can be found by solving the corresponding Euler–Jacobi equation [2].

## References


[1] A.V.Dmitruk, Quadratic order conditions of a weak minimum for singular regimes in optimal control problems, *Soviet Math. Doklady,* 1977, v. 18, No. 2.

[2] A.V.Dmitruk, Jacobi Type Conditions for Singular Extremals, *Math. Methods in Optimal Control, (A. Korytowski, ed.),* Springer, 2007 (to appear).


# Launching trajectories with singular arcs: a shooting method approach.


*Author(s):*

P. Martinon
INRIA FUTURS, CMAP Ecole Polytechnique

F. Bonnans
INRIA FUTURS, CMAP Ecole Polytechnique

E. Trélat
Université d'Orléans, MAPMO



We study optimal trajectories for launcher problems, where the control is the thrust force, and the objective is to maximize the payload (final mass). Due to the presence of aerodynamic forces (drag), optimal trajectories may not have a pure bang-bang (on/off) thrust law. Namely, singular arcs can occur, along which the norm of the thrust is neither zero nor maximal. The resolution approach we choose here consists in combining a shooting method with an homotopic method. The homotopic approach implies the progressive introduction of the aerodynamic forces, as well as a quadratic regularization of the problem. It provides strong hints about the control structure, and a suitable starting point for the shooting merthod. Numerical simulations are carried out for the generalized (3D) Goddard problem, and for a more realistic multi-stage heavy launcher.

## References


[1] H.M. Robbins, *A generalized Legendre-Clebsch condition for the singular case of optimal control.* **IBM J. of Research and Development**, 11:361–372, 1967.

[2] A.E. Bryson and Y.C. Ho, *Applied optimal control*, Hemisphere Publishing, New-York, 1975.

[3] E. Allgower and K. Georg, *Numerical Continuation Methods*, Springer-Verlag, Berlin, 1990.

[4] H.J. Oberle, *Numerical computation of singular control functions in trajectory optimization.* **Journal of Guidance, Control and Dynamics**, 13:153–159, 1990.

[5] J. Gergaud and P. Martinon, *"An application of PL continuation methods to singular arcs problems"*, Proceedings of the 12th FGS Conf. on Optimization, Avignon, 2004, Ed. A. Seeger, **Lectures Notes in Economics and Mathematical Systems**, Vol. 563, pp.163-186, Springer, 2006.

[6] F. Bonnans, P. Martinon and E. Trélat, *"Singular arcs in the generalized Goddard's Problem"*, **RR-6157**, 2007.


# Optimality conditions for problems linear in a part of controls: quadratic form and Riccati equation


*Author(s):*

N. Osmolovskii

Systems Research Institute, Polish Academy of Sciences, ul. Newelska 6, 01-447 Warszawa, Poland

H. Maurer

Institut für Numerische und Angewandte Mathematik, Einsteinstr. 62, D–48149 Münster, Germany



The classical second order optimality conditions for an optimization problem with constraints require that the second variation of Lagrangian be positive (semi-)definite on the cone of critical directions. Conditions of such type, both necessary and sufficient, were obtained in [1, 2, 3] for the pure bang-bang case, where all control variables enter linearly to the system dynamics and the control constraint is given by a convex polyhedron. In the present talk, we formulate quadratic optimality conditions of such type for optimal control problems with a vector control variable having two components: a *continuous* unconstrained control *appearing nonlinearly* in the control system and a *bang–bang* control *appearing linearly* and belonging to a convex polyhedron. For the control problem with continuous and bang-bang control components, we define the notions of a Pontryagin local minimum and a bounded-strong local minimum and formulate both necessary and sufficient second order conditions for these types of a minimum. Using a suitable transformation via a Riccati matrix equation, we develop numerical methods to test the positive definiteness of the quadratic form and give criteria for the positive definiteness of the quadratic form on the critical cone in terms of solutions to a matrix Riccati equation which may be discontinuous at the switching times. The results are applied to an economic control problem in optimal production and maintenance which was introduced by Cho, Abad and Parlar. We give another important example of a problem of such type: the planar Earth-Mars transfer with minimal flight time. Moreover, the importance of sufficient second order conditions is due to their crucial role in the sensitivity analysis of parametric optimal control problems.

# References


[1] Milyutin, A.A. and Osmolovskii, N.P. *Calculus of Variations and Optimal Control*, Translations of Mathematical Monographs, 180, American Mathematical Society, Providence, 1998.

[2] Maurer, H. and Osmolovskii, N.P. Second order optimality conditions for bang–bang control problems. *Control and Cybernetics*, 32(3): 555-584, 2003.

[3] Maurer, H. and Osmolovskii, N.P. Second order sufficient conditions for time optimal bang–bang control problems *SIAM J. Control and Optimization*, 42: 2239–2263, 2004.

# Minisymposium
# PDEs and image processing

Organised by
E. Prados

# Tomography and Reconstruction via boundary measurement

*Author(s):*

A.K. Nandakumaran

Department of Mathematics - Indian Institute of Science - Bangalore- 560 012 - India. - Email: nands@math.iisc.ernet.in

Hari M. Verma and R. M. Vasu

Department of Instrumentation - Indian Institute of Science - Bangalore- 560 012 - India.

Our intention is to study Diffraction tomographic reconstruction of refractive index distribution and diffuse optical correlation Tomography for the reconstruction of visco-elastic properties. This has applications in many area including medical imaging. First, we present a method which can reconstruct the complex refractive index distributions from intensity-based measurements. We have implemented an iterative algorithm which requires efficient implementation of a forward wave propagation equation and sensitivity matrices . An efficient method for estimation of the sensitivity matrices is given and also the forward operator. The results of numerical experiments shows that different reconstruct respectively the imaginary and real part of the refractive index distribution. The basic equation, we are as follows:

The propagation of monochromatic wave of wavelength $\lambda_0$ through a medium of refractive index distribution $n(\vec{r})$is governed by the Helmholtz equation

$$\nabla \cdot \nabla u(\vec{r}) + k^2 u(\vec{r}) = 0 \tag{14}$$

Here $u(\vec{r})$ is the complex amplitude of the wave and $k$ is the modulus of the propagation vector,which is $\mid \vec{k} \mid = n(\vec{r})\frac{2\pi}{\lambda_0}$. Considering $n(\vec{r}) = 1 + n_\delta(\vec{r})$ where $n_\delta(\vec{r})$ is a small perturbation to the background medium which is air whose refractive index is one we can approximate the above equation as,

$$\nabla \cdot \nabla u(\vec{r}) + k_0^2(1 - f(\vec{r}))u(\vec{r}) = 0 \tag{15}$$

Our future plan is to work diffuse optical correlation tomography. We consider the propagation of the unnormalized field autocorrelation function $G_1(r,\tau) =< E(\vec{r},t)E^*(\vec{r},t+\tau) >$ of near infrared light, inside a highly scattering medium like tissue. The propagation of $G_1(\vec{r},\tau)$ is governed by certain pde. We wish to do certain numerical computations, mathematical analysis as well as experiments.

# Contributions to the deformable models and variational framework for some computer vision and image processing applications.

*Author(s):*

J. P. Pons

Deformable models constitute a flexible framework to address various shape reconstruction problems in image processing. They have been initially proposed for the purpose of image segmentation, but they have also proven successful in many other contexts in computer vision and in medical imaging, including region tracking, stereovision, shape from shading and shape from unstructured point sets. The key elements of this framework are the design of an energy functional, the choice of a minimization procedure and of a geometric representation. In this talk, we consider these three elements, with the objective of increasing the applicability and efficiency of deformable models and we consider some associated applications in the fields of medical imaging (unfolded representations of the cerebral cortex and segmentation of several head tissues from MRI) and of computer vision (multi-view stereovision and scene flow estimation).

## Hamilton-Jacobi Equations for the photometric reconstruction of tridimensional shape.

*Author(s):*

E. Prados

Inria Rhône-Alpes, Montbonnot, France

We are interested in the reconstruction of the tridimensional shape of a surface from 2D images of that surface. When this reconstruction is directly based on photometric properties of the surface and when we try to really exploit them, then this yields in resolving a Partial Differential Equation of Hamilton-Jacobi type, or more generally in the case of the most complex scenari, this yields in a system of nonlocal integro-differential equations. We then propose to study some scenari, to detail the associated PDEs, and to illustrate some fundamental theoretical questions about these equations and to understand their impact in the computer vision field.

## Fast Anisotropic Smoothing of Multi-Valued Images using Curvature-Preserving PDEs.

*Author(s):*

D. Tschumperlé

This talk focuses on PDE's (Partial Differential Equations) in order to smooth Multi-Valued Images in an anisotropic manner. We point out the pros and cons of the different existing equations, then we introduce a tensor-driven PDE, regularizing images while better preserving the curvatures of important image structures. A direct link is made between our proposed equation and a continuous formulation of the LIC's (Line Integral Convolutions as introduced by [Cabral & Leedom:93]). It leads to the design of a very fast and stable algorithm that implements our regularization method, by successive integrations of pixel values along curved integral lines. The scheme numerically performs with a sub-pixel accuracy and outperforms classical finite differences discretization schemes. We finally illustrate the various applications and the efficiency of our generic curvature-preserving approach - in terms of speed and visual quality with results for color images denoising, inpainting and image resizing by nonlinear interpolation.

# Minisymposium
# Shadow equations

Organised by
W. Hayes

## A New Containment Method For Rigorous Shadowing

*Author(s):*

A. Goldsztejn

University of California, Irvine, CA, USA

W. B. Hayes

University of California, Irvine, CA, USA

A reliable simulation usually refers to a simulation that presents a small global error. This study of reliability is called forward error analysis. However, this kind of analysis is useless when one studies chaotic systems, because such systems will present exponential growth of global errors no matter how small the local error. In this context, where the forward error analysis does not provide any interesting information, the backward error analysis may allow extracting information from simulations that diverge exponentially from the exact solution. The backward error analysis consists of finding a modified problem P' for which the simulation, which diverges exponentially from the exact solution of P, is a good approximation of the exact solution of P'. Among other backward error analysis techniques, shadowing allows modifying the problem by changing its initial condition, while disallowing changes in the defining equation. Therefore, the question asked by shadowing error analysis is "Given a dynamical system, an initial condition and a simulation of this system (which certainly diverges exponentially), can we find a different initial condition for which our simulation is accurate?" We will introduce the shadowing backward analysis and present our new containment algorithm for the rigorous proof of the existence of a shadow. This algorithm results of an original application of the interval analysis for the rigorous verification of the hypotheses of a containment theorem. Our method is both simpler and more efficient than the previous containment algorithms. Applications to the rigorous proof of chaos in discrete dynamical systems are reported.

## Reliability of galaxy simulations

*Author(s):*

W. B. Hayes

University of California, Irvine, CA, USA

Numerical simulations of collisionless gravitational systems form the backbone of our theoretical understanding of galaxy, galaxy cluster, and cosmological evolution. Simulation provides the crucial link between our microscopic understanding of gravity (Newtonion + Relavitistic), and the macroscopic dynamical evolution of gravitational systems. Such simulations have been used to test and even invalidate theories. As such, establishing their trustworthiness is absolutely critical.

Gravitational systems are chaotic, and display sensitive dependence on initial conditions (SDIC), so that numerical errors become exponentially magnified with time. Although the existence of SDIC has been known for decades, its effect on macroscopic properties of solutions is still not well understood.

A shadow is an exact solution that remains close to a numerical solution for a long time. If a shadow solution exists, then the numerical solution can be viewed as an observation of an exact solution, and thus its dynamical properties can be trusted, to within "observational" error. In this talk, I will discuss recent results on shadowing a million-particle simulation of a collision between two galaxies.

## Accurate particle tracing in realistic flows by finite time shadowing

*Author(s):*

E.D. Svensson

Department of Mathematical Sciences, Chalmers University of Technology, SE-412 96 Göteborg, Sweden; Current address: erik.svensson@skf.com

We consider computed particle trajectories in flows defined by continuum models but given as approximate velocity data, and derive finite time shadowing error estimates, cf. [1]. In particular we consider finite element approximations to Stokes flows and compare classical a posteriori error estimates with the provided finite time shadowing error estimate, according to which accurate particle tracing is possible for large times even in dynamically unstable flows. As an application we briefly show how the error estimate could be used to define a quantitative measure for mixing of fluids in the absence of diffusion.

# References

[1] Rigorous computational shadowing of orbits of ordinary differential equations. *Numer. Math.*, 69:401–421, 1995.

# Minisymposium
# Software issues

Organised by
L. Brugnano, F. Mazzia

## MATLAB Interface to Test Set for IVP Solvers

*Author(s):*

J. Kierzenka

The MathWorks, Inc., Natick, USA

In this talk we describe the MATLAB interface to problems in the Test Set for IVP Solvers [1].

The Test Set contains a collection of initial value problems for differential equations. A uniform FORTRAN interface to all test problems makes them an easy to use tool for testing and profiling general purpose ODE solvers.

The latest Revision 2.3 of the Test Set has been enhanced with a MATLAB interface to all problems in the collection. In this talk we discuss our motivation for developing that interface and provide an overview of its functionality. We will demonstrate how the test problems can be used to profile MATLAB solvers. The discussion will be illustrated with performance data gathered during our experiments with solvers from the MATLAB ODE Suite. We will conclude with remarks on the problems available in the collection, features of MATLAB interface and MATLAB solvers, and possible directions of future developments.

## References

[1] Francesca Mazzia, Cecilia Magherini, and Felice Iavernaro, *Test Set for Initial Value Problem Solvers,* Technical Report 43, Department of Mathematics, University of Bari, 2006. Available at `http://pitagora.dm.uniba.it/~testset/`

## Computation of Consistent Initial Values for Properly Stated Index 3 DAEs

*Author(s):*

R. Lamour

Humboldt-University of Berlin, Berlin, Germany

F. Mazzia

Università di Bari, Italy

The computation of consistent initial values is one of the basic problems solving initial or boundary value problems of DAEs.
The difficulties to compute consistent initial values start before a numerical computation. For a given DAE it is not obvious how to formulate the initial conditions which leads to a uniquely solvable IVP.
The existing algorithms for the determination of consistent initial values are designed for fixed indexes or need a special structure of the DAE or need more than the given data (e.g. additional differentiations).
We propose an algorithm which delivers the necessary data to formulate the initial conditions and which works for nonlinear DAEs up to index 3. Illustrative examples are given.

## References

[1] P. Amodio and F. Mazzia. An algorithm for the computation of consistent initial values for differential-algebraic equations. *Numerical Algorithms*, 19:13–23, 1998.

[2] R. Lamour. Index determination and calculation of consistent initial values for daes. *Comp. Math. with Appl.*, 50:1125–1140, 2005.

## Implementation of the BS-methods for the numerical solution of BVPs

*Author(s):*

F. Mazzia
Università di Bari, Italy

D. Trigiante
Università di Firenze, Italy

A. Sestini
Università di Firenze, Italy

The BS linear multistep methods have been introduced in [1] where the properties of the numerical schemes are studied in case of uniform stepsize and in [2, 3] where the methods have been generalized for a non-uniform mesh.

An important property of these methods is that it is easy to compute a continuous extension using the B-spline basis which has the derivatives globally continuous up to order $k$, if $k$ is the number of steps of the method. The convergence properties of the continuous extension have been studied in [3] where an economical strategy for the computation of the spline coefficients has been introduced.

These methods have been implemented in the new release of the code TOM, written in Matlab. The code TOM is designed for the numerical solution of Boundary Value Problems (BVPs). The distinguishing characteristics of the code are: the use of the conditioning in the mesh selection strategy, that allows the code to solve efficiently singularly perturbed BVPs; the use of a quasi-linearization strategy to handle non linearity and the use of BVMs (Top Order and BS methods) as underlying numerical schemes. The effectiveness of the implementation of these strategies is demonstrated by means of numerical examples.

## References

[1] F. Mazzia, A. Sestini and D. Trigiante (2006), B-spline Multistep Methods and their Continuous Extensions, SIAM J. Numer Anal. 44, No. 5, 1954-1973.

[2] F. Mazzia, A. Sestini and D. Trigiante (2006), BS Linear Multistep Methods on Non-uniform Meshes, JNAIAM 1, 131-144.

[3] F. Mazzia, A. Sestini and D. Trigiante (2006), The continuous extension of the BS linear multistep methods on non-uniform meshes, submitted.

## Explicit two-step peer methods

*Author(s):*

R. Weiner
University of Halle, Germany

B.A. Schmitt
University of Marburg, Germany

H. Podhaisky
University of Halle, Germany

We discuss $s$-stage explicit two-step peer methods for nonstiff differential equations. These methods compute at each step $s$ numerical approximations of the same order. We derive order conditions and present a construction principle for methods of order of consistency $p = s$. By a special ansatz optimal zero stability of the methods is ensured. The methods are convergent of order $s$. An additional condition allows to construct superconvergent methods of order $p = s + 1$ for variable stepsizes.

The methods are implemented in Nordsieck form, what allows an easy error estimation and stepsize changes. We present numerical results for superconvergent peer methods with $s = 4, ..., 7$ stages on well-known test problems and compare the methods with the state of the art Runge-Kutta codes DOPRI5 and DOP853 [1]. The results show the efficiency of the proposed two-step methods.

# References

[1] E. Hairer, S.P. Nørsett and G. Wanner, *Solving Ordinary Differential Equations, I. Nonstiff Problems*, second revised edition, Springer, Berlin, 1993.

# Minisymposium
# Software issues II

Organised by
L. Brugnano, F. Mazzia

# Numerical solution of Bordered ABD linear systems arising from Boundary Value Problems

*Author(s):*

P. Amodio

Dipartimento di Matematica, Università di Bari, Italy

I. Gladwell

Department of Mathematics, Southern Methodist University, Dallas, Texas, U.S.A.

G. Romanazzi

School of Computing, University of Leeds, United Kingdom

The most time-consuming part of any software for the numerical solution of BVPs is the linear algebra one, where the solution of several systems with a well defined sparsity pattern is needed. In general numerical methods for BVPs require the solution of ABD linear systems, that is systems with the nonzero elements grouped in block rows and with no intersection between the nonzero columns of two nonconsecutive block rows [1]. This is the case, for example, of some Runge-Kutta methods and orthogonal spline collocation methods. For these reasons, several codes for ABD systems (see, for example, SOLVEBLOK and COLROW) have been developed and used inside these packages.

If the considered BVPs have nonseparated boundary conditions, then the structure of the obtained linear systems shows an additional nonnull block in the left-lower (or right-upper) corner and no ABD solver may be used. In such a case all the BVP packages require that the number of ODEs is doubled in order to derive separated boundary conditions.

We will analyze the application of the recently published package BABDCR [3] to some of the most used softwares for BVPs. BABDCR solves BABD linear systems with blocks of the same size and with the same overlap (for example, the linear systems obtained in the package MIRKDC). We will also consider the solution of systems with a more general BABD structure [2] and a straightforward distributed memory parallel implementation of BABDCR based on MPI procedures.

## References

[1] P. Amodio, J.R. Cash, G. Roussos, R.W. Wright, G. Fairweather, I. Gladwell, G.L. Kraut, M. Paprzycki, *Almost block diagonal linear systems: sequential and parallel solution techniques, and applications*, Numer. Linear Algebra Appl. **7** (2000), pp. 275–317.

[2] P. Amodio, I. Gladwell, G. Romanazzi, *Numerical solution of general Bordered ABD linear systems by cyclic reduction*. Journal of Numerical Analysis, Industrial and Applied Mathematics **1** (2006), pp. 5-12.

[3] P. Amodio, G. Romanazzi, *BABDCR: a Fortran 90 package for the solution of Bordered ABD systems*. ACM Trans. Math. Software, **32** (2006), no. 4, pp. 597–608.

# Linear Analysis of Convergence for Splittings Solving ODE Problems

*Author(s):*

L. Brugnano

Università di Firenze, Italy

C. Magherini

Università di Pisa, Italy

In the nineties, Van der Houwen et al. (see, e.g., [4, 5, 6]) introduced a linear analysis of convergence for studying the properties of the iterative solution of the discrete problems generated by implicit methods for ODEs. This linear convergence analysis has been recently completed [2], in order to provide a useful quantitative tool for the analysis of splittings for solving such discrete problems. Moreover this tool, in its complete form, has been actively used when developing the computational codes `BiM` and `BiMD` [1, 3]. Further examples of application, aimed to compare different iterative procedures, are also presented.

## References


[1] L. Brugnano, C. Magherini. The BiM Code for the Numerical Solution of ODEs, *Jour. Comput. Appl. Math.* **164-165** (2004) 145–158.
Code available at: `http://www.math.unifi.it/~brugnano/BiM/index.html`

[2] L. Brugnano, C. Magherini. Recent Advances in Linear Analysis of Convergence for Splittings for Solving ODE Problems, *(submitted).*

[3] L. Brugnano, C. Magherini, F. Mugnai. Blended implicit methods for the numerical solution of DAE problems, *Jour. Comput. Appl. Math.* **189** (2006) 34–50.

[4] P. J. van der Houwen, B. P. Sommeijer, J. J. de Swart. Parallel predictor-corrector methods. *Jour. Comput. Appl. Math.* **66** (1996) 53–71.

[5] P. J. van der Houwen, J. J. B. de Swart. Triangularly Implicit Iteration Methods for ODE-IVP Solvers, *SIAM J. Sci. Comput.* **18** (1997) 41–55.

[6] P. J. van der Houwen, J. J. B. de Swart. Parallel Linear System Solvers for Runge-Kutta Methods, *Adv. Comput. Math.* **7**,1-2 (1997) 157–181.


# A Fortran-Matlab code for Second Order Differential Equations


*Author(s):*

S. González-Pinto

Dpto Analisis Matematico, University of La Laguna, 38208 La Laguna, Tenerife, Spain, spinto@ull.es

S. Pérez-Rodríguez

Dpto Analisis Matematico, University of La Laguna, 38208 La Laguna, Tenerife, Spain, sperezr@ull.es

L. Randez

Dpto Matematica Aplicada, University of Zaragoza, 50009 Zaragoza, Spain, randez@unizar.es

R. Rojas-Bello

Area de Matematicas, UNEG, Puerto Ordaz, Venezuela, rrrojas@ull.es



We present a standard Fortran 90 code, intended for the numerical solution of initial value problems for second order diferential equations of the special type $y''(t) = f(t, y)$. It can also be used, after some minor modifications, for boundary value problems by shooting techniques. The code, that is of general scope, can cope satisfactorily with oscillatory problems specially when the low frequencies are dominant and low to medium accuracy is required. It is of interest for medium to large dimensional problems when banded Jacobian matrices arise from the discretization in space via MoL of some time-dependant partial differential equations. The code is equipped with a reliable global error estimate and it is based on the two-stage Runge-Kutta Gauss method, where the internal stages are solved by a special Newton-type iteration with predictors carefully chosen to minimize the number of iterations of the iterative process. It also incorporates an automatic selection of the initial step-size and a variable step-size policy. A continuous solution with no extra computational cost it is provided. The code

is based on the papers [1, 2, 3] and it can be downloaded from [4]. Also the `Matlab` version with similar user interface will be presented. This version uses the facility of `Matlab` to handle matrices to avoid different calls to the full-matrix solvers and also makes use of the specialized sparse-matrix linear algebra subroutines. The software developed has the following features: Easy to use, Plot the numerical solution against time and Plot the phase-space in the plane. The performance of the code on some interesting second order problems will be exhibited.

