ICMAT Workshop

Topics in Numerical Analysis for Differential Equations (TNADE2013)

July 8-12, 2013

Sergio BLANES¹ · Fernando CASAS² ·
Alfredo DEAÑO³ · Kurusch EBRAHIMI-FARD⁴ ·
Ander MURUA⁵

27th June 2013

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Abstract Differential equations play a fundamental role in many different fields, e.g., engineering, fluid dynamics, chemical reaction kinetics, molecular dynamics, electronic circuits, population dynamics, finance. Therefore, the art of approximating or computing solutions of differential equations, partial as well as ordinary, linear as well as non-linear, is of particular importance in applied mathematics.

The meeting aims at bringing together leading experts working in numerical analysis of differential equations and related areas. It is composed of five sessions. Each session of the workshop is organized around a specific topic:


The background and current status of each field is introduced in a plenary talk by specifically chosen leading experts:

Jesús Sanz-Serna (Valladolid), Arieh Iserles (Cambridge), Christian Lubich (Tübingen), David Martín de Diego (ICMAT-CSIC), and Hans Munthe-Kaas (Bergen).

Beside the plenary speech, each session includes research talks, where recent progress in the field is reported. In addition, discussion roundtables will take place in the afternoons, which are of specific importance, as they shall give researchers from all subjects a platform to discuss common problems, current open questions, as well as future perspectives of each subject. Young researchers and PhD students are invited to participate in this meeting.

¹Univ. Politècnica de València, ²Univ. Jaume I, Castellón, ³Univ. Carlos III de Madrid, ⁴ICMAT-CSIC, ⁵Univ. del País Vasco, San Sebastián
1 Topics and Plenary Speakers

- Topic I:
  Geometric Numerical Integration
  Jesús M. Sanz-Serna  Univ. de Valladolid, Spain
e-mail: sanzserna@mac.uva.es
  http://sanzserna.org/

- Topic II:
  Highly Oscillatory Problems
  Arieh Iserles  Univ. of Cambridge, UK
e-mail: A.Iserles@damtp.cam.ac.uk
  www.damtp.cam.ac.uk/user/na/people/Arieh/

- Topic III:
  Splitting Methods and Time Integration of Partial
  Differential Equations
  Christian Lubich  Univ. Tübingen, Germany
e-mail: lubich@na.uni-tuebingen.de
  http://na.uni-tuebingen.de/~lubich/

- Topic IV:
  Discrete Mechanics and Control Theory
  David Martín de Diego  ICMAT-CSIC, Spain
e-mail: david.martin@icmat.es
  www.icmat.es/dmartin

- Topic V:
  Algebraic Structures in Numerical Integration
  Hans Munthe-Kaas  Univ. of Bergen, Norway
e-mail: hans.munthe-kaas@math.uib.no
  http://hans.munthe-kaas.no/

1.1 Committees

Scientific Committee  Organizing Committee

Arieh Iserles  Sergio Blanes (Valencia, Spain)
Christian Lubich  Fernando Casas (Castellón, Spain)
David Martín de Diego  Alfredo Deaño (Madrid, Spain)
Hans Munthe-Kaas  Kurusch Ebrahimi-Fard (Madrid, Spain)
Jesús M. Sanz-Serna  Ander Murua (San Sebastian, Spain)
2 Speakers, Participants and Schedule

2.1 Speakers

1) Gil Ariel (Ramat-Gan, Israel)
2) Elena Celledoni (Trondheim, Norway)
3) Philippe Chartier (Rennes, France)
4) François Gay-Balmaz (Paris, France)
5) Vasile Gradinaru (Zürich, Switzerland)
6) Robert Grossman (Chicago, USA)
7) Ernst Hairer (Geneva, Switzerland)
8) Eskil Hansen (Lund, Sweden)
9) Marlis Hochbruck (Karlsruhe, Germany)
10) Daan Huybrechs (Leuven, Belgium)
11) Arieh Iserles (Cambridge, UK)
12) Marin Kobilarov (Baltimore, USA)
13) Ben Leimkuhler (Edinburgh, UK)
14) Melvin Leok (La Jolla, USA)
15) Christian Lubich (Tübingen, Germany)
16) Simon Malham (Edinburgh, UK)
17) Dominique Manchon (Clermont-Ferrand, France)
18) David Martín de Diego (ICMAT-CSIC, Madrid, Spain)
19) Hans Munthe-Kaas (Bergen, Norway)
20) Sina Ober-Blöbaum (Paderborn, Germany)
21) Brynjulf Owren (Trondheim, Norway)
22) Jesús M. Sanz-Serna (Valladolid, Spain)
23) Mechthild Thalhammer (Innsbruck, Austria)
24) Gerhard Wanner (Geneva, Switzerland)
25) Anke Wiese (Edinburgh, UK)
26) Antonella Zanna (Bergen, Norway)
2.2 Participants

1) Andreas Ansheim (Cambridge, UK)
2) Miguel Atencia (Málaga, Spain)
3) Philipp Bader (Valencia, Spain)
4) María Barbero Liñán (ICMAT-UC3M, Spain)
5) Sergio Blanes (Valencia, Spain)
6) Giancarlo Breschi (ICMAT-CSIC, Spain)
7) Manuel Calvo (Zaragoza, Spain)
8) Begoña Cano (Valladolid, Spain)
9) Maria-José Cantero (Zaragoza, Spain)
10) Fernando Casas (Castellón, Spain)
11) Leonardo Colombo (ICMAT-CSIC, Spain)
12) Charles H. Curry (Edinburgh, UK)
13) Alfredo Deaño (Madrid, Spain)
14) François Demoures (Lausanne, Switzerland)
15) Kurusch Ebrahimi-Fard (Madrid, Spain)
16) Utku Erdoğan (Usak, Turkey)
17) Daniel Fox (UPM, Madrid, Spain)
18) Elisa Lavinia Guzman Alonso (La Laguna, Spain)
19) Dhia Mansour (Tübingen, Germany)
20) Håkon Marthinsen (Trondheim, Norway)
21) Juan Ignacio Montijano (Zaragoza, Spain)
22) María Jesús Moreta, (UCM, Madrid, Spain)
23) Ander Murua (San Sebastian, Spain)
24) Luis Randez (Zaragoza, Spain)
25) Hector Salas (Mayaguez, Puerto Rico)
26) Pranav Singh (Cambridge, UK)
27) Muaz Seydaoglu (Valencia, Spain)
2.3 Schedule

Opening on Monday, 09:00am.  PT = Plenary TALK (60 + 15 min.)
Closing on Friday, 05:00pm.  ST = Session TALK (45 + 15 min.)
DS = Discussion SESSION
YRS = Young Researchers Session

<table>
<thead>
<tr>
<th>Schedule</th>
<th>Mon.</th>
<th>Tue.</th>
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<tbody>
<tr>
<td>09:15</td>
<td>Topic I</td>
<td>Topic II</td>
<td>Topic III</td>
<td>Topic IV</td>
<td>Topic V</td>
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<td>10:30</td>
<td>Sanz-Serna</td>
<td>Iserles</td>
<td>Lubich</td>
<td>Martin de Diego</td>
<td>Munthe-Kaas</td>
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<td>11:00</td>
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<td>12:00</td>
<td>Zanna</td>
<td>Huybrechs</td>
<td>Thalhammer</td>
<td>Ober-Blöbaum</td>
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<td>Hansen</td>
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<td>16:00</td>
<td>Chartier</td>
<td>Ariel</td>
<td>Hochbruck</td>
<td>Kobilarov</td>
<td>Grossman</td>
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<td>17:00</td>
<td>ST4</td>
<td>DS2</td>
<td>DS3</td>
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<td>Leok</td>
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<td>DS1</td>
<td>Poster</td>
<td>YRS 1</td>
<td>YRS 2</td>
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Young Researchers Session