## References


[1] M. Calvo, S. González-Pinto and J.I. Montijano, *Global error estimation based on the tolerance proportionality for some adaptive Runge-Kutta codes*, Accepted in J. Comput. Appl. Math. (2007), doi: 10.10.16/j.cam.2007.02.034

[2] S. Gonzalez-Pinto, S. Pérez-Rodriguez and R. Rojas-Bello, Efficient iterations for Gauss methods on second order problems,*J. Comput. Appl. Math.*,**189** (2006), 80–97.

[3] S. Gonzalez-Pinto and R. Rojas-Bello, A code based on the two-stage Gauss method for second order problems, preprint at *http : //pcmap.unizar.es/numerico/* submitted for publication.

[4] S. Gonzalez-Pinto, S. Pérez-Rodriguez, L. Rández and R. Rojas-Bello, *gauss2.tgz* in *http : //www.netlib.org/ode/*, see also *http : //pcmap.unizar.es/numerico/software.php*


# Design and implementation of a coordinate projection integrator in SUNDIALS


*Author(s):*

R. Serban

Lawrence Livermore National Laboratory, Livermore, USA


This talk introduces CPODES, a coordinate projection integrator for ODEs with invariants. CPODES was designed and implemented within the framework provided by SUNDIALS, the SUite of Nonlinear and DIfferential/ALgebraic equation Solvers.

SUNDIALS [1] is a suite of advanced computational codes for solving large-scale problems that can be modeled as a system of nonlinear algebraic equations, or as initial-value problems in ordinary differential or differential-algebraic equations. The basic versions of these codes are called KINSOL, CVODE, and IDA, respectively, and sensitivity-enabled solvers are also included (CVODES) or under development (IDAS). The codes are written in ANSI standard C and are suitable for either serial or parallel machine environments.

CPODES is a coordinate projection-based solver [2] for systems of ODEs with invariants (either in explicit or implicit form). It implements a variable-order, variable-step BDF method combined with several methods for the projection onto the invariant manifold, including the option of user-supplied projection functions. For the nonlinear systems arising in the application of the implicit LMM, CPODES provides a choice of functional iteration or Newton iteration, in the latter case combined with one of the many linear solver modules provided within SUNDIALS. The internal projection algorithm can use one of several decompositions of the constraint Jacobian; e.g. LU, QR, QR with pivoting, etc.

The main motivation for developing CPODES was the solution of index-3 DAEs as arising in the modeling of multibody systems. CPODES is currently used in conjunction with SimTK in Simbios, an NIH Center for Biomedical Computation at Stanford.

We discuss the main design and implementation characteristics of CPODES as related to and imposed by those of the SUNDIALS suite, present some typical problems and their solution with CPODES, and conclude with future devlopments.

# References

[1] Alan C. Hindmarsh, Peter N. Brown, Keith E. Grant, Steven L. Lee, Radu Serban, Dan E. Shumaker, and Carol S. Woodward. SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers. *ACM Transactions on Mathematical Software*, 31(3):363–396, 2005.

[2] E. Eich Convergence Results for a Coordinate Projection Method Applied to Mechanical Systems with Algebraic Constraints. *SIAM Journal on Numerical Analysis*, 30(5):1467–1482, 1993.

# Minisymposium
# Splitting and Lie-group methods

Organised by
F. Casas, B. Owren

## On the BCH formula and related expansions

*Author(s):*

F. Casas

Departament de Matemàtiques, Universitat Jaume I, 12071 Castellón, Spain

In the theory of Lie-group methods and in general in geometric numerical integration, an important role is played by the Baker–Campbell–Hausdorff (BCH) formula on the composition of exponentials [3]. It allows, in particular, to obtain the order conditions to be satisfied by the coefficients of composition ad splitting methods [1].

There are at least two other expansions which are closely related to the BCH formula. The first is the Magnus expansion [2], also called the continuous analogue of the BCH formula, with several important applications in mathematical physics, control theory and numerical analysis. The second is the so-called Zassenhaus formula [2, 4], which is essentially the dual of the BCH formula, in the sense that it expresses the exponential of an element in a Lie algebra as an infinite product of exponentials.

In this talk we will review some of the most recent contributions in the analysis of these expansions, including new derivations and a detailed treatment of their convergence.

## References

[1] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, 2nd Edition, Springer, 2006.

[2] W. Magnus, On the exponential solution of differential equations for a linear operator, *Commun. Pure and Appl. Math.* **7** (1954), 649-673.

[3] W. Magnus, A. Karrass, and D. Solitar, *Combinatorial Group Theory*, Dover, 1976.

[4] R.M. Wilcox, Exponential operators and parameter differentiation in quantum physics, *J. Math. Phys.* **8** (1967), 962-982.

## Geometric integrators for the Camassa-Holm equation

*Author(s):*

D. Cohen

NTNU Trondheim, Trondheim, Norway

We will present some initial attempts to develop geometric integrators for the Camassa-Holm equation. We will focus the talk on some multi-symplectic formulations of this nonlinear partial differential equation.

This is a joint work with Xavier Raynaud and Brynjulf Owren.

## Observations on Gaussian bases for Schrödingers Eigenproblem

*Author(s):*

I. Degani

Department of Mathematics, university of Bergen, Norway.

One of the few methods for generating efficient function spaces for multi-D Schrödinger equations is given by Garashchuk and Light [1]. Their Gaussian basis functions are wider and sparser in high potential regions, and narrower and denser in low ones. A modification of their approach will be discussed based on the following observation: In very steep potential regions which are near wells, wide, sparse, Gaussians should be avoided even if their centers have high potential values. Numerical results will be shown illustrating that a dramatic improvement in accuracy may be obtained in this way. Some observations will be given regarding the use of collocation together with Gaussian basis functions in Schrödinger Eigenproblems.

## References


[1] S. Garashchuk and J.C. Light, *Quasi random distributed Gaussian bases for bound problems,* J.Chem.Phys. 114 (2001) 3929.


# Geometric integration methods for the computation of the Evans function


*Author(s):*

J. Niesen
La Trobe University, Melbourne, Australia

S. Malham
Heriot–Watt University, Edinburgh, Scotland


The spectral stability of travelling wave solutions of partial differential equations is determined by the spectrum of the differential operator linearized around the travelling wave. The Evans function is a tool for locating the eigenvalues of this operator. The main step in the computation of the Evans function is the computation of the fundamental solution of a linear ordinary differential equation (ODE). Unfortunately, the straightforward approach will suffer from numerical stability problems [4].

A possible solution is to lift the ODE to an exterior product space [1, 2]. The question arises how to preserve the geometry of the product space. Specifically, the ODE evolves on a Grassmannian manifold, which we wish to preserve. Both splitting methods and Lie-group methods achieve this feat. Specifically, the discretization used by these methods commutes with the lift to the exterior product space.

A disadvantage of this approach is that the dimension of the exterior product space can be exorbitantly large. Humpherys and Zumbrun [3] have proposed an alternative approach, based on continuous orthogonalization, which projects the equation on a Stieffel manifold. Again, Lie-group methods show us how to preserve this manifold.

## References


[1] A. L. Afendikov and T. J. Bridges. Instability of the Hocking–Stewartson pulse and its implications for three-dimensional Poiseuille flow. *Proc. R. Soc. Lond. A*, 457:257–272, 2001.

[2] L. Q. Brin. Numerical testing of the stability of viscous shock waves. *Math. of Comput.*, 70(235):1071–1088, 2000.

[3] J. Humpherys and K. Zumbrun. An efficient shooting algorithm for Evans function calculations in large systems. *Physica D*, 220(2):116–126, 2006.

[4] B. Sandstede. Stability of travelling waves. In B. Fiedler, editor, *Handbook of Dynamical Systems II*, pages 983–1055. North-Holland, 2002.

# Minisymposium
# Stable and conservative general linear methods

Organised by
J. Butcher, Z. Jackiewicz

## Order arrows and some applications

*Author(s):*

J.C. Butcher

Department of Mathematics, University of Auckland, New Zealand

The famous theory of order stars has been crucial in resolving many questions related to the conflicting aims of order and stability. A related approach, using order arrows, has similar applications and some of these will be surveyed. In particular a generalization of the Ehle barrier to multivalue-multiderivative methods, first formulated as a conjecture by Fred Chipman and the author, will be discussed and an outline proof will be given.

## Algebraically stable DIMSIMs

*Author(s):*

L.L. Hewitt

Department of Mathematics, University of Bath, England

A.T. Hill

Department of Mathematics, University of Bath, England

DIMSIMs are a class of general linear methods with diagonally implicit stage equations. To solve nonlinear and time-varying stiff systems, it is desirable to use an algbraically stable method. Here, we give conditions for DIMSIMs to be algebraically stable and construct some example methods.

## $G$-symplectic general linear methods

*Author(s):*

A.T. Hill

Department of Mathematics, University of Bath, England

J.C. Butcher

Department of Mathematics, University of Auckland, New Zealand

L.L. Hewitt

Department of Mathematics, University of Bath, England

Symplectic Runge-Kutta methods preserve quadratic invariants of the form $u^T Su$. $G$-symplectic general linear methods preserve $y^T(G \bigotimes S)y$, where $y$ is the vector of update vectors for the method, and $G$ is a symmetric positive definite matrix, (see Hairer, Lubich & Wanner, 2002 & 2006, and Butcher in *Acta Numerica*, 2006). Here, we present several different properties and characterisations of $G$-symplectic methods.

## Exponential general linear methods for large systems of equations

*Author(s):*

W.M. Wright

Department of Mathematics, La Trobe University, Melbourne, Australia

In this talk we will describe a class of exponential general linear methods, constructed for the time integration of large systems of differential equations. To enable a cost efficient implementation we use Krylov techniques. We also discuss several implementation details such as error estimation, variable stepsize, variable Krylov subspace size and possibly variable order. These methods are compared on large scale problems with the MATLAB implementation `ode15s` and the exponential integrator `exp4`.

# Minisymposium
# Stiff problems

Organised by
G. Russo

## On a Class of Uniformly Accurate IMEX Runge-Kutta Schemes and Applications to Hyperbolic Systems with Relaxation

*Author(s):*

S. Boscarino

University of Catania, Catania, Italy

We develop new Implicit-Explicit (IMEX) Runge-Kutta (R-K) schemes for hyperbolic systems of conservation laws with stiff relaxation that are uniformly accurate with respect to the stiffness parameter. IMEX R-K schemes have been widely used for the time evolution of hyperbolic partial differential equations, however the schemes existing in literature do not exibit uniform accuracy with respect to the stiffness parameter $\varepsilon$. The new schemes were obtained by imposing new additional order conditions to guarantee better accuracy over a wide range of the stiffness $\varepsilon$. In particular, we propose the construction of an uniformly accurate IMEX R-K scheme of type CK. In two test problems, these schemes confirm, with a fixed spatial and temporal discretization, the accuracy for all range of the stiffness $\varepsilon$.

## Stage value predictors for stiff problems

*Author(s):*

I. Higueras

Departamento de Ingeniería Matemática e Informática, Universidad Pública de Navarra, Pamplona, Spain,
higueras@unavarra.es

When ordinary differential equations (ODEs) are solved with implicit Runge-Kutta (RK), the computational effort is dominated by the cost of solving nonlinear systems. Usually these systems are solved with an iterative scheme that requires good starting values to begin the iterations. Over the last few years, a great development has been done in the study and construction of stage value predictors for different classes of RK schemes and differential problems (ODEs and differential algebraic equations). A first criterion to construct these predictors is order. However, for stiff ODEs a stability criterion should also be taken into accout.

In this talk we explore stage value predictors for stiff problems.

This is joint work with T. Roldán, from Universidad Pública de Navarra, Pamplona, Spain.

Supported by Research Project MTM2005-03894 from Ministerio de Educación y Ciencia, Spain.

## References

[1] González-Pinto, S.; Montijano, J. I.; Pérez-Rodríguez, S. *On the starting algorithms for fully implicit Runge-Kutta methods*. BIT 40 (2000), no. 4, 685–714.

[2] González-Pinto, S.; Montijano, J. I.; Pérez-Rodríguez, S. *Stabilized starting algorithms for collocation Runge-Kutta methods*. Comput. Math. Appl. 45 (2003), no. 1-3, 411–428.

[3] Laburta, M. P. *Starting algorithms for IRK methods*. J. Comput. Appl. Math. 83 (1997), no. 2, 269–288.

[4] Higueras, I.; Roldán, T. *IRK methods for index 2 and 3 DAEs: starting algorithms*. BIT 43 (2003), no. 1, 67–92.

[5] Higueras, I.; Roldán, T. *Starting algorithms for a class of RK methods for index-2 DAEs*. Comput. Math. Appl. 49 (2005), no. 7-8, 1081–1099.

[6] Roldán, T.; Higueras, I. *IRK methods for DAE: starting algorithms*. J. Comput. Appl. Math. 111 (1999), no. 1-2, 77–92.

## Accelerating the Convergence of Spectral Deferred Correction Methods

*Author(s):*

M. Minion

University of North Carolina, Chapel Hill, NC, USA

Spectral deferred correction methods (SDC) for ODEs have been shown to possess favorable accuracy and stability properties even for versions with very high order of accuracy. Unfortunately, for very stiff problems, SDC methods exhibit order reduction for a range of time-step values. I will show that for linear problems, the iterations in the SDC algorithm are equivalent to constructing a preconditioned Neumann series expansion for the solution of the standard collocation discretization of the ODE. I will explain the connection between order reduction and the convergence of this series. These observations motivate the use of Krylov subspace methods to accelerate the convergence of SDC. The resulting methods possess increased stability and efficiency compared to the original SDC approach, and the acceleration effectively eliminates order reduction in the preliminary linear and nonlinear numerical experiments studied thus far.

## High-Order Implicit-Explicit Linear Multistep Methods with General Monotonicity Properties

*Author(s):*

S. Ruuth

Simon Fraser University, Burnaby, Canada

For solving hyperbolic systems with stiff sources or relaxation terms, it is natural to seek time-stepping methods which exhibit favorable monotonicity properties for shocks and steep solution gradients while still yielding good stability properties for stiff terms. In this talk we discuss some new implicit-explicit linear multistep methods that are appropriate for this type of system. Our methods are based on recent explicit methods with general monotonicity and boundedness properties. Numerical comparisons are made with several implicit-explicit Runge-Kutta methods.

This is joint work with Willem Hundsdorfer.

# Minisymposium
# Stochastic computation (ODE's)

Organised by
T. Mitsui, K. Ritter

## Linear and nonlinear approximation of stochastic processes

*Author(s):*

J. Creutzig
TU Darmstadt

M. Lifshits
Saint-Petersburg

K.Ritter
TU Darmstadt

T. Müller Gronbach
Hagen

We study approximation of stochastic processes by linear and nonlinear methods. More specifically, we ask how well a process might be approximated e.g. by splines of a given order, and how the approximation error behaves if the number of allowed knots tends to infinity. Special attention is paid to the question whether nonlinear (i.e., free choice of knots) will yield advatanges over linear (fixed knots) methods. While in several classical cases (Brownian motion/diffusions, fractional Brownian motion) we find that the error rates coincide for both kinds of approximation, Levy processes (notably stable ones) do enjoy benefits from nonlinear approximation schemes.

## References

[1] J. Creutzig, T. Müller-Gronbach, K. Ritter *Free-Knot Spline Approximation of Stochastic Processes*. J. Comp.,to appear.

[2] J. Creutzig, M. Lifshits, *Free-Knot Spline Free-Knot Spline Approximation of fractional Brownian Motion*. Proceedings of the MCQMC Ulm 2007, to appear.

[3] J. Creutzig, *Free-knot spline approximation and quantization of stochastic processes*, in preparation.

## Constructive Quantization of Scalar SDEs

*Author(s):*

T. Müller-Gronbach
FernUniversität Hagen

K. Ritter
TU Darmstadt

We study $L_p$-quantization of the solution $X$ of a scalar sde on the unit interval, i.e., approximation of $X$ by a random variable with finite range in the path space $L_p([0,1])$. We present an algorithm for this problem, which is easy to implement and performs asymptotically optimal. Our approach is based on a suitable quantization method for the Brownian bridge and exploits key ideas from optimal step-size control for strong approximation of $X$.

## Multiple stochastic integrals with Mathematica

*Author(s):*

A. Tocino

Multiple stochastic integrals with integrand identically equal to 1 appear in Itô and Stratonovich Taylor expansions. In the construction of numerical methods for solving stochastic differential equations, it becomes necessary to calculate products of these multiple integrals as well as their expectations. Well-known recursive relationships between multiple integrals make possible to express any product of them as linear combination of integrals of the same type. Exploiting the symbolic character of Mathematica, these expressions for multiplications of Itô or Stratonovich multiple integrals can be accomplished. From here, a routine that calculates the expectation of any polynomial in multiple stochastic integrals is obtained.

## References

[1] Burrage, P.M.: Runge-Kutta methods for stochastic differential equations, PhD thesis, University of Queensland, Brisbane, Australia, 1995.

[2] Gaines, J.G.: *A basis for iterated stochastic integrals*, Mathematics and Computers in Simulation 38(1-3), (1995), 7-11.

[3] Kendall, W.S.: *Stochastic Integrals and Their Expectations* Mathematica J. 9 (2005), 757-767.

[4] Kloeden, P.E.; Platen, E.: *Numerical Solution of Stochastic Differential Equations*, Springer-Verlag, Berlin, 1992.

[5] Wolfram, S.: *The Mathematica book*. Cambridge University Press, Cambridge, 1999.

# Practical variance reduction via regression for simulating diffusions

*Author(s):*

M.V. Tretyakov

Department of Mathematics, University of Leicester, Leicester, UK

G.N. Milstein

Department of Mathematics, Ural State University, Ekaterinburg, Russia

The stochastic approach to solving problems of mathematical physics is based on probabilistic representations of their solutions with making use of the weak-sense numerical integration of stochastic differential equations (SDEs) and the Monte Carlo (MC) technique. In this approach we have two main errors: the error of SDEs numerical integration and the MC error. The first error essentially depends on the choice of a method of numerical integration and the second one depends on the choice of the probabilistic representation. While the error of numerical integration is well studied in the systematic theory of numerical integration of SDEs which allows us to propose suitable effective methods for a lot of typical problems, in connection with the MC error there is no systematic constructive method of variance reduction.

The well-known variance reduction methods, the method of important sampling and the method of control variates, can be exploited if an approximation of the required solution is known. However, until now there have been no systematic methods for getting such approximations in a constructive efficient way. In [1] we employ conditional probabilistic representations of solutions together with the regression method to obtain sufficiently inexpensive (although rather rough) estimates of the solution and its derivatives. These estimates can effectively be used for significant reduction of variance and further accurate evaluation of the required solution. The developed approach is supported by numerical experiments.

# References

[1] G.N. Milstein, M.V. Tretyakov. *Practical variance reduction via regression for simulating diffusions*. Technical Report No. MA-06-19. School of Mathematics and Computer Science, University of Leicester, Leicester, 2006, 24 pp. (sumitted).

# Minisymposium
# Stochastic Modelling

Organised by
M. Hairer, D. Talay

## Local wind simulation by using a stochastic particle method

*Author(s):*

F. Bernardin

Laboratoire Régional des Ponts et Chaussées, Clermont-Ferrand, France

M. Bossy

Projet Tosca, INRIA, Sophia-Antipolis, France

A. Rousseau

Projet Moïse, INRIA, Grenoble, France

T. Salameh

LMD, Ecole Polytechnique, Palaiseau, France

P. Drobinski

LMD, Ecole Polytechnique, Palaiseau, France

A Lagrangian stochastic model is introduced in order to describe the local behavior of the wind. Based on some data given by a large scales meteorological model (MM5), and thanks to particles driven by stochastic differential equations, we propose a numerical method allowing to improve the MM5 simulations at small scales, without requiring too much additional computational cost.

Consider a $3D$ box (for example a cell of MM5 mesh) where the three components $(u; v; w)$ of the velocity field are given on each side. We use a Lagrangian approach to describe the time evolution of a generic fluid particle, to get some information at smaller scales (inside the box). To this aim, we run a particle in cell numerical algorithm, which consists in splitting our domain into cells $C_i$, in which we drop $K$ particles having Langevin dynamics. Then, we compute some local (i.e. for a cell) characteristics of the fl uid by averaging the corresponding attributes of the particles being in the considered cell.

We use a Lagrangian stochastic model developped by S.B. Pope [1] which describes the behavior of the fluid generic particle in the considered domain $\mathcal{D} \subset \mathbb{R}^3$. Denoting by $(X_t; \mathcal{U}_t; \omega_t)$ the position, velocity and turbulence frequency of the particle, the model consists in writing a stochastic differential equation (SDE) that describes the dynamic of the process $(X_t; \mathcal{U}_t; \omega_t)_{t \geq 0}$. The numerical algorithm that we develop takes into account both the continuous time evolution in the domain and the boundary conditions (given by MM5) that are expressed thanks to conditional expectations.

## References

[1] S.B. Pope. Lagrangian pdf methods for turbulent ows. Annu. Rev. Fluid Mech., 26:23-63, 1994.

## Nonparametric Drift Estimation for Diffusion Processes

*Author(s):*

Y. Pokern,

University of Warwick, Coventry, UK

A. M. Stuart

University of Warwick, Coventry, UK

E. Vanden-Eijnden

Courant Institute, New York University, New York, USA

In applications such as molecular dynamics it is of interest to fit Smoluchowski and Langevin equations to data. Practitioners often achieve this by a variety of *ad hoc* procedures such as fitting to the empirical measure generated by the data, and fitting to properties of auto-correlation functions. Statisticians, on the other hand, often use estimation procedures which fit diffusion processes to data by applying the maximum likelihood principle to the path-space density of the desired model equations, and through knowledge of the properties of the quadratic variation. In this note we show that these procedures used by practitioners and statisticians are, in fact, closely related. We do this by introducing a nonparametric approach to estimation for diffusion processes. Furthermore, we present the results of numerical experiments which probe the relative efficacy of the two approaches to model identification and compare them with other methods such as the minimum distance estimator.

## Title to be announced

*Author(s):*

C. Schütte

Freie Universität Berlin, Berlin, Germany

## A stochastic particle model of age-structured population

*Author(s):*

C. Tran

MODAL'X, Université Paris 10 - Nanterre

A continuous-time individual-centered population model with age structure is presented. Individuals reproduce asexually, age and die. The death rate takes interactions of logistic type into account. Adapting the approach of Fournier and Méléard [1], we show that in a large population limit, the microscopic process converges to the deterministic measure-valued solution of an equation that generalizes the Gurtin-McCamy PDE in demography. On compact time intervals, the stochastic process behaves like its deterministic approximation, but dissemblance can occur in the long time. The stochastic microscopic process gets extinct almost surely. When the limiting equation admits a non trivial stationary stable solution, we give estimates for the time at which the stochastic process leaves the neighborhood of its large population equilibrium.

These results are applied to the theory of adaptive dynamics in evolution. They allow us to separate the time scales of ecology (birth and death events) and evolution (mutation events) for populations with age and trait structures, by following the work of Champagnat [2]. We then obtain new generalizations of the famous Trait Substitution Sequence Process and Canonical Equation that have been introduced by Metz et al. [3] and Dieckmann and Law [4].

## References

[1] N. Fournier, S. Méléard, A Microscopic Probabilistic Description of a Locally Regulated Population and Macroscopic Approximations, *Ann. Appl. Probab.*, 14:1880–1919, 2006.

[2] N. Champagnat, A Microscopic Interpretation for Adaptative Dynamics Trait Substitution Sequence Models, *Stoch. Proc. App.*, 2006.

[3] J.A.J. Metz, S.A.H. Geritz, G. Meszéna, F.A.J. Jacobs, J.S. Van Heerwaarden, Adaptative Dynamics, a Geometrical Study of the Consequences of Nearly Faithful Reproduction, *S.J. Van Strien & S.M. Verduyn Lunel (ed.), Stochastic and Spatial Structures of Dynamical Systems,* 45:182–231, 1996.

[4] U. Dieckmann, R. Law, The Dynamical Theory of Coevolution: a Derivation from Stochastic Ecological Processes, *J. Math. Biol.*, 34:579–612, 1996.

# Minisymposium
# Stochastic PDE's

Organised by
A. Debussche, M. Hairer

## G-NI discretization methods for stochastic boundary-value problems incorporating geometric uncertainties

*Author(s):*

C. Canuto
Dipartimento di Matematica, Politecnico di Torino, I-10129 Torino, ITALY

We will discuss several stochastic boundary-value problems of elliptic or parabolic type. They share the feature that the spatial domain in which they are set, or a portion of it, is described by stochastic variables or depends implicitly upon stochastic variables.

Various techniques are used to handle the geometric uncertainties, whereas Generalized Polynomial Chaos expansions (Askey Chaos) allow us to convert each problem into a deterministic one, in the typical framework of spectral methods. Discretization is performed by a G-NI (Galerkin with Numerical Integration) approach. The choice of the quadrature formulae will be carefully analyzed, as it is crucial to guarantee accuracy and efficiency; in certain cases, the discretization is indeed equivalent to a collocation scheme.

Applications to Wind Engineering (joint work with D. Fransos) and to Phase Transition problems (joint work with T. Kozubek) will be presented.

## Uncertainties Quantities in electromagnetism: Stochatic Finite Element with Polynomial Chaos

*Author(s):*

R. Gaignaire
ENSAM, L2EP, France

Electrical engineering often deals with global quantities as current, magnetic flux, difference of potentials, power or torque. Previous works have shown that Stochastic Finite Element Method SFEM it possible to predict the propagation of some uncertainties in the input data (material characteristics) towards the magnetic field distribution. The next step consists in deriving the global quantities from the random magnetic field distribution. The calculation of current has been implemented in the extended stochastic version of the 3D FEM software dedicated to electromagnetic field computation. The approach has been successfully validated on a 3D electrical current density problem by comparing with Monte Carlo Simulation Method and the convergence has been shown on an industrial application.

## Sparse Second Moment Analysis of Elliptic Problems in Stochastic Domains

*Author(s):*

C. Schwab
ETH Zurich, Zurich, Switzerland

H. Harbrecht
Kiel, Germany

R. Schneider
Bonn, Germany

We consider the numerical solution of Elliptic problems in domains with a class random boundary perturbations. Assuming perturbations with small amplitude and known mean field and two-point correlation function, we derive, using a second order shape calculus, deterministic equations for the mean field and the two-point correlation function of the random solution for the Dirichlet problem in the stochastic domain.

Using a variational boundary integral equation formulation on the unperturbed, 'mean' boundary and a wavelet discretization, we present and analyze an algorithm to approximate the random solution's two-point correlation function at essentially optimal order in essentially $\mathcal{O}(N)$ work and memory, where $N$ denotes the number of unknowns required for consistent discretization of the boundary of the domain.

# Order Reduction for Discretisation Schemes for SPDEs

*Author(s):*

J. Voss

University of Warwick, Coventry, UK

We compare different ways to discretise the differential operator in a Stochastic Partial Differential Equation (SPDE) and, in particular, study the effect the choice of discretisation has on statistical properties of the discretised SPDE. We study the stochastic heat equation, driven by the Laplace operator, and consider how close the stationary distribution of the discretised SPDE is to the exact stationary distribution. It transpires that one looses one order of accuracy for the stationary distribution when using second-order finite difference approximation as compared to the (also second order) finite element discretisation.

# Minisymposium
# Stochastic simulation in systems biology

Organised by
K. Burrage

## Modelling intrinsic noise and delays in cellular processes

*Author(s):*

K. Burrage

Advanced Computational Modelling Centre, University of Queensland, Brisbane, Australia

Understanding the roles of noise in cellular dynamics is a crucial driver of Cell Biology. The Stochastic Simulation Algorithm (SSA) is an important technique for simulating the interactions of small numbers of molecules in cellular environments and in particular genetic regulation. In this talk we will show how both noise and delay can be modelled in a discrete and continuous setting. We will illustrate these ideas by modelling delays in transcription and translation via both the Hes 1 gene regulatory clock in mouse and the Her1/Her7 gene complex for oscillating cells in contact with one another through delta-notch signalling.

## Pseudo-random variables for numerical Stochastic Differential Equations

*Author(s):*

P.M. Burrage

Advanced Computational Modelling Centre, University of Queensland, Brisbane, Australia

When solving Stochastic Differential Equations (SDEs) numerically with weak-order methods, very many simulations must be obtained in order to determine properties of the numerical solution (for example, the mean or variance). By analysing the required moment properties of discrete pseudo-random numbers and applying this information to the construction of such pseudo-random numbers, the number of numerical simulations can be significantly reduced. Consequently weak numerical approximations can be obtained with much reduced computational cost.

## Title to be announced

*Author(s):*

M. Carletti

## Diffusion-limited reaction in one dimension

*Author(s):*

G. Lythe

Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK

We study the following dynamics in one space dimension:

1. Point particles are nucleated at random times and positions
   (a) either in pairs with separation $b$ at rate $\Gamma$,
   (b) or one at a time at rate $Q$.
2. Once born, particles diffuse independently with diffusivity $D$.
3. Particles annihilate on collision.

Classical treatment produces a hierarchy of particle correlation functions without an exact solution. It is possible to sidestep this hierarchy and find an exact solution for the mean number of particles per unit length as a function of time. We review this exact method and derive an exact rate equation in terms of the correlation function. The exact method of analysis permits exact calculation of the steady state density and its time evolution in terms of the three parameters describing the microscopic dynamics: the nucleation rate, the initial separation of nucleated pairs and the diffusivity of a particle. For paired nucleation at sufficiently small initial separation the nucleation rate is proportional to the square of the steady state density. For unpaired nucleation, and for paired nucleation at sufficiently large initial separation, the nucleation rate is proportional to the cube of the steady state density. In addition, the distribution of particle lifetimes is calculated under a "constant-killing-rate" approximation that compares favourably with the results of numerical experiments.

## References


[1] Salman Habib, Katja Lindenberg, Grant Lythe, and Carmen Molina-París. Diffusion-limited reaction in one dimension: paired and unpaired nucleation. *J. Chem. Phys.*, 115:73–89, 2001.

[2] Thomas O. Masser and Daniel ben Avraham. Method of intervals for the study of diffusion-limited annihilation. *Physical Review E*, 63:006108, 2001.

[3] Grant Lythe. Diffusion-limited reaction in one dimension. *Physica D*, 222:159–163, 2006.


# Peripheral T cell repertoire maintenance the quasi-stationary probability distribution


*Author(s):*

C. Molina-París

Department of Applied Mathematics, School of Mathematics, University of Leeds, Leeds LS2 9JT, UK

Hugo van den Berg

Warwick Systems Biology Centre, University of Warwick, Coventry CV4 7AL, UK


A protective immune system requires a T cell population that can respond to foreign antigens. Given that the host cannot predict the precise pathogen-derived antigens that will be encountered in the future, the immune system uses self peptides (i) to select a T cell receptor repertoire in the thymus by means of positive and negative selection and (ii) to keep the naive T cells alive and "ready for action" in the periphery [1].

There is immunological evidence that peripheral naive T cells are maintained by (1) output of mature thymocytes from the thymus and (2) cell division due to survival signals received by APCs presenting self pMHC complexes. Furthermore, there is evidence that the number of naive T cells in the periphery is under homeostatic regulation. This implies that the mature T cell repertoire consists of a constant number of cells distributed over a large number of different T cell clonotypes [2]. T cells compete for survival signals provided by self APPs and the immune system guarantees coexistence and persistence of different T cell clonotypes [3]. Finally, centenarians have an extremely low number of naive T cells.

In this talk I introduce a stochastic model to study T cell repertoire diversity maintenance. The model incorporates the concept of survival stimuli emanating from self antigen presenting cells and in the mean field approximation clonotype extinction is guaranteed. Extinction times of T cell clonotypes without thymic input are computed and the concept of mean niche overlap is introduced. Finally, I make use of the quasi-stationary probability distribution [4] to compute average clonotype numbers for different values of the niche overlap.

# References


[1] A. A. Freitas and B. Rocha. Peripheral T cell survival. *Curr. Opin. Immunol.*, 11:152-156, 1999.

[2] A. W. Goldrath and M. J. Bevan. Selecting and maintaining a diverse T cell repertoire. *Nature*, 402, 1999.

[3] D. Mason. A very high level of crossreactivity is an essential feature of the T-cell repertoire. *Immunol. Today*, 19:395-404, 1998.

[4] I. Nasell Extinction and quasi-stationarity in the Verhulst logistic model. *J. Theor. Biol.*, 211:11-27, 2001.

# Minisymposium
# Time integration of PDE's

Organised by
F. Castella, S. Descombes, S. Reich

## Constraint preserving schemes for some gauge invariant wave equations

*Author(s):*

S. Christiansen

University of Oslo, Oslo, Norway

We study discretizations of the Maxwell-Klein-Gordon equation as an example of a constrained geometric nonlinear evolution partial differential equation. Gauge invariance entails, by Noether's theorem, conservation of electric charge. We discuss schemes capable of conserving electric charge even though the Galerkin spaces are not invariant under gauge transformations.

## Explicit local time stepping for second-order wave equations

*Author(s):*

J. Diaz

Magique 3D, Inria Futurs, Pau, France

M. Grote

Department of Mathematics, University of Basel, Basel, Switzerland.

Adaptivity and mesh refinement are certainly key for the efficient numerical solution of partial differential equations. However, locally refined meshes impose severe stability constraints on explicit time-stepping schemes, where the maximal time-step allowed by a CFL condition is dictated by the smallest elements in the mesh. When mesh refinement is restricted to a small region, the use of implicit methods, or a very small time step in the entire computational domain, are very high a price to pay. To overcome that stability restriction, we propose local time-stepping schemes, which allow arbitrarily small time steps where small elements in the mesh are located. In this talk, we will consider the semi-discretized wave equation :

$$M\frac{d^2y}{dt^2} + Ky = F, \tag{16}$$

where $M$ and $K$ are obtained from a specific symmetric finite element discretization in space, so that the mass matrix $M$ is essentially diagonal (for instance Interior Penalty DG elements [1] or finite elements with mass lumping [2]). Starting from the standard second order "leap-frog" scheme, time integrators of second order of convergence are derived, based on the method proposed in [3, 4] for the resolution of ordinary differential equations. The resulting fully discrete scheme is explicit and exactly conserves a discrete energy. The CFL condition of the new scheme is usually comparable to that of the standard leap-frog scheme without local refinement. If a small overlap across at most three elements is allowed into the coarse region immediately next to the refined region, the CFL condition is optimal, in the sense that the same time step can be used. Numerical experiments illustrate the efficiency of these methods and validate the theory.

## References

[1] M.J. Grote, A. Schneebeli, and D. Schötzau, *Discontinuous Galerkin finite element method for the wave equation*, SIAM Numer. Analysis **44** (2006), 2408–2431.

[2] G. Cohen, P. Joly, J.E. Roberts, and N. Tordjman, *Higher order triangular finite elements with mass lumping for the wave equation*, SIAM Numer. Analysis **38** (2001), 2047–2078.

[3] B. Leimkuhler and S. Reich, *Simulating Hamiltonian dynamics*, Cambridge Monographs on Applied and Computational Mathematics, 2004.

[4] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration*, 2nd edition, Springer-Verlag Berlin Heidelberg, 2006

## Exponential integrators for oscillatory second-order differential equations

*Author(s):*

M. Hochbruck

Heinrich-Heine-University, Düsseldorf, Germany

V. Grimm

Heinrich-Heine-University, Düsseldorf, Germany

In this talk, we analyse a family of exponential integrators for second-order differential equations in which high-frequency oscillations in the solution are generated by a linear part. We characterise methods which allow second-order error bounds by presenting a unified error analysis for the whole family of methods. A major advantage of our analysis is that it does not require bounds for point-wise products of matrices and therefore, generalises to abstract differential equations, where the linear part is an unbounded operator with infinitely many large eigenvalues directly.

## Preconditioned Runge-Kutta schemes

*Author(s):*

M. Schatzman

CNRS, Université de Lyon

The time integration of discretized partial differential equations by implicit schemes is usually a very stiff problem, which is usually solved numerically with the help of a preconditioner.

In this talk, we will present some examples of implicit-explicit Runge-Kutta schemes, which contain their preconditioner, with the property that numerical resolutions take place only for systems containing the preconditioner, while the scheme is explicit with respect to the discretized partial differential equation operator.

The properties of stability and convergence of these methods will be explored, and numerical examples will be given.

# Minisymposium
# Validated computing

Organised by
D. Stoffer, P. Zgliczynski

## Verified computations of the error in the finite element methods with applications to nonlinear PDEs

*Author(s):*

M.T. Nakao

Faculy of Mathematics, Kyushu University, Japan

In this talk, we first consider the guaranteed a proiri error estimates in the finite element method for Poisson's equation and for bi-harmonic problems. Next, as an application of the results, we show a numerical verification method of solutions for nonlinear elliptic problems and Navier-Stokes equations as well as other applications. The special emphasis of our method is that we can obtain the finite element solution with guaranteed error bounds even if we have no information about the existence of exact solutions for the original equations such as noncoercive or nonlinear problems. Several numerical examples which confirm the actual effectiveness of our method will be presented.

## References

[1] Nakao, M.T., A numerical approach to the proof of existence of solutions for elliptic problems, Japan Journal of Applied Mathematics 5 (1988), 313-332.

[2] Nagatou, K., Hashimoto, K, Nakao, M.T., Numerical verification of stationary solutions for Navier-Stokes problems, Journal of Computational and Applied Mathematics 199 (2007), 424-431.

[3] Hashimoto, K., Kobayashi, K., Nakao, M.T., Verified numerical computation of solutions for the stationary Navier-Stokes equation in nonconvex polygonal domains, MHF Preprint Series, Kyushu University, MHF2007-2, 2007, 15 pages.

[4] Nakao, M.T. and Hashimoto, K., Constructive error estimates of finite element approximations for noncoercive elliptic problems and its applications, MHF Preprint Series, Kyushu University, MHF2007-5, 2007, 12 pages.

## A computer-assisted existence proof for photonic band gaps

*Author(s):*

M. Plum

Karlsruhe, Germany

V. Hoang, Ch. Wieners

The investigation of monochromatic waves in a periodic dielectric medium ("photonic crystal") leads to a spectral problem for a Maxwell operator. It is well known that the spectrum is characterized as a countable union of compact real intervals ("bands") which may or may not be separated by gaps, and the occurrence of such gaps is of great practical interest but difficult to prove analytically. In this talk, we will attack this problem, for the 2D case of polarized waves, by computer-assisted means. First we reduce the problem, using an analytical perturbation type argument, to the computation of enclosures for finitely many eigenvalues of finitely many periodic eigenvalue problems. This task is then carried out by computer-assisted variational methods.

## A Proof of Chaotic Behaviour via Shadowing

*Author(s):*

D. Stoffer

The aim is to prove chaotic behaviour of a given discrete dynamical system. A construction of a hyperbolic set is given. the key element is the knowledge of two adjacent points generating two approximate hyperbolic periodic orbits. A shadowing theorem is derived. All the assumptions of this theorem are formulated in terms of computable quantities. At this point validated computing is needed. It is explained how the Bernoulli shift system may be embedded into the given system. This establishes the existence of chaotic behaviour. Some applications are addressed.

# A geometric method for proving the existence homoclinic and heteroclinic solutions.

*Author(s):*

D. Wilczak

Institute of Computer Science, Jagiellonian University, Cracow, Poland

I would like present a geometric method which can be use for proving the existence of homoclinic or heteroclinic solutions which appear for isolated parameter values in parameterized family of ODEs. The method has been applied to the Michelson system

$$\begin{cases} \dot{x} &= y \\ \dot{y} &= z \\ \dot{z} &= c^2 - y - \frac{1}{2}x^2 \end{cases} \tag{17}$$

in order to prove the following results. Put $c_{\min} = 0.8285$ and $c_{\max} = 0.861$.

1. For each parameter value $c \in [c_{\min}, c_{\max}]$ the Michelson system (17) is $\Sigma_4$ chaotic, i.e. a suitable Poincaré map is semiconjugated to the full shift on four symbols.
2. There exists a countable infinite set of parameter values $c \in [c_{\min}, c_{\max}]$ for which the system (17) possesses a heteroclinic orbit connecting $(-\sqrt{2}c, 0, 0)$ with $(\sqrt{2}c, 0, 0)$ along one dimensional unstable-stable manifolds.
3. For all parameter values $c \in [c_{\min}, c_{\max}]$ there exist infinitely many heteroclinic solutions connecting $(\sqrt{2}c, 0, 0)$ with $(-\sqrt{2}c, 0, 0)$.
4. There exists a countable infinite set of parameter values $C_h \subset [c_{\min}, c_{\max}]$ for which the Michelson system (17) possesses a pair of homoclinic orbits to the equilibrium points.

Details can be found in [1, 2].

## References

[1] D. Wilczak, The existence of Shilnikov homoclinic orbits in the Michelson system: a computer assisted proof, *Foundations of Computational Mathematics.*, 6:495–535, 2006.

[2] D. Wilczak, P. Zgliczyński, Topological method for symmetric periodic orbits for maps with a reversing symmetry, *Discrete and Continuous Dynamical Systems - Series A*, 17:629–652, 2007.

# Contributed Talks

# Approximate Solutions of Differential Algebraic Equations by Splines

*Author(s):*

M. Ahmadinia

Department of Mathematics, University of Qom, Qom, Iran

In the recent paper [1] Ahamadinia-Loghmani , showed that some anti-periodic boundary value problems can be solved by slpine functions. In this talk, we generalize this idea for differential algebraic equations $f(t, x(t), x'(t), \cdots, x^{(n)}(t)) = 0$ on $(a, b)$ ($t \in [a, b]$ and $f$ continuous) with initial conditions $x(a) + x'(a) + \cdots + x^{(n-1)}(a) = 0$ . We will show that for every $\varepsilon > 0$, there exist a positive integer $k$ and a linear combination $v_k$ of spline functions such that $||f(t, v_k(t), v_k'(t), \cdots, v_k^{(n)}(t))||_{L^2([a,b])} < \varepsilon$ and $v_k$ satisfies the exact initial condition conditions and also, we change the inintial condition to some other forms of boundary conditions as in [2, 3].

## References

[1] M. Ahmadinia and G. B. Loghmani. Splines and Anti-periodic Boundary Value Problems. *Int. J. Computer. Math.*, (to appear).

[2] M. Ahmadinia and M. Radjabalipour. Application of Least Square Method to Non-linear Partial Differential Equations with Boundary Conditions, Another paper. *The 2nd International Conference on Scientific Computing and Partial Differential Equations and The First East Asia SIAM Symposium* , (Baptist University, Hong Kong, 12-16 December, 2005).

[3] G. B. Loghmani and M. Ahmadinia. Numerical solution of sixth order boundary value problems with sixth degree B-spline functions. *J. Appl. Math. Comp.*, (to appear).

# Multi-dimensional Piecewise Deterministic Markov Processes: a first order numerical treatment.

*Author(s):*

M. Annunziato

Dipartimento di Matematica e Informatica, Università degli Studi di Salerno, via Ponte Don Melillo 84084 Fisciano (SA), Italy.