Wednesday, July 10, 2013
17:30 – 17:45: Ph. Bader
17:50 – 18:05: M.J. Cantero
18:10 – 18:25: P. Singh

Thursday, July 11, 2013
17:30 – 17:45: Ch. Curry
17:50 – 18:05: H. Marthinsen
18:10 – 18:25: D. Mansour

Talks will take place in AULA AZUL, which is equipped with blackboards and beamer.
3 Titles

NOTE: Abstracts can be found on the workshop website.

http://www.icmat.es/congresos/tnade2013/TNADE2013.html

Geometric Numerical Integration

Geometric Integration and Monte Carlo Methods
J.M. Sanz-Serna (Valladolid Univ., Spain)

Integral preserving Lie group integrators
E. Celledoni, (NTNU, Trondheim, Norway)

Uniformly accurate numerical schemes for highly oscillatory nonlinear Schrödinger equations
Ph. Chartier (INRIA Rennes & ENS Cachan, France)

Geometric properties of Kahan’s method
B. Owren, (NTNU, Trondheim, Norway)

Generating forms and volume-preserving numerical integrators
A. Zanna (Bergen Univ., Norway)

Highly Oscillatory Problems

Expansion of ODEs forced by irregular highly oscillatory terms with stationary points
A. Iserles (Cambridge Univ., UK)

A multiscale method for highly oscillatory dynamical systems using a Poincaré map type technique
G. Ariel (Bar Ilan Univ., Ramat-Gan, Israel)

A numerical approach to the semiclassical Schrödinger equation for nuclei
V. Gradinaru (ETHZ, Zürich, Switzerland)

Complex-plane methods for oscillatory integrals
D. Huybrechs (K.U. Leuven, Belgium)

Splitting Methods and Time Integration of Partial Differential Equations

Operator splitting for partial differential equations with Burgers nonlinearity
Ch. Lubich (Univ. Tübingen, Germany)

Splitting for nonlinear parabolic equations
E. Hansen (Lund Univ., Sweden)
Error analysis of implicit Runge–Kutta methods for discontinuous Galerkin discretizations of linear Maxwell’s equations
M. Hochbruck, T. Pažur (Karlsruhe Institute of Technology, Germany)

Convergence analysis of high-order time-splitting generalized Laguerre–Fourier–Hermite pseudo-spectral methods for rotational Gross–Pitaevskii equations
M. Thalhammer (Innsbruck Univ., Austria)

Discrete Mechanics and Control Theory

Discrete mechanics and optimal control theory
D. Martín de Diego (ICMAT-CSIC, Madrid, Spain)

On the use of variational integrators in geophysical fluid dynamics
F. Gay-Balmaz (École Normale Sup., Paris, France)

Symplectic Algorithms for Mechanics and Control of Multi-body Systems
M. Kobilarov (Johns Hopkins Univ., USA)

Variational integrators of higher order in optimal control theory
S. Ober-Blöbaum (Univ. of Paderborn, Germany)

Algebraic Structures in Numerical Integration

Algebraic Structures in Numerical Integration
H. Munthe-Kaas (Univ. of Bergen, Norway)

Hopf Algebras of Trees and the Symbolic and Numeric Computations of Flows
R. Grossman (Univ. of Chicago, USA)

Grassmannians, superpotentials and applications
S. Malham (Heriot–Watt Univ., Edinburgh, Scotland)

Rooted trees, non-rooted trees and Hamiltonian B-series
D. Manchon (CNRS, Clermont–Ferrand, France)

Lévy processes and the algebra of stochastic integrals
A. Wiese (Heriot–Watt Univ., Edinburgh, Scotland)
4 Young Researchers Session

Geometric integrators for Schrödinger equations
Ph. Bader (Valencia, Spain)

In this talk, I will present some problems which are addressed in my PhD thesis. The Schrödinger equation and its varieties (time-dependent, semiclassical, imaginary, nonlinear) are of great interest among theorists and practitioners and I will explain some of their properties and peculiarities that come with their numerical solution. We have developed numerical methods which are specifically adapted to the equations in question following the general idea of Splitting methods and Magnus expansions and the central ideas are summarized.