We consider a numerical treatment of the following Liouville - Master Equation (LME):

$$\partial_t F_s(\overrightarrow{x}, t) + \sum_{k=1}^{d} A_s^{(k)}(x_k) \cdot \partial_{x_k} F_s(\overrightarrow{x}, t) = \sum_{j=1}^{S} Q_{sj} F_j(\overrightarrow{x}, t), \tag{18}$$

for the unknown distribution functions $F_s(\overrightarrow{x}, t)$, $\overrightarrow{x} = x_1, \ldots x_d$. Eq. (18) is related to a $d$-dimensional piecewise deterministic Markov process [1], described by the system of ODE's:

$$\frac{dX_k}{dt} = A_s^{(k)}(X_k) \qquad k = 1, \ldots, d, \tag{19}$$

where $A_s^{(k)}(X_k)$ is chosen randomly from a set of $s = 1, \ldots, S$ known functions with $d$-components and one independent variable, and it is subject to a Markov process of stochastic transition matrix $q_{ij}$, $i, j = 1, \ldots, S$, and Poisson statistics of transition rates $\mu_s$. The importance of LME is that it provides an alternative way to a direct Monte Carlo simulation of Eq. (19) when extracting the statistical properties of the process. Eq. (18) is solved for Cauchy conditions $F_s(\overrightarrow{x}, 0) = F_s^{(0)}(\overrightarrow{x})$, and boundary conditions: $\lim_{\{x_1,\ldots,x_d\}\to\infty} F_s(\overrightarrow{x}, t) = 1$, $\lim_{\{x_1,\ldots,x_d\}\to-\infty} F_s(\overrightarrow{x}, t) = 0$, $\lim_{x_k\to\infty} F_s(x_1, \ldots, x_k, \ldots, x_d, t) \leq 1$. The one-dimensional case has been

studied in [2], for which convergence and monotonicy has been prooved and tested for the upwind method, under the Courant-Friedrichs-Lewy (CFL) condition. An extended CFL condition can guarantee that the upwind produces a convergent solution for the $d$-dimensional case (18). Some numerical tests are performed for $d = 2$, showing the time dependent density probability distribution function $p(x_1, x_2, t) = \partial_{x_1 x_2} \sum_s F_s(x_1, x_2, t)$ for processes having a statistical equilibrium.

[The author acknowleges the *"Gruppo Nazionale per il Calcolo Scientifico"* (GNCS) for the financial support.]

# References

[1] M.H.A. Davis. Markov Models and Optimizations, Chapman & Hall/CRC, London 1993.

[2] M. Annunziato,*A finite difference method for piecewise deterministic Markov processes*, Preprint 10-2006, Dipartimento di Matematica e Informatica, Università degli Studi di Salerno.

[3] M. Annunziato, *A finite difference method for piecewise deterministic processes with memory,* Mathematical Modelling and Analysis, 12 (2) 2007, 157-178.

# On the Definition and Comparison of the Information Efficiency of Iterative Methods for solving Systems of Non Linear Equations

*Author(s):*

D.K.R. Babajee

MPhil/Ph.D student at the University of Mauritius, Reduit, Mauritius.
The work of the first author is partly financed by Tertiary Education Commission, TEC and University of Mauritius.
Email: rajiv.nishi@intnet.mu.

M.Z. Dauhoo

Department of Mathematics, Faculty of Science, University of Mauritius, Reduit, Mauritius.

Email: m.dauhoo@uom.ac.mu.

The Informational Efficiency [1] is commonly used to compare the efficiency of iterative methods for the solution of scalar non linear equations of the form $\mathbf{F}(\mathbf{x}) = \mathbf{0}$. It is defined as $EFF = q^{1/d}$, where $q$ is the order of the method and $d$ is the number of function evaluations per iteration. However, for systems of $n$ equations with $n$ variables the function $\mathbf{F}$ is now a $n \times 1$ vector and the $p$th derivative $\mathbf{F}^{(p)}$ is a $\underbrace{n \times n \times .... \times n}_{(p+1) \text{ times}}$ matrix with $n^{p+1}$ values. Taking this remark into consideration, we alter the definition of $d$ which is now dependent on $n$. That is, $d$ must be defined as $d = d_0 n + \sum_{i=1}^{p} d_i \; n^{i+1}$, where $d_0$ and $d_i$ represent the number of times $\mathbf{F}$ and $\mathbf{F}^{(i)}$ is to be evaluated respectively. The definition of the Informational Efficiency is given by $EFF^* = q^{1 \Big/ \left( d_0 n + \sum_{i=1}^{p} d_i \; n^{i+1} \right)}$. Obviously, the case $n = 1$ reduces to the Informational Efficiency for scalar equation. We also note that $\lim_{n \to +\infty} EFF^* = 1$. This explains why iterative methods have little practical utility for large system of non linear equations.

In this work, we compare the Informational Efficiency of the second order Newton ($NM$) method with those of the third order Halley ($HM$) method and the third order two-point Arithmetic Mean Newton ($AM$) method. We then show that using our definition of Informational Efficiency that the $m$-step composite Newton ($mNM$) method with constant Jacobian is the most effective method as compared to the $NM$, $HM$ and $AM$ methods.

Finally, we conduct numerical experiments in which we solve the 1-D and 2-D Bratu problems and the Hammerstein equations (These arise frequently in connection with boundary value problems for differential equations) using $mNM$ method and compare the resulting Informational Efficiencies.

# References

[1] J. F. Traub., *Iterative Methods for the Solution of Equations.* Prentice Hall, Englewood Cliffs, New Jersey, 1976.

# Stochastic Runge-Kutta Methods for Equations with Small Noise

*Author(s):*

E. Buckwar
Department of Mathematics, Technical University Berlin

A. Roessler
Department of Mathematics, Technical University Darmstadt

R. Winkler
Department of Mathematics, Humboldt University Berlin

This talk is concerned with the numerical approximation of solutions of Itô stochastic differential equations. Quite often fluctuations which affect a physical system are quite small, e.g., if thermal noise is included in a physical model. We express the smallness of the noise by means of a small factor $\epsilon$ in the diffusion coefficient of the stochastic differential equation. In general, numerical schemes for stochastic differential equations that include only information on the increments of the Wiener process have an asymptotic rate of strong convergence of 1/2, for additive or commutative noise it may be 1. However, when the noise is small, the error behaviour is much better. In fact, the errors are still dominated by the deterministic terms as long as the step-size is large enough.

In this talk we start with a discussion of *stochastic Runge-Kutta Maruyama schemes* for small noise Itô stochastic differential equations. Such methods complement a deterministic Runge-Kutta-formula for the drift-part of the stochastic differential equation by a Maruyama-type term that discretizes the diffusion part of the SODE. One obtains that the global error is of order $\mathcal{O}(\epsilon^2 h^{1/2} + \epsilon h + h^p)$, where $p$ is the deterministic order of the method. For $h \ll \epsilon^2$ the term $\mathcal{O}(\epsilon^2 h^{1/2})$ dominates and one observes the asymptotic order of convergence 1/2. For $\epsilon^{1/(p-1)} \ll h$ the term $\mathcal{O}(h^p)$ dominates and reflects the deterministic order of convergence. For step-sizes between these two extreme cases the term $\mathcal{O}(\epsilon h)$ is dominating the global error. One observes order 1 behaviour with a small error constant that is due to the factor $\epsilon$, such that the errors are still considerably smaller than those for the Euler-Maruyama scheme.

Motivated by this observation we aim at improving the methods such that the $\mathcal{O}(\epsilon h)$ term is cancelled out by including suitable terms which involve mixed classical-stochastic integrals in the numerical schemes. We propose a class of *improved stochastic Runge-Kutta schemes*. These methods are constructed in such a way, that the use of derivatives is avoided; and only evaluations of the drift and diffusion coefficients themselves are needed. A careful analysis of the local and global errors yields conditions on the set of parameters in the considered methods such that the global error is of order $\mathcal{O}(\epsilon^2 h^{1/2} + \epsilon h^2 + h^p)$. Further we discuss for which relations of step-size and smallness of the noise these methods are useful and demonstrate their behaviour with numerical simulations.

# Runge-Kutta convolution quadrature methods and discrete transparent boundary conditions

*Author(s):*

M.P. Calvo
Universidad de Valladolid

E. Cuesta
Universidad de Valladolid

C. Palencia
Universidad de Valladolid

In this talk Runge-Kutta convolution quadrature methods, firstly proposed in [2] and later extended to the nonsectorial case in [1], are used to time integrate the equations with memory arising when discrete transparent boundary conditions for evolutionary partial differential equations in unbounded domains are considered.

Interesting qualitative properties of the numerical solution of the resulting fully discrete problems are obtained by using the representation theorem provided in [1]. Numerical experiments to illustrate these results are also included.

## References


[1] M. P. Calvo, E. Cuesta & C. Palencia, Runge-Kutta convolution quadrature methods for well posed equations with memory. *Numer. Math.*, submitted.

[2] Ch. Lubich & A. Ostermann, Runge-Kutta methods for parabolic equations and convolution quadrature. *Math. Comput. 60*, 105–131, 1993.


# Eulerian and Semi-Lagrangian exponential integrators for convection dominated problems


*Author(s):*

E. Celledoni

Norwegian University of Science and Technology, Trondheim, Norway


We consider a new class of integration methods particularly suited for convection diffusion problems with dominating convection. These methods are exponential integrators and their peculiarity is that they allow for the computation of exponentials of the linearized convection term.

The main reason for developing this type of methods is that as it turns out they can be applied to the numerical integration of the considered PDEs in a semi-Lagrangian fashion. The main challenge in the numerical approximation of convection dominated phenomena is to avoid the occurrence of spurious oscillations in the numerical solution, (numerical dispersion), without adding diffusion. This task is achieved nicely by semi-Lagrangian methods. In these methods linear convective terms are integrated *exactly* by computing first the characteristics corresponding to the gridponts of the adopted discretization, and then producing the numerical approximation via a simple although expensive interpolation procedure.

## References


[1] E. Celledoni, Eulerian and Semi-Lagrangian schemes based on commutator free exponential integrators, CRM Proceedings and Lecture notes, I *CRM Proceedings and Lecture notes, I*, ISSN: 1065-8580, Vol. 39, 2005.

[2] E. Celledoni, *Exponential integrators for convection dominated problems*, in preparation.


# The efficiency of Triple Composition Runge-Kutta methods


*Author(s):*

D.J.L. Chen

Department of Business Administration, Ling Tung University, Taichung, Taiwan

J.C.Chang

Department of Information Management, National Yunlin University of Science Technology, Yunlin, Taiwan, is also a lecturer at the department of Information Technolgy, Ling Tung University, Taichung, Taiwan

T.M.H. Chan

Department of Accounting, National Taichung Institute of Technology, Taichung, Taiwan


A sixth order six-stage explicit Runge-Kutta method is constructed by composing three fifth order five-stage explicit methods. An error estimator using linear combination of stage values and output values over three steps is also derived. Numerical results are presented by testing the new triple over DETEST problems and some financial derivative models show a significant feasibility.

## References


[1] P. Albrecht, A new theoretical approach to Runge-Kutta methods, SIAM J. Numerical Anal. 24, 391-406, 1987.

[2] F. Bornemann, Runge-Kutta methods, Trees, and Mathematica, Selcuk J. Appl. Math, 2, 1-13, 2001.

[3] J. C. Butcher, On the attainable order of Runge-Kutta methods, Math. Comp. vol. 19, 408-417, 1965.

[4] J. C. Butcher, The effective order of Runge-Kutta methods, Conference on the Numerical Solution of Differential Equations, Lecture Notes in Math., 109, 133-139, 1969.

[5] J. C. Butcher, An Algebraic theory of integration methods, Math. Comp. 26, 79-106, 1972.

[6] J. C. Butcher, An introduction to "Almost Runge-Kutta" methods, Appl. Numerical Math., vol.24, pp.331-342, 1997.

[7] J. C. Butcher, Numerical Methods for Ordinary Differential Equations. John Wiley & Sons, 2002.

[8] J. C. Butcher, T. M. H. Chan, Multi-step zero approximations for stepsize control, Applied Numerical Mathematics 34, 167-177, 2000.

[9] J. C. Butcher, T. M. H. Chan, Variable stepsize schemes for effective order methods and enhanced order composition methods, Numerical Algorithms 26, 131-150, 2001.

[10] J. C. Butcher, P. Chartier, The effective order of singly-implicit Runge-Kutta methods, Numer. Algorithms, 20, 269-284, 1999.

[11] J. C. Butcher, D. J. L. Chen, ESIRK methods and variable stepsize, Appl. Numerical Math. 28, 193-207, 1998.

[12] T. M. H. Chan, Algebraic structure for the analysis of numerical methods, Thesis submitted for the Degree of Doctor of Philosophy at the University of Auckland, Department of Mathematics, 1998.

[13] A. R. Gifkins, An algebraic approach to Runge-Kutta methods, Thesis submitted for the Degree of Doctor of Philosophy at the University of Auckland, Department of Mathematics, 1972.

[14] S. J. Huang, Jun Yu, On stiffness in Affine Asset Pricing Models, Journal of Computational Finance, 10, 99-123, 2007

[15] B. Stehlikova, D. Sevcovic, On a Volatility Averaging in a Two-Factor Interest Rate Model, Proceedings of ALGORITMY, 325-333, 2005

# Multiple time stepping symplectic integrator for molecular dynamics

*Author(s):*

E. Darve
Stanford University, U.S.A.

One of the numerical challenges of Molecular Dynamics is the presence of multiple time scales from very fast bond vibrations and much slower long-range electrostatic forces. In order to reduce the computational cost, it is common to integrate the equations of motion using multiple time steps for the different terms in the potential energy. We will present a new symplectic integrator, called Asynchronous Variational Integrator (AVI), which is based on a variational principle and uses multiple time steps. The accuracy and stability of the method will be demonstrated mathematically and on practical simulation cases. The superiority of AVI compared to the reversible reference system propagator algorithm (r-RESPA) will be discussed.

# Methods for computing oscillatory integrals involving Bessel functions

*Author(s):*

A. Deaño
Departamento de Matemáticas. Universidad Carlos III de Madrid (Spain). Email: alfredo.deanho@uc3m.es

The computation of integrals of the form

$$\mathcal{H}_\omega(f) = \int_a^b f(x)\, J_\nu(\omega x)\, dx,$$

where $0 \leq a < b$, $\omega$ is a real parameter and $J_\nu(\omega x)$ is a Bessel function of the first kind is analysed. When $a = 0$ and $b = \infty$ this integral is commonly known as the Hankel transform of $f(x)$, and arises in the resolution of differential equations involving cylindrical symmetry. The computation of this kind of integrals when $\omega \gg 1$ is a numerical challenge, since the integrand exhibits high and irregular oscillations. However, recent advances in the study of highly oscillatory integrals have produced different methods whose performance improves in the presence of high oscillation [1]. In particular, in [2], [3] and [4] the problem of quadrature is restated in terms of solving a system of ODEs satisfied by the oscillatory part of the integrand by numerical collocation. Following this approach, several strategies are proposed for the computation of these oscillatory integrals. Numerical examples are provided.

## References


[1] A. Iserles, S.P. Nørsett, S. Olver. *Highly oscillatory quadrature: The story so far.* Proceedings of ENuMath. Springer-Verlag, Berlin (2006), 97–118.

[2] D. Levin. *Procedures for computing one and two-dimensional integrals of functions with rapid irregular oscillations.* Math. Comp. 38 no. 158 (1982), 531–538.

[3] D. Levin. *Fast integration of rapidly oscillatory functions.* J. Comput. Appl. Math. 63 (1995), 95–101.

[4] D. Levin. *Analysis of a collocation method for integrating rapidly oscillatory functions.* J. Comput. Appl. Math. 78 (1997), 131–138.

[5] S. Olver. *Moment-free numerical integration of highly oscillatory functions.* IMA J. Numer. Anal. 26 (2006), 213–227.

[6] S. Olver. *Numerical approximation of vector-valued highly oscillatory integrals.* Report no. NA2006/06, DAMTP, University of Cambridge, to appear in BIT.


# Convergence of stochastic Runge–Kutta methods that use an iterative scheme to compute their internal stage values


*Author(s):*

K. Debrabant

Darmstadt University of Technology,Department of Mathematics

A. Kværnø

Norwegian University of Science and Technology, Department of Mathematical Sciences


In the modeling of many applications, e.g., in chemical reaction systems and electrical circuits, taking stochastic effects into account often leads to stochastic differential equations (SDEs) of the form

$$X(t) = x_0 + \int_{t_0}^{t} g_0(X(s))ds + \sum_{l=1}^{m} \int_{t_0}^{t} g_l(X(s)) \star dW_l(s)$$

which can be stiff, i. e., explicit approximation methods do not work efficiently, and implicit methods have to be considered. An important class of derivative free approximation methods for solutions of SDEs are stochastic Runge–Kutta (SRK) methods. In the last years, implicit SRK methods have been developed both for strong and weak approximation. For these methods, the stage values are only given implicitly. However, in practice these implicit equations are solved by iterative schemes like simple iteration, modified Newton iteration or full Newton iteration. For ordinary differential equations, using the theory of B-series and rooted trees, Jackson et. al. have proved that the iteration error can be accurately described in terms of certain growth functions defined on trees. In our talk, this theory will be extended to the SDE case. In particular, the order of weak convergence of the overall scheme will be discussed.

# A numerical model for coupling chemistry and transport


*Author(s):*

C. de Dieuleveult

IRISA/ANDRA, France

J. Erhel

IRISA/INRIA, France


One mission of ANDRA is to contribute to both national and international R&D projects related to deep repositories for Long-Lived High Level radioactive waste. The behaviour of potential sites of storage is governed by many complex physico-chemical mechanisms. In this context, numerical simulations are carried out in order to contribute to safety evaluations and risk assessment. In this paper we focus on chemistry as well as transport of the aqueous solutions. To take into account simultaneously these two phenomena, we need to consider a coupled model. In the literature, two methods have been described to run simulations for this coupled model : the so-called Sequential Iterative Approach

SIA or the so-called Direct Substitution Approach DSA. In this talk, we present the global DSA approach by using a framework of Partial Differential Algebraic Equations.

Whereas SIA implies the consecutive solution of smaller systems and requires less modifications of the basic components, DSA presents theoretically faster convergence and solves a linearized chemistry. In 1989, Yeh and Tripathi rejected DSA because of time and memory requirements. However, their comparisons were carried out without considering the convergence rates improvement potential. In fact, Steefel and MacQuarrie, in 1996 and Saaltink and al., in 2001, showed that sometimes DSA could be more interesting. The development of this global method requires an important work. In order to set this task up, we start from a system dealing only with homogeneous reactions and heterogeneous reactions related to sorption. Moreover, the chemical reactions are considered at equilibrium. Concerning transport, the tensor of diffusion is supposed independent of species and porosity is constant. The coupled model is a system of Partial Differential and Algebraic Equations. Following the method of lines (Hunsdorfer and Verwer, 2003), we first discretize in space, using a combination of centered and upwind scheme for the convective part and a finite difference approximation for the diffusive part. We thus obtain a system of algebraic differential equations of index 1. The system is then discretized in time by a Backward Differentiation Formula method with variable order and variable time step. For each time step, the nonlinear algebraic system obtained is then solved by a modified Newton method. Currently, we consider one dimensional problems. The software developed is used to simulate example 11 from the user guide of the PhreeqC software. The results obtained are consistent with the results of the software PhreeqC itself. Moreover, other tests are currently realized.

In the future, we plan to study more complex models, in particular by introducing precipitation-dissolution reactions. Also 2D and 3D domains will be considered.

## Normal form and long-time behavior of splitting methods for the linear Schroedinger equation

*Author(s):*

G. Dujardin
IRISA/INRIA-Rennes Campus Scientifique de Beaulieu 35042 RENNES FRANCE

E. Faou
IRISA/INRIA-Rennes Campus Scientifique de Beaulieu 35042 RENNES FRANCE

We consider the linear Schroedinger equation in one periodical space dimension with real analytic potential, and solve it numerically by a time splitting method. This very basic example shows that the resonances that appear do not allow to get uniform long-time estimates for the numerical solution that would permit to derive energy conservation properties by backward error analysis (see for instance [2]). However, we show by a perturbative approach that it is possible to prove a normal form theorem for the splitting propagator under a non-resonance condition similar to the ones used in [2, 3] in the finite dimensional case. This theorem then allows us to derive the conservation over exponentially long time of coupled energies associated with the double eigenvalues of the Laplace operator.

These results are presented *in extenso* in [1] and are illustrated by several numerical experiments.

# References

[1] G. Dujardin, E. Faou, *Normal form and long time analysis of splitting schemes for the linear Schroedinger equation*, Submitted.

[2] E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration. Structure-preserving Algorithms for Ordinary Differential Equations.* Springer, Berlin, 2002.

[3] Z. Shang *Resonant and Diophantine step sizes in computing invariant tori of Hamiltonian systems* Nonlinearity 13 (2000), 299–308.

## Effective Condition Number Estimates for a Class of Initial Value Solvers

*Author(s):*

W. Enright
Department of Computer Science, University of Toronto

When solving the initial value problem (IVP),

$$y' = f(x, y), \;\; y(a) = y_0, \;\; \text{for} \;\; x \in [a, b],$$

most numerical methods will now return a discrete approximation, $\{x_i, y_i\}_{i=0}^{N}$, as well as a piecewise polynomial, $Z(x) \in C^1[a, b]$ which will interpolate the discrete approximation and have an associated global error, $y(x) - Z(x)$, that is proportional to a specified error tolerance, $TOL$. We have recently implemented (see [1]) a class of very reliable Continuous Runge-Kutta methods (CRKs) of this type, of orders four through eight, which attempt to ensure that the numerical solution, $Z(x)$, will satisfy the perturbed IVP,

$$Z' = f(x, Z) + \delta(x), \;\; Z(a) = y_0, \;\; \text{for} \;\; x \in [a, b],$$

where $\|\delta(x)\| \leq TOL$. The methods we have developed tend to require up to twice as many derivative evaluations per step (compared with the cost of generating only the underlying discrete solution), but extensive testing has demonstrated that the associated estimate of the maximum of $\|\delta(x)\|$ on each step is within one percent of the true maximum eighty percent of the time and the true maximum of the associated $\|\delta(x)\|$ for $x \in [a, b]$ very rarely exceeds $TOL$.

For these methods, as well as for any method that produces a piecewise approximation $Z(x)$ to $y(x)$, the global error, $u(x) = y(x) - Z(x)$, is the exact solution of the IVP,

$$u' = f(x, Z + u) - Z'(x), \;\; u(a) = 0, \;\; \text{for} \;\; x \in [a, b].$$

One can therefore estimate the global error associated with $Z(x)$ by approximating the solution of this companion IVP. One is free to choose the same initial value solver to approximate $u(x)$ or to use a different solver and/or a different accuracy request.

In this talk we will report on how this approach can be used to not only produce effective estimates of the global error of $Z(x)$, but also estimates of the condition number of the underlying ODE. An "iterative refinement" technique where $V(x)$, the approximate solution of the companion IVP, can be used to improve the numerical solution $Z(x)$ will also be discussed. Numerical results on some well-known test problems will be presented to illustrate the usefulness and cost of the approach.

# References


[1] Robust and Reliable Defect Control for Runge Kutta Methods. *ACM Trans. Math. Soft.*, 33,1: 1–19, 2007.


# A family of eighth order, eighth stages Explicit Numerov type methods for second order IVPs with oscillating solutions.


*Author(s):*

I. Th. Famelis

Assistant Professor, Department of Mathimatics, TEI of Athens, Greece, E-Mail:ifamelis@teiath.gr


The initial value problem of second order

$$y'' = f(y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \tag{20}$$

especially when the solution is oscillating, is of continued interest in many fields of celestial mechanics, quantum mechanics, scattering theory, theoretical physics and chemistry, and electronics. When solving (20) numerically we have to pay attention in the algebraic order of the method used, since this is the main factor of achieving higher accuracy with lower computational cost, i.e. this is the main factor of increasing the efficiency of our effort. If we also feel that the solution of (20) is of periodic nature it is essential to consider *phase-lag* (or dispersion) and *amplification* (or dissipation). These are actually two types of truncation errors. The first is the angle between the true and the approximated solution, while the second is the distance from a standard cyclic solution.

In this work a new family of explicit hybrid Numerov type methods

$$\begin{aligned} y^{[k+1]} &= 2y^{[k]} - y^{[k-1]} + h^2 \cdot (b \otimes I_8) \cdot f(Y) \\ Y &= (e-c) \otimes y^{[k]} + c \otimes y^{[k-1]} + h^2 \cdot (A \otimes I_8) \cdot f(Y) \end{aligned} \tag{21}$$

is presented. These eighth order methods have a cost of eight stages per step while their phase lag order is 18 and partly satisfy the dissipation order conditions. The construction procedure is analyzed and a very efficient representative of such methods is compared to its competitive methods found in the literature. Numerical testing is performed in a variety of problems found in the literature revealing the good characteristics of the new method.

# References


[1] Ch. Tsitouras Explicit eighth order two-step methods with nine stages for integrating oscillatory problems. *International Journal of Modern Physics C*, 17:861–876, 2006.

[2] G. Papageorgiou et. al. Explicit eighth order two-step methods with nine stages for integrating oscillatory problems. *International Journal of Modern Physics C*, 12:657–666, 2001.

[3] I. Famelis, Ch. Tsitouras Symbolic Derivation of Order Conditions for Hybrid Numerov-type methods solving $y'' = f(x, y)$ *Submitted* .


## On longitudinal vibration of thick bars


*Author(s):*

I. Fedotov

Department of Mathematics and Statistics P.B.X680, Pretoria, 0001 FIN-40014 Tshwane University of Technology (Pretoria), South Africa, fedotovi@tut.ac.za

M. Shatalov

CSIR Manufacturing and Materials P.O. Box 395, Pretoria 0001, CSIR, and Department of Mathematics and Statistics P.B.X680, Pretoria, 0001 FIN-40014 Tshwane University of Technology (Pretoria), South Africa, mshatlov@csir.co.za

S. Joubert

Department of Mathematics and Statistics P.B.X680, Pretoria, 0001 FIN-40014 Tshwane University of Technology (Pretoria), South Africa, JoubertSV@tut.ac.za



Longitudinal vibration of bars are normally considered in mathematical physics in terms of classical model described by the wave equation under assumptions that the bar is thin and relatively long structure. More general theories were formulated taking in consideration the effect of lateral motion of relatively thick bar. Mathematical formulation of these models includes fourth order derivatives in the equation of their motion. Rayleigh did the simplest generalization of the classical model in 1894, by including the effects of lateral motion and neglecting the shear stress. Bishop obtained the next generalization of the theory in 1952. The Rayleigh-Bishop model is described by a forth order partial differential equation not containing the forth time derivative. He taken into accounts the effects of shear stress. Both Rayleighs and Bishops theories consider lateral displacement being proportional to the longitudinal strain. The Bishops model was generalized by Mindlin and Herman. They considered the lateral displacement proportional to an independent function of time and longitudinal coordinate. This result is formulated as a system of two differential equations of second order, which could be replaced by a single equation of forth order resolved with respect to the highest order time derivative. The Greens functions for all these models are constructed.


## Discrete variational derivative method: one of structure preserving methods for numerical integration of PDEs


*Author(s):*

D. Furihata

Osaka University, JAPAN

Recently we have proposed a method to construct numerical schemes for PDEs which have some dissipative or conservative properties. This method, we refer to it as discrete variational derivative method(DVDM), is a kind of structure preserving methods for PDEs.

The key idea of DVDM is to discretise the variational structure of PDEs which is essence of those properties using rigorous definitions of discrete variational derivative. It follows that constructed schemes inherit the property of integral functional of PDEs.

For example, we are able to construct dissipative or conservative properties preserving schemes for

$$\partial u/\partial t = (\partial/\partial x)^{\alpha}(\delta G/\delta u),$$

$$\partial^2 u/\partial t^2 + C\partial u/\partial t = (\partial/\partial x)^{\alpha}(\delta G/\delta u),$$

and other kind of PDEs. Examples of concrete PDEs are Swift-Hohenberg equation, Cahn-Hilliard equation, KdV equation, Camassa-Holm equation and so on.

Due to preserving properties we able to expect that those schemes have preferable properties such as numerical stability and solution uniqueness. In fact, we have obtained mathematical theorems for such properties of some our schemes. Not only applying DVDM to PDEs but we also have studied DVDM carefully to extend it, for instance, to obtain higher order of precision, to use other than finite difference method, to apply higher space dimension and so on. We will talk and indicate result of our effort.

# References


[1] D. Furihata. Finite difference schemes for equation $\partial u/\partial t = (\partial/\partial x)^{\alpha}(\delta G/\delta u)$ that inherit energy conservation or dissipation property, *J. Comput. Phys.*, 156:181–205, 1999.
the Cahn-Hilliard Equation,

[2] T. Matsuo and D. Furihata. Dissipative or Conservative Finite Difference Schemes for Complex-Valued Nonlinear Partial Differential Equations, *J. Comput. Phys.*, 171:425–447, 2001.

[3] D. Furihata. Finite difference schemes for nonlinear wave equation that inherit energy conservation property, *J. Comput. Appl. Math.*, 134:35–57, 2001.

[4] T. Matsuo, M. Sugihara, D. Furihata and M. Mori. Spatially accurate dissipative or conservative finite difference schemes derived by the discrete variational method, *Jpn. J. Indust. Appl. Math.*, 19:311–330, 2002.
Difference Scheme for the Cahn-Hilliard Equation,


## A modified least-squares FEM with quadrature for nonlinear advection-diffusion-reaction equations


*Author(s):*

M. Ganesh

Colorado School of Mines, Golden, Colorado, USA



We present, analyse, and implement a modified least-squares fully discrete finite element method (FEM) with quadrature for strongly nonlinear advection-diffusion-reaction equations on smooth and polygonal domains (satisfying a maximum interior angle condition at the corners). The quadrature FEM algorithm and analysis are applicable for a large class of nonlinear functions (including exponentials and polynomials of odd and even degrees) in the unknown variables. In addition, the algorithm requires solutions of only a linear system at each time step, avoiding the expensive Newton iterations. We prove the stability of the modified least-squares solutions by including the effect of the quadrature in computer implementation, and also prove and demonstrate the optimal order convergence of the approximate solutions. (This is a joint work [1] with K. Mustapha.)


# References


[1] M. Ganesh and K. Mustapha, A fully discrete $H^1$-Galerkin method with quadrature for nonlinear advection-diffusion-reaction equations. *Numer. Algorithms*, **43** (2007), 355–383.

# On multistep methods of Adams type for fractional differential equations

*Author(s):*

R. Garrappa

Department of Mathematics - University of Bari - Bari - Italy

L. Galeone

Department of Mathematics - University of Bari - Bari - Italy

In the last decade, new algorithms have been suggested for solving differential equations of fractional (i.e. non integer) order. Recently, an increasing attention has been dedicated to generalize classical multistep methods of Adams type for solving fractional differential equations too.

Adams multistep methods for ordinary differential equations can be generated according two equivalent approaches: the replacement of the state function by a suitable interpolating polynomial or the evaluation of the first coefficients in the expansion of a generating function. When applied to fractional differential equations, the above approaches give raise to two different classes of algorithms (e.g. see [1, 2, 3, 4, 5]).

We consider implicit and explicit schemes in both classes of methods and we present some techniques for evaluating their coefficients. Hence we study some properties of resulting algorithms, with main emphasis on the analysis of linear stability. Furthermore, we make a comparison between methods generated according the two approaches.

## References

[1] Kai Diethelm, Neville J. Ford, and Alan D. Freed. Detailed error analysis for a fractional Adams method. *Numer. Algorithms*, 36(1):31–52, 2004.

[2] Luciano Galeone and Roberto Garrappa. Fractional Adams–Moulton methods. Technical Report 19/2007, Department of Mathematics, University of Bari, 2007.

[3] Roberto Garrappa. On explicit Adams multistep methods for fractional differential equations. Submitted.

[4] Christian Lubich. Discretized fractional calculus. *SIAM J. Math. Anal.*, 17(3):704–719, 1986.

[5] Christian Lubich. A stability analysis of convolution quadratures for Abel-Volterra integral equations. *IMA J. Numer. Anal.*, 6(1):87–101, 1986.

# The perturbation and ADAE index of a degenerated hyperbolic system modelling a heat exchanger

*Author(s):*

M. Hanke

Royal Institute of Technology, Stockholm

T. Reis

Technical University of Berlin

In a recent paper [1], a reduced model for the heat exchangers appearing in a heat pump has been developed. It consists essentially of the zero-Mach number limit of the compressible Euler equations. This degenerated hyperbolic system turns out to be a coupled hyperbolic/parabolic equation. In the cited paper, energy estimates for a (simplified) frozen coefficient system transformed to a certain normal form are derived. In fact, the system is weakly ill-posed. In terms of the perturbation index, the time index is 1, while the space index is 2. This statement depends essentially on the fact that time-independent boundary conditions are used exclusively. This is an unrealistic assumption for practical simulations. In case of time-dependent boundary conditions, the time index is known not to exceed 2 [2]. Numerical experiments in [2] indicate that this is an overestimate of the time index.

In the present paper we will show that the perturbation index od the linearized system is one with respect to time and two with respect two space even for time-dependent boundary conditions. The main tool is the theory of abstract differential-algebraic equations [3]. The estimates will be provided in the original physical variables such that they can be interpreted immediately.

## References


[1] M. Hanke, K.H.O. Olsson, M. Strömgren: Stability analysis of a degenerate hyperbolic system modelling a heat exchanger, *Math. Comp. in Simulation,* 74 (2007), 8–19.

[2] M. Strömgren: *Some PDAE aspects of the numerial simulation of a $CO_2$ heat pump*, Licentiate Thesis, Royal Institute of Technology, Stockholm 2006.

[3] T. Reis: Consistent initialization and perturbation analysis for differential-algebraic equations, *Math. Control Signals System*, to appear, 2007.


# A Theoretical Framework for Backward Error Analysis on Manifolds


*Author(s):*

A. Hansen
University of Cambridge



Backward Error Analysis (BEA) has been a crucial tool when analyzing the long-time behavior of numerical integrators, in particular, one is interested in the geometric properties of the perturbed vector field generated by a numerical method. In this talk we present a new framework for BEA on manifolds. We extend the previously known "exponentially close" estimates from $\mathbb{R}^n$ to smooth manifolds and also provide an abstract theory for classifications of numerical integrators in terms of their geometric properties. Classification theorems of type: symplectic integrators generate symplectic perturbed vectorfields are known to be true in $\mathbb{R}^n$. We present a general theory for proving such theorems on manifolds by looking at the preservation of smooth $k$-forms on manifolds by the pull-back of a numerical integrator. This theory is related to classification theory of subgroups of diffeomorphisms. We also look at other subsets of diffeomorphisms that occur in the classification theory of numerical integrators. Typically these subsets are symmetric spaces and anti-fixed points of involutions.


# The stability of BDF methods with variable stepsize


*Author(s):*

A. Heard
The University of Auckland, New Zealand

John Butcher
The University of Auckland, New Zealand



This paper is concerned with the stability of BDF methods when used with variable stepsize. The stability is dependent on the formulation of the method as well as on the method itself. Theoretical analysis of the underlying one-step method for the Nordsieck form is considered, and the application of the 'scale and modify' approach, introduced by J. Butcher and Z Jackiewicz for General Linear Methods (in the paper referenced below) and since developed further, is included.


## References


[1] A new approach to error estimation for general linear methods *Numer. Math.* ., 95: 487-502, 2003.


# Multi-symplectic Runge-Kutta Type Methods for Hamiltonian Partial Differential Equations


*Author(s):*

J. Hong
State Key Laboratory of Scientific and Engineering Computing,
Institute of Computational Mathematics and Scientific/Engineering Computing,
Academy of Mathematics and Systems Science,
Chinese Academy of Sciences,
P.O.Box 2719, Beijing 100080, P. R. China
Email: hjl@lsec.cc.ac.cn

In this talk we present some new developments of multi-symplectic Runge-Kutta type methods for Hamiltonian partial differential equations (PDEs), which play an important role in scientific and engineering computing. These developments include:

-The symplecticity of partitioned Runge-Kutta methods and Nyström methods and the corresponding discrete multi-symplectic conservation laws.

-The analysis of energy and momentum, the discrete charge conservation law of multi-symplectic Runge-Kutta type methods for Hamiltonian PDEs.

-The theory of generating functions for multi-symplectic Runge-Kutta type methods which are closely related to Donde-Weyl Hamilton-Jacobi theory.

-The construction of explicit multi-symplectic schemes for some special Hamiltonian PDEs in some scientific and engineering fields.

-Some applications of multi-symplectic Runge-Kutta methods to Klein-Gordon- Schrödinger equations and Dirac equations in quantum physics.

## Linearly stable and time-reversible integration methods for classical mechanics

*Author(s):*

T. Hundertmark
Universität Potsdam

S. Reich
Universität Potsdam

Numerical integration in classical mechanics holds several problems which need to be addressed. In terms of conservation laws the Störmer-Verlet (SV) scheme is the most popular method. However, the restriction on the time step is a major drawback. Fully implicit algorithms are known to be unconditionally stable, but in turn, they are often computationally too expansive. We propose a linearly implicit method that is based on a regularization of the fast forces, combined with a SV time-stepping for the regularized equations. The proposed scheme is time-reversible, linearly stable and only requires one additional matrix inversion per SV time step. A similar regularization approach has previously shown good results in applications from fluid dynamics. Here we can show further promising results for an example from molecular dynamics.

## On the efficient evaluation of multivariate highly oscillatory integrals

*Author(s):*

D. Huybrechs
K.U. Leuven, Dept. of Computer Science. Address: Celestijnenlaan 200A, BE-3001 Leuven, Belgium. E-mail: daan.huybrechs@cs.kuleuven.be

S. Vandewalle
Same address. E-mail: stefan.vandewalle@cs.kuleuven.be

We consider the problem of evaluating a multivariate highly oscillatory integral of the form

$$I[f] := \int_S f(\mathbf{x}) e^{i\omega g(\mathbf{x})} \mathrm{d}s,$$

where both $f$ and $g$ are smooth $n$-dimensional functions and $\omega$ is a large parameter. Oscillatory integrals of this form abound in methods of science and engineering, most notably in mathematical models describing wave phenomena. The motivation for this study has been the solution of the Helmholtz equation for wave scattering problems in acoustics.

The method we describe has a number of interesting properties. First of all, the accuracy of the method improves as the frequency of the integrand increases. This is quite contrary to the rapid deterioration of classical cubature approaches

for increasingly oscillatory integrals. Second, the method is quite efficient. One formulation takes the form of a simple cubature rule involving derivatives,

$$I[f] \approx Q[f] := \sum_{j=1}^{N} \sum_{|\alpha| \leq s} w_{\alpha,j} \frac{\partial^\alpha f}{\partial \mathbf{x}^\alpha}(\mathbf{x}_j),$$

where we have used a multi-index $\alpha$ to denote the partial derivatives of $f$. The set of cubature points $\{\mathbf{x}_j\}$ can be surprisingly small. For example, when $S$ is the three-dimensional unit ball and $g(\mathbf{x}) = \mathbf{x}$ is the Fourier oscillator, only two function evaluations of $f$ are required. In that case, one obtains an absolute error of $10^{-8}$ at $\omega = 1600$. The numerical integration of highly oscillatory integrals can be very effective indeed.

The method is based on a numerical interpretation of the method of steepest descent. The approach is described for one-dimensional integrals in [1]. The extension to multivariate integrals exhibits some new features not found in the 1D case and is described in [2].

# References


[1] Huybrechs, D. and Vandewalle S. On the efficient evaluation of highly oscillatory integrals by analytic continuation. *SIAM J. Numer. Anal.*, 44:1026–1048, 2006.

[2] Huybrechs, D. and Vandewalle S. The construction of cubature rules for multivariate highly oscillatory integrals. *Math. Comp.*, to appear.


## Difference forms for finite difference schemes


*Author(s):*

P. Hydon
University of Surrey

E Mansfield
University of Kent


Many important systems of differential equations are most naturally written in terms of differential forms on a manifold. Qualitative errors commonly occur when a numerical approximation fails to preserve this structure and the topology of the underlying manifold (in some sense). Error analysis shows the approximation to be locally accurate, but global features of the original system are not reproduced correctly. This observation has recently led to the development of *discrete differential forms* [1] (and related finite element methods) which can be used when a domain is partitioned into simplices.

Any simplicial decomposition essentially retains the underlying continuity of the domain. By contrast, finite difference approximations retain only the ordering of adjacent points in each direction – continuity is lost. However, for some systems, difference equations provide the most natural class of approximations. This raises some questions. Is it possible to construct finite difference analogues of differential forms? If so, can they help us to preserve global features of an approximated system?

We have recently found that both of these questions have a positive answer [2], which is surprising in view of the complete loss of continuity. Furthermore, the *difference forms* that occur can be tailored to suit various numerical schemes that are used for geometric integration, including Gauss-Legendre and Preissman schemes.

This talk is an introduction to difference forms and their applications; it is aimed at a general audience.

# References


[1] Desbrun, M., Kanso, E. & Tong, Y., 2005, Discrete differential forms for computational modelling, ACM SIGGRAPH '05 course notes on Discrete Differential Geometry.

[2] Mansfield, E. L. & Hydon, P. E., Difference forms, (submitted to *Found. Comp. Math.*).

# Normal-mode-constrained Molecular Dynamics (NMC)

*Author(s):*

J.A. Izaguirre

Computer Science and Engineering, University of Notre Dame

NMC is a method that can propagate the slow dynamics of a protein using 100 times longer time steps for a real speedup of nearly 50 over conventional MD. NMC stands for Normal-Mode-Constrained MD. This method periodically diagonalizes a time-averaged Hessian and propagates the true dynamics of a subset of the slower modes. Very long times are needed between rediagonalizations, which happen upon significant conformational changes. We have developed a metric based on perturbation theory to detect when rediagonalization is needed. Processes of biological interest may take several microseconds (e.g., conformational change), which are thus made more accessible. I will present an application of NMC to compute commitor probabilities for transition path sampling of a protein undergoing slow conformational exchange. NMC can also be used to accelerate replica-exchange simulations, since the effective number of degrees of freedom is reduced, and thus can be used to sample the conformational space of biomolecules.

# Numerical solutions for highly oscillatory ODEs

*Author(s):*

M. Khanamiryan

University of Cambridge

The work presents efficient numerical approximation to linear and nonlinear systems of highly oscillatory ODEs given in the vector form $\boldsymbol{y}' = A_\omega \boldsymbol{y} + \boldsymbol{f}$, where $A_\omega$ is a constant nonsingular matrix, $\|A_\omega\| \gg 1$, $\sigma(A_\omega) \subset \mathrm{i}\mathbb{R}$, $\boldsymbol{f}$ is a smooth vector-valued function and $\omega$ is an oscillatory parameter. We show how an appropriate choice of quadrature rule improves the accuracy as $\omega \to \infty$. We present a Filon–type method to solve highly oscillatory linear systems and WRF method, a special combination of the Filon–type method and the waveform methods, for nonlinear systems. The work is accompanied by numerical examples.

# Solution of the inverse problem of the determination of hydrodynamic flow profiles from electric currents measured at two electrodes in a microfluidic channel

*Author(s):*

O.V. Klymenko

Kharkov National University of Radioelectronics, Mathematical and Computer Modelling Laboratory,14 Lenin Avenue, Kharkov, 61166, Ukraine

C. Amatore

Ecole Normale Superieure, Department de Chimie, UMR CNRS 8640 "PASTEUR", 24 rue Lhomond, 75231 Paris Cedex 05, France

A. Oleinick

Ecole Normale Superieure, Department de Chimie, UMR CNRS 8640 "PASTEUR", 24 rue Lhomond, 75231 Paris Cedex 05, France

I. Svir

Kharkov National University of Radioelectronics, Mathematical and Computer Modelling Laboratory,14 Lenin Avenue, Kharkov, 61166, Ukraine;

Ecole Normale Superieure, Department de Chimie, UMR CNRS 8640 "PASTEUR", 24 rue Lhomond, 75231 Paris Cedex 05, France

Microfabrications and microfluidic systems are playing an increasing role in modern physical, chemical and biological sciences. These systems provide many advantages and abilities such as reduced analysis duration, enhanced reproducibility, separation, mixing, detection, dilution and other operations, which can be performed within a single integrated device called "lab-on-a-chip" for complete analysis in many applications. However, optimisation of the hydrodynamics in such

devices requires an experimental ability of monitoring in real time the actual intensity and shape of flow streams within them. This is of interest when various microscopic factors (imperfections of fabrication, surface effects such as solution slippage at the walls, etc.) affect the flow pattern leading to distortion of flow profile across the channel with respect to the expected parabolic one [1]. The ability to monitor such distortions would ensure the implementation of feedback control loops so that the flow can be tailored precisely to fulfil the desired application. An approach for flow profile reconstruction in a two-dimensional rectangular cross-section of a microfluidic channel equipped with one or two microband electrodes [2, 3, 4] is developed and the system geometrical and hydrodynamic parameters are optimised to achieve the best performance of the method. The unknown flow profile function is determined on the basis of electrochemical currents measured at the band electrodes, thus being the solution of the inverse electrochemical mass transport problem. The spline representation of the flow profile function permitted the sensitivity analysis of the problem at hand leading to the determination of the area in the three-parameter space of the system (the parameters being the dimensionless electrode width, $W$, interelectrode gap, $G$, and the Peclet number, $Pe$) where the flow profile shape may be reliably reconstructed from experimental current data [5]. The results of this analysis confirm previously predicted area of high sensitivity to flow profile shape based on physical considerations.