From orthogonal polynomials on the unit circle to functional equations via generating functions
M.J. Cantero (Zaragoza, Spain), A. Iserles (Cambridge, UK)

We study a family of orthogonal polynomials on the unit circle by derive two generating functions. The first can be represented in terms of sums of a q-hypergeometric type and used to derive explicitly the underlying orthogonal polynomials, while the second obeys a functional differential equation and can be used to determine the asymptotic behaviour of these polynomials. These constructs allow us to study the Caratheodory function and examine the underlying orthogonality measure.

Quasi-shuffle algebras and Lévy processes
Ch. H. Curry (Edinburgh, UK)

A finite family of independent Lévy processes having finite moments generates a quasi-shuffle algebra. We demonstrate this construction and explore its implications for strong approximations of stochastic differential equations driven by Lévy processes.

Gauss–Runge–Kutta time discretization of wave equations on evolving surfaces
D. Mansour (Tübingen, Germany)

A linear wave equation on a moving surface is discretized in space by the evolving surface finite element method. Discretization in time is done by Gauss–Runge–Kutta (GRK) methods, aiming for higher-order accuracy in time and unconditional stability of the fully discrete scheme. The latter is established in the natural time-dependent norms by using the algebraic stability and the coercivity property of the GRK methods together with the properties of the spatial semi-discretization. Under sufficient regularity conditions, optimal-order error estimates for this class of fully discrete methods are shown. Numerical experiments are presented to confirm some of the theoretical results.
Symplectic Lie group methods
H. Marthinsen (Trondheim, Norway)

A unified approach to obtain arbitrarily high order symplectic integrators on $T^*G$ from Lie group integrators on a Lie group $G$ will be presented.

Effective approximation for the linear time-dependent Schrödinger equation
P. Singh (Cambridge, UK)

The computation of the linear Schrödinger equation presents major challenges because of the presence of a small parameter. Assuming periodic boundary conditions, the standard approach consists of semi-discretisation with a spectral method, followed by an exponential splitting. We follow an alternative strategy: our analysis commences from the investigation of the free Lie algebra generated by the operations of differentiation and multiplication with the interaction potential. It turns out that this algebra possesses structure that renders it amenable to a very effective form of asymptotic splitting: exponential splitting where consecutive terms are scaled by increasing powers of the small parameter. The number of terms of the splitting increases linearly with time accuracy. This leads to methods that attain high spatial and temporal accuracy and whose cost scales like $O(N \log N)$, where $N$ is the number of degrees of freedom.
Numerical selfsimilar solutions to Smoluchowski’s coagulation equation with gelling kernels
Giancarlo Breschi (ICMAT-CSIC, Madrid, Spain)

Smoluchowski’s coagulation equation is a mean field model describing cluster growth. Let the function $c(x,t)$ represent the mean amount of $x$-mass polymers per unit volume at a given time $t$. Then, the variation of $c$ is expressed by a non-linear, integrodifferential equation:

$$\frac{\partial c(x,t)}{\partial t} = \frac{1}{2} \int_{0}^{x} K(x-y,y) c(x-y,t) c(y,t) \, dy - c(x,y) \int_{0}^{\infty} K(x,y) c(y,t) \, dy$$

where the first convolution integral accounts for clusters of smaller sizes aggregating to form a new cluster of size $x$ and the second integral represents the loss of $x$-mass clusters coagulating to form heavier ones. Smoluchowski’s equation has been used in a very wide set of applications, ranging from physical chemistry to astrophysics and population dynamics. For a good introductory survey, see [2] and the references therein.

Many dynamical properties depend on the integration kernel $K(x,y)$, which determines the reactivity between couples of masses. It is known that, for certain kernels such as $K_\ast = xy$, a singularity in finite time occurs: the solution develops a heavy tail in finite time and the total mass is no longer conserved. This phenomenon is called gelation and represents the formation of a cluster with infinite density that drains mass from the coagulating system.