# References


[1] V.G. Levich. Physicochemical hydrodynamics. USSR Academy of Sciences, Moscow, 1952.

[2] C. Amatore, A. Oleinick, O.V. Klymenko, I. Svir. *ChemPhysChem*, 6:1581–1589, 2005.

[3] C. Amatore, O.V. Klymenko, I. Svir. *ChemPhysChem*, 7:482–487, 2006.

[4] O.V. Klymenko, A.I. Oleinick, C. Amatore, I. Svir. *Electrochim. Acta*, in press.

[5] C. Amatore, O.V. Klymenko, A. Oleinick, I. Svir. *ChemPhysChem*, submitted.


## Fully implicit stochastic Runge-Kutta methods for stochastic differential equations with a scalar Wiener process


*Author(s):*

Y. Komori

Kyushu Institute of Technology


Recently, a very general stochastic Runge-Kutta (SRK) family has been proposed for weak approximations to solutions of Stratonovich type stochastic differential equations (SDEs) [1], and new explicit SRK schemes of weak order 2 have been derived from the family for not only commutative SDEs but also non-commutative SDEs [2, 3].

In this talk, on the basis of the family, new fully implicit SRK schemes of weak order 1 or 2 will be addressed for SDEs with sufficiently smooth drift and diffusion coefficients and a scalar Wiener process [4]. The schemes have the following features:

- They are A-stable in mean square in the case that $\Re(\sigma) = 0$ or $\Im(\lambda) = \Im(\sigma) = 0$ for the scalar test equation

$$\mathrm{d}y(t) = \lambda y(t)\mathrm{d}t + \sigma y(t) \circ \mathrm{d}W(t), \qquad y(0) = x_0, \qquad \lambda, \sigma \in \boldsymbol{C},$$

  where $W(t)$ is a scalar Wiener process, $x_0$ is independent of $W(t) - W(0)$ for $t \geq 0$, and $\circ$ means the Stratonovich formulation.

- With any step size $h > 0$, they generate asymptotical mean square preserving approximate solutions for the multi-dimensional SDE with additive noise [5]

$$\mathrm{d}\boldsymbol{y}(t) = A\boldsymbol{y}(t)\mathrm{d}t + \boldsymbol{b} \circ \mathrm{d}W(t), \qquad \boldsymbol{y}(0) = \boldsymbol{x}_0.$$

Their convergence order and stability properties will be confirmed in numerical experiments.

## References


[1] Y. Komori. Multi-colored rooted tree analysis of the weak order conditions of a stochastic Runge-Kutta family. *Appl. Numer. Math.*, 57 (2): 147–165, 2007.

[2] Y. Komori. Weak order stochastic Runge-Kutta methods for commutative stochastic differential equations. *J. Comput. Appl. Math.*, 203 (1): 57–79, 2007.

[3] Y. Komori. Weak second-order stochastic Runge-Kutta methods for non-commutative stochastic differential equations. *J. Comput. Appl. Math.*, 206 (1): 158–173, 2007.

[4] Y. Komori. Weak first- or second-order implicit stochastic Runge-Kutta methods for stochastic differential equations with a scalar Wiener process. Submitted for publication.

[5] H. Schurz. Preservation of probabilistic laws through Euler methods for Ornstein-Uhlenbeck process. *Stochastic Anal. and Appl.*, 17 (3): 463–486, 1999.


# Correctly Rounded Numerical Computation of IVPs for ODEs based on Classical Error Estimation


*Author(s):*

T. Kouya

Shizuoka Institute of Science and Technology


Nowadays, validated numerical computation is closed up. Corliss[1] et al. shows that the validated computation of IVPs for ODEs is possible. Because validated computation is based on interval algorithms, which in turn are based on rigorous theories, it can be used to obtain intervals or regions that contain true solutions.

Many numerical computation users, however, do not require such rigorous validation for obtaining their numerical solutions. In the case of IVPs for ODEs, the truncation error in the numerical solutions can be estimated by comparing some solutions that are calculated by using different stepsizes. Further, the round-off error can be obtained by the difference between two numerical solutions by using, for example, IEEE754 double precision and quadruple precision arithmetic. This estimation of truncation and round-off errors, the so-called "classical error estimation", is still the standard technique employed by users who feel that the level of validation obtained by it is sufficient.

Furthermore, many existing numerical libraries do not provide fasilities for validated computation. Therefore, programs to realize validated computation must be rebuilt from scratch. However, such programs are incapable of realizing non-validated computation at a performance that is higher than normal.

In our study, we show that non-validated standard numerical algorithms with classical error estimation can realize unrigorous yet practical precision estimation for the numerical solutions of IVPs for ODEs in both IEEE754 double precision and multiple precision computation environments. Moreover, we demonstrate that correctly rounded numerical solutions over user-required precision for chaotic ODEs such as Lorenz or Rössler models can be automatically obtained with the help of BNCpack[4], our multiple precision numerical computation library based on MPFR[3]/GMP[2].

## References


[1] G.F.Corliss, Guaranteed Error Bounds for Ordinary Differential Equations, Theory and Numerics of Ordinary and Partial Differential Equations, Clarendon Press, 1995.

[2] GNU Multiple Precision Arithmetic Library, `http://gmplib.org/`

[3] MPFR Project, `http://www.mpfr.org/`

[4] BNCpack, `http://na-inet.jp/na/bnc/`


# Exponential operator splitting time integration for pseudospectral methods


*Author(s):*

R. Kozlov

Department of Mathematics, University of Bergen, Jonannes Brunsgate 12, 5008 Bergen, Norway
roman.kozlov@mi.uib.no

Pseudospectral spatial discretization by orthogonal polynomials and Strang splitting method for time integration are applied to second order linear evolutionary PDEs

$$u_t = u_{xx} + p(x)u_x + q(x)u, \qquad u = u(t, x).$$

Transformations of the original PDEs into a suitable for such numerical integration form are found. Trigonometric, Jacobi (and some their special cases), associated Laguerre and Hermite polynomials are considered.

A double representation of polynomials (by coefficients with respect to set of orthogonal basis functions and by values at the nodes associated with a suitable quadrature formula) is used for numerical implementation so that it is possible to avoid calculations of matrix exponentials. This framework is suitable reaction-convection-diffusion problems and Schrödinger equation.

# Criticism of Asymptotic Global Error Expansion with a New Extrapolation Theory

*Author(s):*

G. Kulikov

University of the Witwatersrand, Johannesburg, South Africa

In this paper we discuss existence of the asymptotic global error expansion for numerical solutions obtained from general one-step methods applied to ordinary differential equations. The asymptotic global error expansion was discovered independently by Henrici [1], Gragg [2] and Stetter [3] in 1962, 1964 and 1965, respectively. It is an important theoretical background for extrapolation methods. We draw attention to some flaws in that theory and show that such an expansion is likely to fail to work in practice. Therefore we give another substantiation for extrapolation methods. The Richardson extrapolation technique is a key means to explain how extrapolation methods perform. Additionally, we prove that the Aitken-Neville algorithm works for any one-step method of an arbitrary order s under suitable smoothness.

## References

[1] P. Henrici. *Discrete variable methods in ordinary differential*, John Wiley & Sons, Inc., New York-London-Sydney, 1962.

[2] W.B. Gragg. *Repeated Extrapolation to the Limit in the Numerical Solution of Ordinary Differential Equations*, PhD. thesis, University of California, 1964.

[3] H.J. Stetter. Asymptotic expansions of the error of discretization algorithms for non-linear functional equations. *Numer. Math.*, 7:18–31, 1965.

# Discrete Square-Root Filtering Algorithms for Likelihood Gradient Evaluation

*Author(s):*

M. Kulikova

University of the Witwatersrand, Johannesburg, South Africa

In this paper we consider discrete-time linear stochastic systems and discuss the problem of efficient evaluation of Log-Likelihood Gradient, which is used in system identification. The problem leads to implementation of a Kalman filter, which is known to be numerically unstable. Some insights about numerical properties of the different Kalman filter implementations can be found in [1].

In this paper we present four algorithms for efficient evaluation of the Log-Likelihood Gradient that are based upon the, so called, array square-root filters developed for dealing with the problem of numerical instabilities arising from roundoff

errors [2]. This allows us to avoid the use of the Kalman filter and, apart from numerical advantages, we may mention that array algorithms are better suited to parallel implementation. With the theoretical results we give some examples of ill-conditioned problems and compere the performance of the conventional Kalman filter and algorithms introduced in this paper. The preliminary analysis indicates that our methods outperform the conventional approach for accuracy.

The new results can be used for efficient calculations in gradient-search algorithms for maximum likelihood estimation of the unknown system parameters.

# References


[1] M. Verhaegen and P.V. Dooren. *Numerical Aspects of Different Kalman Filter Implementations*, IEEE Trans. Automat. Contr., vol. AC-31, pp. 907–917, Oct. 1986.

[2] P. Park and T. Kailath. *New square-root algorithms for Kalman filtering*, IEEE Trans. Automat. Contr., vol. 40, pp. 895–899, May 1995.


## Dynamic behavior of moving mesh partial differential equations


*Author(s):*

A. Kværnø
Norwegian University of Science and Technology, Trondheim, Norway

R. D. Russell
Simon Fraser University, Vancouver, Canada


In this talk we discuss discretized moving mesh partial differential equations (MMPDEs) based on the equidistribution principle. We present examples in which the MMPDEs demonstrate quite unexpected behavior, like sudden jumps or rapid oscillations of the grid points. The behavior can be explained by considering the MMPDE as a dynamical system and by computing the corresponding bifurcation diagrams. For certain situations, the diagrams exhibit multiple stable and unstable steady state solutions, as well as bifurcating periodic orbits. The branch of steady state solutions do not depend on the choice of MMPDEs (among those we consider here), but the stability properties do. The bifurcation diagram will also clearly reveal the effect of smoothing techniques.

## Efficient computation of high Sturm-Liouville eigenvalues


*Author(s):*

V. Ledoux
Ghent University

M. Van Daele
Ghent University

G. Vanden Berghe
Ghent University


A classical Sturm-Liouville problem is a real second-order linear differential equation

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=\lambda w(x)y, \quad a<x<b, \tag{22}$$

with boundary conditions at the endpoints as appropriate. A value of the parameter $\lambda$ for which there is a nontrivial solution subject to the boundary conditions, is called an eigenvalue, and the solution is the corresponding eigenfunction. The determination of the eigenvalues of such Sturm-Liouville problems is of great interest in mathematics, classical physics and quantumphysics. However most eigenvalue problems cannot be solved analytically, and computationally efficient approximation techniques are of great applicability.

Finding the eigenvalues can be a computationally challenging task, especially when a large set of eigenvalues is sought, or just when particularly large eigenvalues are sought. The highly oscillatory behaviour of the solutions corresponding to high eigenvalues forces a naive integrator to take increasingly smaller steps. In this talk we will discuss some techniques that yield uniform approximation over the whole eigenvalue spectrum and can take large steps even for high eigenvalues. In particular, we will focus on the important principle of coefficient approximation [1], the addition of a perturbation technique to construct higher order methods (the so-called Piecewise Perturbation Methods [2, 3]), but also on some more recent advances as e.g. the use of a Magnus or Neumann expansion and how to do this to ensure the accuracy for high eigenvalues.

## References


[1] Pruess, S. Estimating the eigenvalues of Sturm-Liouville problems by approximating the differential equation. SIAM J. Numer. Anal. 10 (1973).

[2] L. Ixaru, Numerical Methods for Differential Equations and Applications, Reidel, 1984.

[3] V. Ledoux, M. Van Daele and G. Vanden Berghe, CP methods of higher order for Sturm-Liouville and Schrdinger equations, Comp. Phys. Commun., 162 (2004).


# Symplectic integrators for highly oscillatory Hamiltonian systems


*Author(s):*

F. Legoll

LAMI, Ecole Nationale des Ponts et Chausées, Paris, France

C. Le Bris

CERMICS, Ecole Nationale des Ponts et Chausées, Paris, France


We introduce here a class of symplectic schemes for the numerical integration of highly oscillatory Hamiltonian systems. The bottom line for the approach is to exploit the Hamilton-Jacobi form of the equations of motion. We perform a two-scale expansion of the solution of the Hamilton-Jacobi equation. We thus compute an approximation of the generating function, from which we obtain a symplectic integration scheme. Several numerical examples will be presented, that demonstrate the efficiency of the approach.

## References


[1] C. Le Bris, F. Legoll, Dérivation de schémas numériques symplectiques pour des systèmes hamiltoniens hautement oscillants, C. R. Acad. Sci. Paris, Série I, vol. 344 (4), 277-282, 2007.


# Sampling the canonical measure: some numerical comparisons


*Author(s):*

F. Legoll

LAMI, Ecole Nationale des Ponts et Chausées, Paris, France


Several dynamics have been proposed in the litterature to compute canonical averages: some are fully deterministic (such as the Nosé-Hoover or Nosé-Poincaré methods), while other ones are stochastic (such as the Langevin or the Hybrid Monte-Carlo methods). We will compare the efficiency of all these methods for a benchmark model of linear alkane molecules [1].

Next, we will turn to a different problem. Collective variables are routinely introduced in order to have a better understanding of a system which explores many metastable wells. We will report on ongoing works aiming at defining a dynamics on these collective variables.

This work is joint with E. Cancès, T. Lelièvre and G. Stoltz.

## References


[1] E. Cancès, F. Legoll, G. Stoltz, Theoretical and numerical comparison of some sampling methods for molecular dynamics, Mathematical Modelling and Numerical Analysis (M2AN), in press.


# Calculation of free energy differences using stochastic dynamics


*Author(s):*

T. Lelièvre

CERMICS, Ecole Nationale des Ponts et Chauses, Paris, France

Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. Many recent methods rely on complex Markov processes (non-homogeneous or non-linear processes). Examples of such methods are exponential reweighting of non-equilibrium paths (Jarzynski equality) and Adaptive Biasing Force (ABF) techniques. We present some mathematical analysis of these two methods for stochastic dynamics, for transitions between states defined through values of a reaction coordinate. More precisely, we extend the traditional Jarzinski equality in this context using constrained stochastic dynamics. Concerning the ABF method, we present a proof of the longtime convergence as well as an implementation using an interacting particle system with birth death processes. A unifying presentation of adaptive methods is also proposed.

## Virtual Internal Bond Model and Coarse Grained Molecular Dynamics in Material Fracture

*Author(s):*

P. Lin

Department of Mathematics, National University of Singapore

A virtual internal bond (VIB) model was proposed recently in the mechanical engineering literature for simulating dynamic fracture. The model is a nonlinear conservation law of mixed type (hyperbolic or elliptic). A discrete model in material analysis and simulation is the molecular dynamics (MD) model. Because the number of particles (atoms) is huge for a MD model, in practice people often take a much smaller number of particles (coarse grained). We consider the relationship between the coarse grained solution and the MD solution by using the continuous VIB model as a framework. A modified MD scheme is used to simulate dynamic fracture. Shock wave solutions related to the model are analyzed and numerically demonstrated. Instability in the elliptic region of the model is also expected and observed.

## Adaptive, Fast and Oblivious Convolution in Evolution Equations with Memory

*Author(s):*

M. López-Fernández

Departamento de Matemáticas, Universidad Autónoma de Madrid, C/ Francisco Tomás y Valiente 7, 28049 Madrid, Spain. E-mail: `maria.lopez@uam.es`.

C. Lubich

Mathematisches Institut, Universität Tübingen, Auf der Morgenstelle 10, D–72076 Tübingen, Germany. E-mail: `lubich@na.uni-tuebingen.de`.

A. Schädle

ZIB Berlin, Takustr. 7, D-14195 Berlin, Germany. E-mail: `schaedle@zib.de`.

To approximate convolutions which occur in evolution equations with memory terms, a variable-stepsize algorithm is presented for which advancing $N$ steps requires only $O(N \log N)$ operations and $O(\log N)$ active memory, in place of $O(N^2)$ operations and $O(N)$ memory for a direct implementation. A basic feature of the fast algorithm is the reduction, via contour integral representations, to differential equations which are solved numerically with adaptive step sizes. Rather than the kernel itself, its Laplace transform is used in the algorithm. The algorithm is illustrated on two examples: a blow-up example originating from a Schrödinger equation with concentrated nonlinearity [1] and chemical reactions with inhibited diffusion [2, 4]. Details can be found in [3], where the algorithm is also applied to a viscoelasticity model with a fractional order constitutive law.

# References

[1] R. Adami, A. Teta. A simple model of concentrated nonlinearity. *Mathematical results in quantum mechanics, Prague, Czech Republic (1998), Oper. Theory Adv. Appl., Birkhäuser, Basel.*, 108:183–189, 1999.

[2] X. Cao, K. Burrage, and F. Abdullah. A variable stepsize implementation for fractional differential equations. *Report*, 2006.

[3] M. López-Fernández, C. Lubich, and A. Schädle. Adaptive, Fast and Oblivious Convolution in Evolution Equations with Memory. *Preprint*, 2006.

[4] S. B. Yuste, L. Acedo, K. Lindenberg. Reaction front in an A+B → C reaction-subdiffusion process. *Phys. Rev. E* 69:036126, 2004.

## Construction of Conservative or Dissipative Galerkin Schemes Using Discrete Partial Derivatives

*Author(s):*

T. Matsuo
University of Tokyo

Numerical integration of a certain partial differential equations (PDEs) that have energy dissipation or conservation property, such as the nonlinear Schroedinger equation, the Korteweg-de Vries equation, or the Cahn-Hilliard equation, is considered. For such PDEs, numerical schemes that retain the energy dissipation or conservation property ("dissipative" or "conservative scheme") are generally prefered in that they often imply physically better and numerically stabler results. Thus so far many studies to seek for dissipative/conservative schemes have been done in this context. Among them, quite recently an unified approach to find dissipative/conservative Galerkin schemes has been proposed by the present author. In this talk, this approach is first briefly reviewed, and its extension and several new application examples of the approach are discussed.

## References

[1] T. Matsuo, Dissipative conservative Galerkin Method using Discrete Partial Derivatives for Nonlinear Evolution Equations, submitted,
`http://www.keisu.t.u-tokyo.ac.jp/research/techrep/data/2006/METR06-50.pdf`

## BDF Methods for Differential Riccati Equations arising in Optimal Control for Parabolic PDEs

*Author(s):*

H. Mena
Departamento de Matemáticas, Escuela Politécnica Nacional, Quito, Ecuador.

P. Benner
Fakultät für Mathematik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany.

The numerical treatment of linear-quadratic regulator problems on finite time horizons for parabolic partial differential equations (PDEs) requires the solution of large-scale differential Riccati equations (DREs), [1]. The task of solving large-scale DREs appears also in nonlinear optimal control problems of tracking type and stabilization problems for classes of nonlinear instationary PDEs based on receding horizon formulations. There, linearized problems on small time frames are solved using LQG design, [1, 4]. The coefficient matrices of the resulting DRE have a given structure (e.g. sparse, symmetric or low rank). Typically, DREs arising from discretization of parabolic PDEs exhibit stiff behavior. Thus, we investigate a matrix-valued implementation of the BDF methods [2, 3], based on a low-rank version of the alternating direction implicit (ADI) iteration for Lyapunov equations [5, 6]. Besides an efficient way of storing the solution matrices, we focus on suitable step size and order selection strategies .

## References

[1] P. Benner and S. Görner and J. Saak Numerical solution of optimal control problems for parabolicsystems In K.H. Hoffmann and A. Meyer, editors, *Parallel Algorithms and Cluster Computing. Implementations, Agorithms, and Applications.* Lecture Notes in Computational Science and Engineering, Springer-Verlag, Berlin/Heidelberg, Germany, 2006.

[2] C. Choi and A.J. Laub. Efficient matrix-valued algorithms for solving stiff Riccati differential equations. *IEEE Trans. Automat. Control*, 35:770–776, 1990.

[3] L. Dieci. Numerical integration of the differential Riccati equation and some related issues. *SIAM J. Numer. Anal.*, 29(3):781–815, 1992.

[4] K. Ito and K. Kunisch Receding Horizon Control with Incomplete Observations *SIAM J. Control Optim.*, 45(1):207–225, 2006.

[5] J.R. Li, J. White Low rank solution of Lyapunov equations *SIAM J. Matrix Anal. Appl.*, 260–280, 2002.

[6] T. Penzl A cyclic low rank Smith method for large sparse Lyapunov equations *SIAM J. Sci. Comp.*, 1401–1418, 2000.

## Linear Stability of Generalized Linear Multistep Methods for Delay Integro-Differential Equations

*Author(s):*

T. Mitsui
Professor Emeritus, Graduate School of Information Science, Nagoya Univ.

K. Mitsuda, T. Koto
Graduate School of Information Science, Nagoya Univ.

C. Suzuki
Department of Computer Science, Shizuoka Institute of Science and Technology

We are concerned with the $k$-step generalized linear multistep methods (GLMMs, [1]), which is given by

$$\begin{cases} \displaystyle\sum_{i=0}^{k} \alpha_i \boldsymbol{y}_{n+i} + h \sum_{i=0}^{k} \beta_i \boldsymbol{f}_{n+i} + h\gamma \boldsymbol{f}_{n+s} = 0, \\ \boldsymbol{y}_{n+s} = \displaystyle\sum_{i=0}^{k} \hat{\alpha}_i \boldsymbol{y}_{n+i} + h \sum_{i=0}^{k} \hat{\beta}_i \boldsymbol{f}_{n+i} \end{cases}$$

when applied to ODE $\boldsymbol{y}' = \boldsymbol{f}(x, \boldsymbol{y})$. We are interested how to apply a GLMM to the delay integro-differential equations (DIDEs) with a constant delay and what is its stability behaviour in that case. Taking the linear test equation given by

$$\boldsymbol{y}'(x) = \boldsymbol{L}\boldsymbol{y}(x) + \boldsymbol{M}\boldsymbol{y}(x-\tau) + \boldsymbol{K}\int_{x-\tau}^{x} \boldsymbol{y}(t)dt,$$

where $\boldsymbol{L}, \boldsymbol{M}, \boldsymbol{K}$ are constant complex matrices, we can conclude that the stability of GLMMs for DIDEs closely relates with that of the underlying method for ODE, provided the method is associated with an adequate quadrature rule for the integral term of the equation.

## References

[1] Mitsuda K. and Suzuki C., $A$-stable and stiffly-stable formulas in generalized linear multistep methods for ordinary differential equations, IPSJ Journal, **45**, (2004), 311–319.

[2] Zhang C. and Vandewalle S., Stability analysis of Volterra delay-integro-differential equations and their backward differentiation time discretization, J. Comput. Appl. Math., **164-165**, (2004), 797–814.

## Explicit adaptive integration of Poisson systems based on splitting

*Author(s):*

K. Modin
SKF Engineering Research Centre, Göteborg, Sweden

G. Söderlind
Department of Numerical Analysis, Lund University, Sweden

Implementation of adaptive step size control for geometric numerical integration schemes is non-trivial. Indeed, for e.g. symplectic and/or reversible methods, conventional step size strategies destroy the structure preserving properties which give their excellent long time behaviour. The common approach is instead to introduce a dynamic time transformation of the original system, and then to utilize a structure preserving discretization of the transformed system.

An explicit fully reversible integrating step size control algorithm for reversible systems is suggested in [1]. The idea is to consider an augmented dynamical system, with an additional first integral that corresponds to the step size control objective, and then to carry out explicit reversible discretization of this system. Theoretical justification is given of the good long time behaviour of the algorithm when applied to integrable reversible systems. However, when applied to Hamiltonian systems, the resulting adaptive integrator is not symplectic.

In the talk we show that, when applied to Poisson systems, the time transformed augmented system used as a basis in [1] admits a generalized Poisson structure. Furthermore, we show that the suggested methods, in particular the adaptive Störmer–Verlet scheme, can be viewed as a splitting method of such a generalized Poisson system. This allows a theoretical analysis of the resulting adaptive integrators within the framework of Poisson integrators, without considering reversibility. As a guiding example, adaptive structure preserving numerical integration of the free rigid body is demonstrated.

## References

[1] E. Hairer and G. Söderlind. Explicit, time reversible, adaptive step size control. *SIAM J. Sci. Comput.*, 26:1838–1851, 2005.

# Conformal Multi-Symplectic Integration Methods

*Author(s):*

B. Moore

The University of Central Florida

Conformal symplecticity is generalized to forced-damped multi-symplectic PDEs in 1+1 dimensions. Since a conformal multi-symplectic property has a concise form for these equations [1], numerical algorithms that preserve this property are readily available. In effect, standard multi-symplectic methods do not exactly preserve this property, but applying splitting methods in both space and time yields methods that do. (This is a generalization of preserving conformal symplecticity for ODEs [2].) Such methods work best for problems where the dissipation coefficients are small, and it is shown that standard multi-symplectic methods nearly preserve the conformal multi-symplectic property in this case. The numerical solution behavior is analyzed using a modified equations approach [4], and we find that the numerical methods behave as conformal multi-symplectic PDEs to higher order [3]. More importantly, if the dissipation coefficients are large relative to the mesh, then then the splitting methods yield incorrect rates of energy/momentum dissipation, while the standard multi-symplectic methods yield the correct rates of dissipation, provided the method is not unstable because the problem is stiff. A forced-damped semi-linear wave equation is considered as an example. Numerical results show that the structure-preserving algorithms yield more accurate solutions on long time intervals than higher order non-conservative schemes, and standard multi-symplectic methods are more advantageous than splitting methods for stiff problems.

## References

[1] T.J. Bridges and S. Reich. Multi-symplectic integrators: Numerical schemes for Hamiltonian PDEs that conserve symplecticity. *Physics Letters A*, 284:184–193, 2001.

[2] R.I. McLachlan and G.R.W. Quispel. What kinds of dynamics are there? Lie pseudogroups, dynamical systems and geometric integration. *Nonlinearity* 14:1689–1705, 2001.

[3] B.E. Moore. *A Modified Equations Approach for Multi-Symplectic Integration Methods*. PhD Thesis, University of Surrey, 2003.

[4] B.E. Moore and S. Reich. Backward error analysis for multi-symplectic integration methods. *Numer. Math.* 95:625–652, 2003.

# Uniform stability for a wide class of difference equations

*Author(s):*

Y. Muroya
Department of Mathematics, Waseda University

E. Ishiwata
Department of Mathematical Information Science, Tokyo University of Science

It is important to study the stability of numerical methods for Volterra integro-differential equations (see for example, [1]-[4]).

In this talk, we investigate the sufficient conditions for the uniform asymptotic stability of the zero solution for a wide class of difference equations, for example, the following difference equations with unbounded delays:

$$\begin{cases} x_{i+1} = qx_i - \displaystyle\sum_{j=-\infty}^{i} a_{i,j} f_{i-j}(x_j), & i = 0, 1, 2, \cdots, \\ x_j = \varphi_j, & -\infty < j \leq 0, \end{cases}$$

where $0 < q < 1$ and $f_j(x)$ $(0 \leq j < +\infty)$ belongs to a wide class of suitable functions. Considering nonlinear terms instead of linear terms of the equations (cf. [1]-[4]), we improve the known results.

## References

[1] S. N. Elaydi and S. Murakami. Asymptotic stability versus exponential stability in linear Volterra difference equations of convolution type. *J. Differ. Equations Appl.*, 2;401-410, 1996.

[2] Ch. Lubich. On the stability of linear multistep methods for Volterra convolution equations. *IMA J. Numer. Anal.*, 3;439–465, 1983.

[3] Y. Song and C. T. H. Baker. Qualitative behaviour of numerical approximations to Volterra integro-differential equations. *J. Comput. Appl. Math.*, 172;101–115, 2004.

[4] A. Vecchio. Stability of backward differentiation formulas for Volterra integro-differential equations. *J. Comput. Appl. Math.; Proceedings of the 8th International Congress on Computational and Applied Mathematics, ICCAM-98 (Leuven)*, 115;565–576, 2000.

# A new class of two step continuous methods for Ordinary Differential Equations

*Author(s):*

B. Paternoster
Dipartimento di Matematica e Informatica, University of Salerno, Italy

R. D'Ambrosio
Dipartimento di Matematica e Informatica, University of Salerno, Italy

M. Ferro
Dipartimento di Matematica e Applicazioni, University of Naples Federico II, Italy

Z. Jackiewicz
Department of Mathematics and Statistics, Arizona State University, Tempe, USA

We present a new class of two step continuous methods which provides a uniform approximation of order 2m, where m is the number of stages, for the numerical solution of ordinary differential equations. These methods were obtained using collocation approach [2, 5], by relaxing some of the collocation conditions to construct highly–stable methods [1]. We present examples of A–stable methods of order 2m with m stages for m=1 and 2. We also discuss the estimation of local discretization errors and some aspects of variable–stepsize implementation [3, 4].

## References


[1] R. D'Ambrosio, M. Ferro, Z. Jackiewicz and B. Paternoster A new class of two step continuous methods for Ordinary Differential Equations, *in preparation.*

[2] E. Hairer and G. Wanner Solving Ordinary Differential Equations II: Stiff and Differential–Algebraic Problems. *Springer.*, Berlin, 1991.

[3] Z. Jackiewicz General Linear Methods for Ordinary Differential Equations. Monograph. *in preparation.*

[4] Z. Jackiewicz and S. Tracogna A general class of two–step Runge–Kutta methods for ordinary differential equations. *SIAM J. Numer. Anal.*, 32(5):1390–1427, 1995.

[5] S. Martucci and B. Paternoster General two step collocation methods for special second order Ordinary Differential Equations, *Proceedings del 17th IMACS World Congress Scientific Computation, Applied Mathematics and Simulation*, Paper T2-R-00-0131, 2005.


# The Adaptive Biasing Force Method: from efficient calculations of free energies to chemical kinetics


*Author(s):*

A. Pohorille

NASA-Ames Research Center and Department of Pharmaceutical Chemistry, University of California, San Francisco

E. Darve

Mechanical Engineering Department and Institute for Computational and Mathematical Engineering, Stanford University


Calculating free energy in computer simulations is of central importance in statistical mechanics of condensed media and its applications to chemistry and biology not only because it is the most comprehensive and informative quantity that characterizes the equilibrium state, but also because it often provides an efficient route to access dynamic and kinetic properties of a system.

One approach that guarantees nearly optimal efficiency of calculating free energy along a generalized coordinate or on a low dimensional manifold is the Adaptive Biasing Force (ABF) method, recently developed by Darve and Pohorille and applied by several authors to such challenging problems as protein unfolding, protein-protein associations and solute transport across membrane channels. In some instances ABF has been shown to improve efficiency of free energy calculations, compared to alternative methods, by a few orders of magnitude.

ABF consists of two steps: (1) solving a general problem of calculating the thermodynamic force along the specified generalized coordinates in unconstrained dynamics or metadynamics, and (2) subtracting the position-dependent average force from the instantaneous force in an adaptive manner. As a result, the specified coordinates are sampled uniformly. To obtain the free energy changes, the calculated average force is integrated along the coordinates of interest. Recently, we developed a new formulation of ABF, in which the free energy is obtained from first derivatives with respect to the selected generalized coordinates and time only. This not only simplifies calculations but establishes a formal analogy between the statistical equations for the average force and Newton's equations of motion.

Since the ABF procedure eliminates the systematic force acting along the specified coordinates, several dynamic properties, such as position dependent diffusion coefficient, can be estimated directly. From this knowledge, reaction rates can be calculated for a broad class of processes that can be approximated as diffusion in the potential of mean force. We will discuss this approach in examples of protein insertion into membrane mimetic and ion transport through membrane protein channels.

# On solving DAE IVPs with defect-based error control


*Author(s):*

J.D. Pryce

Dept of Information Systems, Cranfield University, Shrivenham Campus, Swindon, UK.

N.S. Nedialkov

Dept of Computing and Software, McMaster University, Hamilton, Canada

W.H. Enright

Dept of Computer Science, University Of Toronto, Canada

N.S. Nedialkov has written a C++ code DAETS to solve differential algebraic equation systems (DAEs) by Taylor series, using the structural analysis pioneered by the speaker, see [3, 4, 5] for theory. The method works on many common classes of DAEs found in practice (though not on all) and DAETS has proved robust and efficient on many examples. To control error in the numerical solution of ODEs, an approach based on monitoring the defect (residual) of an approximate solution is becoming increasingly popular. A defect approach for DAEs appears illuminating, both for comparing different error control strategies and as a strategy in itself. It seems to have first been studied by Enright and Nguyen in 1995 for the semi-explicit index 1 and index 2 case [1]. It is also close to the method used by Ilie, Corless & Reid in 2006 to prove that the complexity of the numerical solution of semi-explicit index 1 DAEs is polynomial in the number of digits of accuracy [2]. This talk shows how the Enright and Nguyen error control can be extended to any DAE that is successfully handled by Pryce's structural analysis method. We are currently planning to test this strategy in DAETS. It also describes how the Ilie complexity result may be extended to apply to an implementation of DAETS that employs this extended error control strategy.

# References

[1] W.H. Enright and H. Nguyen. Defect-based error control schemes for algebraic differential equations. Unpublished technical report, Dept of Computer Science, University of Toronto, Sept. 1995.

[2] S. Ilie, R.M. Corless and G. Reid. Numerical solutions of index-1 differential algebraic equations can be computed in polynomial time. *Numerical Algorithms*, 41:161–171, 2006.

[3] J.D. Pryce. A simple structural analysis method for DAEs. *BIT*, 41:364–394, 2001.

[4] N. S. Nedialkov and J. D. Pryce Solving Differential-Algebraic Equations by Taylor Series (I): Computing Coefficients. *BIT*, 45:561–591, 2005.

[5] N. S. Nedialkov and J. D. Pryce Solving Differential-Algebraic Equations by Taylor Series (II): Computing the System Jacobian. Technical report CAS-05-05-NN, Dept. of Computing and Software, McMaster University, Hamilton, ON, L8S 4L7, Canada, August 2005. To appear in BIT.

# The Stochastic-$\alpha$ Method for Time Integration of Noisy Second Order Dynamics

*Author(s):*

S. Raha

Supercomputer Education and Research Centre, Indian Institute of Science, Bangalore 560012, INDIA

N. Rajan

Supercomputer Education and Research Centre, Indian Institute of Science, Bangalore 560012, INDIA

Unmodeled dynamics and structural behavior in engineering systems contribute to both additive and multiplicative noise. For micro-mechanical systems taking the noise in to account for numerical simulation is essential in order to get estimates of design behavior after manufacturing, thus affecting yield and performance index when operating as sensors. Electrical systems like interconnects on sub-65nm VLSI CMOS design are subjected to process variations so that the noise and uncertainties must be taken into account for interconnect simulation. Modeling of these engineering applications yields second order Stochastic Differential Equations (SDE). In the present work we shall consider equations of the form (in Itô sense)

$$dx = v\,dt \tag{23}$$

$$dv = f(x,v,t)dt + B(x,v,t)\,dW_t \tag{24}$$

where $x, v \in \mathbb{R}^n$, $f : \mathbb{R}^n \times \mathcal{T} \to \mathbb{R}^n$, $B : \mathbb{R}^n \times \mathcal{T} \to \mathbb{R}^{n\times m}$, $t \in \mathcal{T}$; and $\mathcal{T}$ is the time interval $[t_0, t_f]$. Also, $W_t$ is a $m$-dimensional Wiener Process. $B$ is the diffusion coefficient. Such second order engineering systems are often stiff and oscillatory in the drift term $f$. Numerical method for integration of such systems thus needs to handle oscillation efficiently through some reasonable numerical damping. For deterministic dynamical systems, the well-known generalized-$\alpha$ method of Hulbert and Chung and similar schemes have been developed to meet the above requirements and achieve

computational efficiency in terms of numerically damping small amplitude high frequency responses. The generalized $\alpha$ method is stable almost everywhere on the complex plane except two small intervals on the real axis and can take large time step sizes fixed over almost the entire interval of integration. In this work, the stochastic version of the generalized $\alpha$-method is developed with a view to achieving the same efficiency for noisy (especially with multiplicative noise) dynamical systems. The stochastic version uses the special structure of the equations for construction of the numerical scheme to strong order 2.0 accuracy in $x$. The method is stochastically stable for sufficiently small step sizes over the same stability region as its deterministic version. It has efficient (with respect to time step size) stochastic stability in the mean and mean-square. The user-selectable damping parameter introduces stochastic contractivity. This in turn can be used to calibrate the expected numerical dissipation in the method and also deal with small multiplicative noise efficiently. Numerical examples are presented to illustrate the scheme.

## Design of DIRK schemes for solving the incompressible Navier-Stokes-equations

*Author(s):*

J. Rang

Institute for scientific computing, TU Braunschweig, Germany, j.rang@tu-bs.de

The Crank-Nicolson and the fractional-step-$\theta$-scheme are widely used to solve the incompressible Navier-Stokes equations [4, 1]. Both methods can be formulated as diagonal-implicit Runge-Kutta methods (DIRK-methods) [2]. In this context an embedded formula for the fractional-step-$\theta$-scheme can be designed [3] such that automatic time stepsize control is possible.

But unfortunately this scheme has the disadvantage that the convergence order for the pressure component drops down to one. Therefore in this talk new diagonal-implicit Runge-Kutta methods for semi-explicit PDAEs of index 2 are presented. These solvers are stiffly accurate, of order 3 for the ODE-variables and of order 2 for the algebraic variables. They have three and four internal stages and automatic steplength control by the help of embedding is possible. The methods with four internal stages have a stiffly accurate embedded method of order 2 for all variables. The methods are applied on the incompressible Navier-Stokes equations and compared with other DIRK-methods.

## References

[1] V. John. *Large Eddy Simulation of Turbulent Incompressible Flows. Analytical and Numerical Results for a Class of LES Models*, volume 34 of *Lecture Notes in Computational Science and Engineering*. Springer-Verlag Berlin, Heidelberg, New York, 2003.

[2] Rang, J.: A note on implicit $\theta$-schemes applied on the Navier-Stokes-equations. Preprint 06-40, Fakultät für Mathematik, Otto-von-Guericke-Universität Magdeburg (2006)

[3] Rang, J.: Automatic step size selection for the fractional-step-$\theta$-scheme. Preprint 06-45, Fakultät für Mathematik, Otto-von-Guericke-Universität Magdeburg (2006)

[4] S. Turek. *Efficient Solvers for Incompressible Flow Problems: An Algorithmic and Computational Approach*, volume 6 of *Lecture Notes in Computational Science and Engineering*. Springer, 1999.

## Efficient Runge–Kutta methods for stochastic differential equations and mean-square stability analysis

*Author(s):*

A. Rößler

Technische Universität Darmstadt, Fachbereich Mathematik, Schloßgartenstr. 7, D-64289 Darmstadt, Germany

The numerical analysis of stochastic differential equations (SDEs) is very different compared to that of ordinary differential equations (ODEs) due to the stochastic calculus. In the present talk, a new class of stochastic Runge-Kutta (SRK) methods for the weak approximation of the solutions of SDEs is introduced. Conditions for weak convergence with order one and two are calculated explicitly. Therefore, the colored rooted tree analysis for SRK methods converging in the

weak sense is applied [3]. As the main novelty, the introduced class turns out to have significantly lower complexity than well known second order SRK schemes. The reduction of the computational effort is improved considerably especially for high dimensional SDE systems with an multi-dimensional driving Wiener process. Such problems are typical for many applications like computational finance or physics.

The stability features of a numerical scheme are of special importance if the scheme is applied to some stiff problem. Therefore, we analyse the mean-square stability (MS-stability) of the introduced SRK schemes. Further, some coefficients for implicit SRK schemes of weak order two are presented and their mean-square stability is analysed as well [1]. The stability functions are calculated and the domains of MS-stability for some linear test equation with multiplicative noise are presented. This is joint work with K. Debrabant.

## References


[1] K. Debrabant and A. Rößler. Mean–square stability of diagonally drift–implicit Runge–Kutta methods for the weak approximation of stochastic differential equations. *TU Darmstadt*, 2007. (submitted)

[2] A. Rößler. Runge-Kutta Methods for Itô Stochastic Differential Equations with Scalar Noise. *BIT*, 46:97–110, 2006.

[3] A. Rößler. Rooted Tree Analysis for Order Conditions of Stochastic Runge-Kutta Methods for the Weak Approximation of Stochastic Differential Equations. *Stochastic Anal. Appl.*, 24:97–134, 2006.

[4] A. Rößler. Runge-Kutta methods for Stratonovich stochastic differential equation systems with commutative noise. *J. Comput. Appl. Math.*, 164–165:613–627, 2004.


# Stabilizing with a hammer


*Author(s):*

J.M. Sanz-Serna

Universidad de Valladolid, Valladolid, Spain


It has been known for almost a hundred years that an inverted pendulum (with the bob above the suspension point) does not fall if it is subjected to violent vertical oscillations. The underlying principle possesses many applications, including the confinement of charged particles by means of oscillatory electric fields (the Paul's trap that was awarded the 1989 Physics Nobel prize).

I shall study the stabilization of unstable oscillators when they are subjected to violent shocks, including the stochastic case where the waiting time between shocks is a random variable.

# Time-integration methods for high-order discontinuous Galerkin discretisation of the wave equation


*Author(s):*

D. Sármány

Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, Netherlands

M. A. Botchev

Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, Netherlands

J. J. W. van der Vegt

Department of Applied Mathematics, University of Twente, P.O. Box 217, 7500 AE Enschede, Netherlands


The discontinuous Galerkin (DG) method is a powerful tool for approximating partial differential equations which model problems in physics, especially in fluid dynamics and electrodynamics. When the solution is comparatively smooth (e.g. in wave propagation phenomena), it is known that the use of higher-order elements can result in a reduced number of degrees of freedom to achieve a given accuracy. It is not always clear, however, what is the best choice of time-integration methods when we need to solve the semi-discrete system resulting from such discretisation. In order to retain the accuracy of the spatial approximation, one can either use a high-order time-integration method or apply a lower-order scheme and keep the size of the time step small.

In this work–whose details can be found in [3]–we discretise the wave equation in space using the high-order DG method introduced in [1], and we investigate the computational performance of some feasible candidates for time integration. We find that the best choice–perhaps unsurprisingly–is a time-integration method of one order higher than that of the polynomials used in the spatial discretisation. In our case, this is the family of strong-stability-preserving Runge-Kutta (SSP-RK) methods taken from [2]. A numerical Fourier analysis is carried out for the fully discrete system which results from combining the DG discretisation with this time-integration scheme. Although the scheme is both dispersive and dissipative, we show that their corresponding errors converge faster than the error measured pointwise in the $l^2$-norm.

## References


[1] J. S. Hesthaven and T. Warburton. Nodal high-order methods on unstructured grids. I. Time-domain solution of Maxwell's equations. *J. Comput. Phys.*, 181(1):186–221, 2002.

[2] M.-H. Chen, B. Cockburn and F. Reitich. High-order RKDG methods for computational electromagnetics. *J. Sci. Comput.*, 22/23:205–226, 2005.

[3] D. Sármány, M. A. Botchev and J. J. W. van der Vegt. Dispersion and dissipation error in high-order Runge-Kutta discontinuous Galerkin discretisation of the Maxwell equations. Memorandum 1821 Department of Applied Mathematics, University of Twente, Enschede, http://eprints.eemcs.utwente.nl/9168/, submitted to *J. Sci. Comput.*


# Parallel starting procedure for explicit parallel peer two-step methods


*Author(s):*

B.A. Schmitt
University of Marburg, Germany

R. Weiner
University of Halle-Wittenberg, Germany


Parallel peer methods may be quite efficient both in stiff and non-stiff initial value problems and are competitive with standard software in realistic problems, [1]. An explicit parallel peer two-step method uses $s$ stages of equal order and needs $s$ parallel function evaluations of the right-hand side followed by one matrix multiplication and may be implemented in parallel on $s$ processors. However, due to their two-step structure peer methods still relied so far on one-step methods for the computation of its stages in the first step [2]. We describe a parallel starting procedure for explicit peer methods with $s$ parallel Euler steps, where lower order error terms are eliminated in subsequent steps by adjusting certain method parameters achieving full order $s$ after $s-2$ steps ($s \leq 8$). From the information of the initial Euler steps estimates for the starting stepsize are obtained, as well. We also comment on the precise structure of the local error if the stepsize is changed and on appropriate modifications of the stepsize selection scheme. Numerical tests with some expensive problems using OpenMP are included.

## References


[1] B. A. Schmitt, R. Weiner, H.Podhaisky, *Multi-implicit peer two-step W-methods for parallel time integration*, BIT 45 (2005), 197-217.

[2] R. Weiner, K. Biermann, B. A. Schmitt, H.Podhaisky, *Explicit two-step peer methods*, to appear in Comput. Math. Appl.


# Towards nanomechanics of biomolecules


*Author(s):*

Ch. Schütte
Freie Universität Berlin, Institute of Mathematics II

The talk will present a method for learning coarse grained nanomechanical properties (like stiffness along the backbone or effective friction wrt. the heat bath) of peptides, small proteins and DNA fragments from extensive molecular dynamics simulations. The method is efficient for large dimensions, even if multiple conformations of the molecule under consideration have to be explored. The mathematical background as well as applications of the technique to a DNA fragment will be presented.

## Interpolation in Special Orthogonal Groups

*Author(s):*

T. Shingel

DAMTP, Centre for Mathematical Sciences, University of Cambridge

Construction of smooth interpolating curves in non-Euclidean spaces is an interesting theoretical problem which finds many applications in engineering and physics. In the present work, we address the question of interpolating points in Lie groups, focusing on a special orthogonal group SO($n$) due to its practical importance. Our technique is based on the connection between the group and its Lie algebra of skew-symmetric matrices and the fact that the exponential map is onto. There exists several methods and algorithms which solve the interpolation problem. In the case of the SO(3) group, various re-parametrizations of rotation matrices (e.g. rotation axes and angles, unit quaternions) are adopted and cubic spline interpolation is performed on such representations. Very common are modifications of the De Casteljau algorithm, in which the key idea is to replace linear interpolation by geodesic interpolation. However, many of the existing algorithms are applied only to localized set of data points, which we believe falls short of having an adequate approach, since the interpolation problem becomes particularly interesting and challenging in a global sense. Our goal is to develop a computationally inexpensive multi-purpose algorithm.

## Adaptive methods for stochastic differential-algebraic equations

*Author(s):*

T. Sickenberger

Humboldt-Universität zu Berlin, Department of Mathematics, 10099 Berlin, Germany.

R. Winkler

Humboldt-Universität zu Berlin, Department of Mathematics, 10099 Berlin, Germany.

Stochastic differential-algebraic equations (SDAEs) arise as a mathematical model for electrical network equations that are influenced by additional sources of Gaussian white noise.

We discuss adaptive linear multi-step methods for their numerical integration, in particular stochastic analogues of the trapezoidal rule and the two-step backward differentiation formula. We study mean-square consistency, stability in the mean-square sense and we obtain conditions that ensure mean-square convergence for the special case of one- and two-step Maruyama schemes (see [2]). In the case of small noise we develop a local error analysis in terms of the step-size and a small parameter, where the latter quantifies the size (smallness) of the noise. We present a strategy for controlling the step-size in the numerical integration. It is based on estimating the mean-square local errors and leads to step-size sequences that are identical for all simultaneously computed paths (see [1] and [3]).

Secondly, we describe and analyze an algorithm which controls the time as well as the chance discretization. It calculates the optimal number of paths and guarantees a good approximation of the mean-square of the local error. Based on the idea of forward selection in scenario reduction, we select some typical solutions and use them to expand or to reduce the computed paths which directly results in a solution path tree.

We illustrate the potential of the step-size control strategy together with the solution path tree by simulation results for drift-implicit schemes applied to test-SDEs and real-life problems in circuit simulation.

# References

[1] W. Römisch and R. Winkler. Stepsize control for mean-square numerical methods for stochastic differential equations with small noise. *SIAM J. Sci. Comp.*, 28(2):604–635, 2006.

[2] T. Sickenberger. Mean-square convergence of stochastic multi-step methods with variable step-size. To appear in *J. Comput. Appl. Math.*, 2007.

[3] T. Sickenberger, E. Weinmüller and R. Winkler. Local error estimates for moderately smooth problems: Part II - SDEs and SDAEs. Preprint 07-07, Institut für Mathematik, Humboldt-Universität zu Berlin, 2007, and submitted (Part I is published in BIT).

## Functionally fitted explicit pseudo two-step Runge–Kutta methods

*Author(s):*

R.B. Sidje

Advanced Computational Modelling Centre, Department of Mathematics, University of Queensland, Brisbane QLD 4072, Australia. rbs@maths.uq.edu.au.

N.S. Hoang

Department of Mathematics, Kansas State University, Manhattan, KS 66502, USA. nguyenhs@math.ksu.edu.

Explicit pseudo two-step Runge–Kutta (EPTRK) methods belong to the wider class of general linear multistep methods. The particularity of EPTRK methods is that they do not use the last two iterates as conventional two-step methods do. Rather, they predict the intermediate stage values and combine them with the last iterate to obtain the next iterate. EPTRK methods were primarily designed to suit parallel computers [1, 2], but they have been shown to achieve arbitrary high-order and thus can be useful as conventional explicit RK methods on sequential computers as well. We present a new family of functionally fitted EPTRK (FEPTRK) methods aimed at integrating an equation exactly if its solution is a linear combination of a chosen set of basis functions [3, 4, 5]. When the basis functions are chosen as the mononials, the algebraic EPTRK methods are recovered. We use a variation of collocation techniques to show that the new generalized FEPTRK family shares the same accuracy properties as EPTRK. The added advantage is that FEPTRK methods can use specific fitting functions to capitalize on the special properties of the problem that may be known in advance.

## References

[1] N.H. Cong. Explicit pseudo two-step Runge-Kutta methods for parallel computers. *Int. J. Comput. Math*, 73:77–91, 1999.

[2] N.H. Cong, H. Podhaisky, and R. Weiner. Numerical experiments with some explicit pseudo two-step RK methods on a shared memory computer. *Math. Applic.*, 36(2):107–116, 1998.

[3] N.S. Hoang, R.B. Sidje, and N.H. Cong. On functionally-fitted Runge-Kutta methods. *BIT*, 46:861–874, 2006.

[4] N.S. Hoang, R.B. Sidje. Functionally fitted explicit pseudo two-step Runge–Kutta methods In preparation, 2007.

[5] K. Ozawa. Functional fitting Runge-Kutta method with variable coefficients. *Japan J. Indust. App. Math*, 18:105–128, 2001.

## Do we know WENO?

*Author(s):*

R.J. Spiteri

Department of Computer Science, University of Saskatchewan, Saskatoon, SK, Canada

R. Wang

Department of Computer Science, University of Saskatchewan, Saskatoon, SK, Canada

The weighted essentially non-oscillatory (WENO) methods are popular spatial discretization methods for hyperbolic partial differential equations; see, e.g., [2, 1]. These methods are adept at handling the non-smooth features that arise in the solutions to hyperbolic PDEs. For example, although these methods are formally first-order accurate once a shock is present, they still have uniform high-order accuracy right up to the location of the shock [1]. In this talk I will describe some analysis showing that the combination of the widely used fifth-order WENO spatial discretization (WENO5) and the forward Euler time integration method is linearly unstable when numerically integrating hyperbolic conservation

laws. Consequently it is not convergent. Furthermore it can be shown that all two-stage, second-order explicit Runge–Kutta (ERK) methods are linearly unstable (and hence do not converge) when coupled with WENO5. Also all optimal first- and second-order strong-stability-preserving (SSP) ERK methods are linearly unstable when coupled with WENO5. Moreover the popular three-stage, third-order SSP(3,3) ERK method offers no linear stability advantage over non-SSP ERK methods, including ones with negative coefficients, when coupled with WENO5. I present new linear stability criteria for combinations of WENO5 with general ERK methods *of any order*. A sufficient condition for the combination of an ERK method and WENO5 to be linearly stable is that the linear stability region of the ERK method should include the part of the imaginary axis of the form $[-\iota\mu, \iota\mu]$, for some $\mu > 0$. The linear stability analysis also provides insight into the behaviour of ERK methods applied to nonlinear problems and problems with discontinuous solutions. I confirm the assertions of the analysis by means of numerical examples.

Details can be found in the forthcoming paper [3].

# References


[1] G.-S. Jiang and C.-W. Shu, Efficient implementation of Weighted ENO schemes, *J. Comput. Phys.*, 126 (1996), pp. 202–228.

[2] X.-D. Liu, S. Osher, and T. Chan, Weighted essentially non-oscillatory schemes, *J. Comput. Phys.*, 115 (1994), pp. 200–212.

[3] R. Wang and R.J. Spiteri, Linear instability of the fifth-order WENO method, *SIAM J. Numer. Anal.* (to appear).


## Process simulation for sewer systems by a splitting approach


*Author(s):*

G. Steinebach
Bonn-Rhein-Sieg University of Applied Sciences

P. Rentrop, S. Seidl
Munich University of Technology

M. Paffrath, R. Rosen
Siemens AG


Chemical and biological reactions in sewer systems may lead to undesired effects like strong smell or corrosion. These reactions can sometimes be prevented by the injection of additional chemicals into the sewer system. The final objective is the optimization of this expensive addition of chemicals.
In a first step a simulation model must be developed, which can be divided into two parts: A flow model and a model describing the transport and reaction. Moreover these models for the single channel reaches must be coupled to a whole channel network. Comments on an appropriate treatment of the coupling conditions can be found in [2].
Since it is assumed that the chemical substances have no influence on the flow behaviour, the flow solver can be applied at first. The flow is assumed to have a free surface and is described by the well known Saint-Venant equations for channel or river flow [3]. The space discretization scheme is based on the splitting of the Saint-Venant equations in quasilinear and nonlinear components. This approach is advantageous for channels or rivers with strongly varying bottom elevation and cross sections. In the talk numerical results for several test problems and different time-integration schemes are discussed.
The transport and reaction of the chemical substances is described by suitable advection-diffusion-reaction equations. These equations are treated by an appropriate splitting in stiff and nonstiff parts [1]. Numerical results of a case-study with eigth chemical reaction equations are presented.

# References


[1] W. Hundsdorfer, J.G. Verwer, Numerical solution of advection-diffusion-reaction equations, *Springer Series in Comput. Math.* **33**, (2003).

[2] G. Steinebach, S. Rademacher, P. Rentrop, M. Schulz, Mechanisms of coupling in river flow simulation systems. *Journal of Computational and Applied Mathematics* **168(1-2)**, (2004), 459-470.

[3] J.J. Stoker, Water waves, the mathematical theory with applications, *Interscience Publishers Inc.*, New York, 1957.

## Energy-preserving numerical methods for multi-symplectic Hamiltonian systems

*Author(s):*

Y. Sun
Academy of Mathematics and Systems Science,
Chinese Academy of Sciences,
PoBox 2719, Beijing 100080, China

J. Hong
Academy of Mathematics and Systems Science,
Chinese Academy of Sciences,
PoBox 2719, Beijing 100080, China

Discrete gradient integrators are established in [1] for computing the integral-preserving ODEs. In [2, 3], the integrators are bootstrapped to higher order. In this talk, we observe the discrete gradient integrators and apply it to multi-symplectic Hamiltonian systems. The energy-preserving numerical methods for multi-symplectic Hamiltonian systems are constructed and the numerical experiments are presented.

## References

[1] R. McLachlan, R. Quispel and R. Robidoux, Geometric integration using discrete gradient *Phil. Trans. R. Soc. A*, 357:1021–45, 1999.

[2] D. McLaren and R. Quispel, Integral-preserving integrators, *J. Phys. A: Math. Gen.* 37: 489-95, 2004.

[3] D. McLaren and R. Quispel, Boostrapping discrete-gradient integral-preserving integrators to fourth order, 2006, preprint

## Generalized Adams methods revisited

*Author(s):*

Per Grove Thomsen
Informatics and Mathematical Modelling, Danish Technical University, Lyngby, Denmark

The Generalized Adams Methods were introduced by Nørsett [2, 3] and have been further discussed by several authors [1]however an efficient combination in the choice of method parameters and implementation details have not been found. It is the intention of the present paper to fill this gap. In the present paper we consider methods for solving systems of ODEs that appear often in practical applications. The methods have been applied to large scale problems in air pollution modelling where the system consists of transport equations coupled to equations for chemical reactions. In other applications the systems may have some parts that are uncoupled from other parts and these have often been solved by splitting techniques. The present approach makes use of a transformation of the system that reduces the stiffness of the resulting equations. By introducing rational approximations to the exponential of the *Multiple Padé* type we construct an Adams type of method with rational coefficients suitable to systems of high dimensions with sparse Jacobian matrices. As a benchmark test we have selected the pollution problem of [5]. Rational approximations to the matrix exponential is discussed in [6].

## References

[1] J.D. Lawson, *Generalized Runge Kutta Processes for stable systems with large Lipschitz Constants.* ,SIAM J.NA. vol 4 pp. 372 - 380, 1967.

[2] S.P. Nørsett, *Generalized Adams methods* , NTH 1969

[3] S.P. Nørsett and P.G. Thomsen,*Imbedded SDIRK-Methods of basic order three*,BIT, 24, (1984) , p. 634-646.

[4] J.C. Butcher,*The numerical analysis of ordinary differential equations. Runge Kutta and general linear methods*, John Wiley & sons , 1987.

[5] W.M.Lioen and J.J.de Swart, *Test set for initial value problem solvers*, Report MAS-R9832, December 1998, CWI.

[6] C.B. Moler and C.F. Van Loan,*Nineteen Dubious Ways to Compute the Exponential of a Matrix*, SIAM Review vol. 20, pp. 801-836, 1978.

## Magnetohydrodynamic (MHD) Simulations Using Exponential Integrators.

*Author(s):*

M. Tokman
University of California, Merced

Large scale behavior of many astrophysical and laboratory plasmas can be modeled using the system of resistive MHD equations. Due to stiffness, solving this system numerically is a challenging task. In this talk, we discuss how exponential integrators help to more efficiently integrate resistive MHD equations over long time intervals compared to standard explicit and implicit methods. We compare performance of several time integrators on demonstrative examples and present a new three-dimensional model of plasma driven by the boundary motions. This model suggests a new paradigm for describing the evolution of driven large-scale plasma configurations. These simulations provide a better understanding of self-organization of plasmas relevant to phenomena such eruptive activity in the solar corona and the dynamics of plasma in laboratory experiments.

## An algorithm for the construction of complex invariant sets for linear discrete dynamical systems

*Author(s):*

C. Vagnoni
Dipartimento di Matematica Pura e Applicata, Università di Padova, via Trieste 63, 35121 Padova, Italy, vagnoni@math.unipd.it

M. Zennaro
Dipartimento di Matematica e Informatica, Università di Trieste, Via A. Valerio 12/1, 34127 Trieste, Italy, zennaro@univ.trieste.it

The asymptotic behavior of the solutions of a discrete linear dynamical system $x^{(k+1)} = A^{(k)}x^{(k)}$, $k \geq 0$ and $x^{(0)}$ given, is related to the spectral radius $\rho$ of its associated family $\mathcal{F} = \{A^{(k)}\}_{k\geq 0}$. In particular, a system is stable if $\rho \leq 1$ and the family $\mathcal{F}$ is non-defective. In turn, this is equivalent to the existence of an extremal norm, which is an invariant subset for the family $\mathcal{F}$. This kind of systems is important for a large number of applications. In particular, we mention the stability analysis of numerical methods for ordinary differential equations.

In the last decades some algorithms have been proposed in order to find real extremal norms of polytope type in the case of finite families $\mathcal{F}$ (see for example [BT79] and [GZ05]). Anyway, recently it has been observed that it is more useful to consider complex polytope norms (see for example [GWZ05] and [MiSa06]). In this talk, using the theory developed in [GZ07], we extend the algorithm for the construction of the unit ball of real polytope norms to the complex space. However, due to the significant increase in the complexity of the problem, we confine ourselves to examine the two-dimensional case.

## References

[BT79] R.K. Brayton, C.H. Tong, *Stability of dynamical systems: a constructive approach*, IEEE Trans. Circuits Systems, vol.26, pp 224-234, 1979.

[GWZ05] N. Guglielmi, F. Wirth, M. Zennaro, *Complex polytope extremality results for families of matrices*, SIAM J. Matrix Analysis Appl., 27:721-743, 2005.

[GZ05] N. Guglielmi, M. Zennaro, *An algorithm for finding extremal polytope norms of matrix families*, Linear Algebra Appl. (to appear).

[GZ07] N. Guglielmi, M. Zennaro, *Balanced complex polytopes and related vector and matrix norms*, J. Convex Anal., 14, 2007 (to appear).

[MiSa06] S. Miani, C. Savorgnan, *Complex polytopic control Lyapunov functions*, "45th IEEE Conference on Decision and Control", San Diego, CA, USA, 13-15 December 2006, 3198–3203.

# Numerically Optimal Runge–Kutta Pairs and Interpolants

*Author(s):*

J. Verner

Department of Mathematics, Simon Fraser University, Burnaby, Canada (jverner@pims.math.ca)

Since Fehlberg [1] derived pairs of Runge–Kutta methods of adjacent high orders to provide an error estimate at each step, optimal pairs have been selected by attempts to minimize the 2-norm of the local truncation error coefficients of the higher order method. From a modification designed by the author [3], various types of pairs have been classified [4], and algorithms for many of these types have been developed (See [5]). In attempts to reduce the LTE 2-norm, modifications and different types of pairs of methods have been developed by other authors (e.g. [2]). This presentation suggests other attractive features of a pair that can and should be considered in a selection of optimal pairs. The author's algorithms are used to obtain pairs of order p and p-1, p = 6,7,8,9, with interpolants of the same orders that are 'numerically optimal' (LTE 2-norm is small), and with some compromise, some formulas have additional attractive features. For these, the LTE 2-norms are lower than those of previously published formulas, numerically optimal interpolants are provided, and all coefficients can be obtained exactly. (In practice, 40 digit approximations are provided at (www.math.sfu.ca/~jverner), and more accurate coefficients can be provided to interested researchers by email on request.)

While coefficients on the author's website provide 'most efficient' and 'most robust' algorithms which might be used to improve the efficiency of existing software for initial value problems, one of the principal motivations for this project was to obtain the 'most accurate' algorithms possible which may be applied to standard test problems to order to calibrate corresponding test results obtained from two-step Runge–Kutta methods now under development.

## References

[1] E. Fehlberg, *Klassische runge–Kutta-Formeln fünfter und siebenter Ordnung mit Schrittweiten-Kontrolle*, Computing **4** (1969), pp. 93–106.

[2] Ch. Tsitouras, *Optimized explicit Runge–Kutta pair of orders 9(8)*, Appl. Num. Math. **38** (2001), pp. 123–134.

[3] J.H. Verner, *Explicit Runge–Kutta methods with estimates of the local truncation error*, SIAM J. Numer. Anal. **15** (1978), pp. 772–790.

[4] J.H. Verner, *A classification scheme for studying explicit Runge–Kutta pairs*, Scientific Computing: Proc. of the Fifth International Conference, 27-31 January, 1972, Benin City, Nigeria. Ed. S.O. Fatunla, Ada Jane Press, Benin City, Nigeria (1994), pp. 201–225.

[5] J.H. Verner, *High-order explicit Runge–Kutta pairs with low stage order*, Applied Numerical Mathematics **22** (1996), pp. 345-357.

# Dynamics of the generalized Euler equations on Virasoro groups

*Author(s):*

Xingyou Zhang

IFS, Massey University, New Zealand

Robert McLachlan

IFS, Massey University, New Zealand

Since Arnold's pioneering work [1], introducing the geometric approach to study the Euler fluid equation, many papers (e.g., the references in [2]) are devoted to the study of genralised Euler equations.

Let $\mathcal{D}(S^1)$ be the group of orientation preserving Sobolev $H^s$ diffeomorphisms of the unit circle $S^1$, then $\mathcal{D}(S^1)$ has a non-trivial one-dimensional central extension, the Bott-Virasoro group $\widehat{\mathcal{D}}(S^1)$ with the Virasoro algebra $\widehat{Vect}^s(S^1)$, in which the commutator is given by

$$[\widehat{U},\widehat{V}] \equiv \left((u_x v - u v_x)\frac{\partial}{\partial x},\ c(u,v)\right), \quad \text{with } c(u,v) \equiv \int_{S^1} u\partial_x^3 v \mathrm{d}x, \tag{25}$$

where $\widehat{U} = (u\frac{\partial}{\partial x}, a), \widehat{V} = (v\frac{\partial}{\partial x}, b) \in \widehat{Vect}^s(S^1)$ with $a, b \in \mathbb{R}$.

It is known now that the Euler equation on the Virasoro algebra for the $L^2$ metric (or equivalently, the geodesic equation on the Virasoro group of the right invariant metric which is $L^2$ metric at the identity) is the KdV equation [2], and the Euler equation for the $H^1$ metric is the Fuchssteiner-Fokas-Camassa-Holm equation [4]. Recently, A. Constantin et al [3] showed that on the Virasoro group, only the Euler equations for the $L^2$ metric and the $H^1$ metric are bi-Hamiltonian systems (see also [4]).

We study the dynamics of the generalized Euler equations on Virasoro groups $\widehat{\mathcal{D}}(S^1)$ with different Sobolev $H^k$ metric ($k \geq 2$) on the Virasoro algebra, i.e.,

$$m_t + 2u_x m + u m_x = a\partial_x^3 u \qquad \text{on } S^1, \quad \text{with } m = A_k u, \tag{26}$$

where the operator $A_k = 1 - \partial_x^2 + \cdots + (-1)^k \partial_x^{2k}$, $k$ is a positive integer and $a \in \mathbb{R}$.

We first prove that the solutions to generalized Euler equations will not blow up in finite time and then study the stability of some trivial solutions.

# References


[1] V. Arnold. Sur la géométrie différentielle des groupes de Lie de dimension infinie et ses applications à l'hydrodynamique des fluides parfaits. *Ann. Inst. Fourier*, 16:316-361, 1966.

[2] V. Arnold and B. Khesin. Topological methods in Hydrodynamics, Springer-Verlag, New York, 1998.

[3] A. Constantin, B. Kolev. Integability of invariant metric on the diffeomorphism groups of the circle. *Journal of Nonlinear Science*, 16:109-122, 2006.

[4] B. Khesin and G. Misiołek. Euler equations on homogeneous spaces and Virasoro orbits. *Advances in Mathematics*, 176:116-144, 2003.

[5] G. Misiołek. Conjugate points in the Bott-Virasoro group and the KdV equation. *Proceedings of AMS*, 125:935-940, 1997.


# Precise integration for the time-dependent Schrodinger equation with periodic Hamiltonians


*Author(s):*

Suying Zhang



The precise integration method proposed for linear-invariant dynamical system can give precise numerical result approaching to the exact solution at the integration points. In this paper, precise integration methods for time-dependent Schrodinger equation with periodic Hamiltonians are presented based on Magnus expansion of the solution of the system. The methods only calculate one exponential matrix. So these methods are cheap and easy to implement. And they can preserve many of the qualitative properties of the exact solution.