In this work we are considering homogeneous, gelling kernels $K(x,y) = (xy)^\lambda$ with $\frac{1}{2} < \lambda < 1$. For greater $\lambda$, the gelation phenomenon is instantaneous and for smaller ones it does not occur. Since neither analytical solutions nor gelling times are known -except for a few explicit kernels-, and, moreover, it is common in applications to assert that the solutions converge to a self-similar form, there is a strong interest in studying numerically the existence of self-similar solutions. Such self-similar solutions depend on a free exponent that cannot be determined from dimensional considerations -self-similar solution of the second kind, in the notation of Barenblatt [1]-; it can be fixed imposing the behaviour at the origin and infinity. We present a numerical scheme to find the self-similar parameter corresponding to self-similar solutions with all its moments bounded.


A complex take on oscillatory ODEs
A. Deaño (Madrid, Spain), D. Huybrechs (Leuven, Belgium)

We present some preliminary work on a complex approach to oscillatory initial value problems posed on the real axis. Much like standard steepest descent analysis for integrals, solving the differential equation along a suitable path in the complex plane can be computationally advantageous since high oscillation does not impose tiny stepsizes on standard ODE solvers. The technique is similar to the well known method of pole vaulting for ODEs with singularities. Linear and nonlinear examples are provided.
A functional fitting Runge–Kutta Method for Oscillatory Problems

U. Erdo˘gan (Usak, Turkey), H. Ko¸cak (Bath, UK)

We propose a two stage functional fitting method with two parameters for solving initial value problem \( \ddot{x} = f(x, \dot{x}, t) \) which may have different types of regimes such as oscillatory and stiff. Local truncation error formula is used to determine these fitting parameters. Stability properties are discussed. Numerical examples are presented to show that the proposed method produces accurate results and preserves some qualitative properties even for relatively large step sizes.

Geometric Numerical Integration of Gradient Systems

Y. Hernandez (Habana, Cuba), Miguel Atencia (Málaga, Spain)

We construct and analyse numerical methods that preserve a Lyapunov function of a dynamical system. Therefore we focus on gradient-like Ordinary Differential Equations:

\[
\frac{d y}{dt} = L(y) \nabla V(y)
\]

where \( L \) is a negative-definite matrix and \( V \) is a scalar function, which fulfills the conditions to be a Lyapunov function, chiefly that it decreases over time. Gradient systems are models of dissipative physical systems, and their trajectories converge towards an asymptotically stable equilibrium. There are few published numerical methods that approximate the original system while preserving the downwards path of the Lyapunov function. We consider discrete-gradient methods [1], defined as:

\[
\frac{y_{k+1} - y_k}{h} = \bar{L}(y_k, y_{k+1}) \nabla V(y_k, y_{k+1})
\]

where \( \bar{L}(y, y) = L(y) \) and \( \nabla \) is a discrete gradient. We choose a particular discrete gradient, namely the coordinate increment, and show that, under mild assumptions, discrete gradient methods are designed that can be computed explicitly. An alternative method, based upon projection, is also described, and the relative merits and shortcomings of each algorithm are brought to light. Numerical results are presented for some simple test equations, supporting the validity of the proposal. For particular examples, the experiments show that discrete gradient methods preserve the Lyapunov function, whereas the Euler rule fails to do so, since periodic solutions appear, and, besides, numerical accuracy of the discrete gradient method is also favourable.

This work has been partially supported by the Spanish Secretaría de Estado de Investigación, Desarrollo e Innovación, project no. TIN2010-16556; the Junta de Andalucía, project no. P08-TIC-04026; and the Agencia Española de Cooperación Internacional para el Desarrollo (AECID), project no. A2-038418-11.


High-order splitting methods for separable non-autonomous parabolic equations

Muaz Seydaoglu and Sergio Blanes (UPV, Valencia, Spain)

High order splitting methods with complex coefficients have been recently used for the numerical integration of separable parabolic equations showing a good performance. Splitting methods with real coefficients of order higher than two necessarily have negative coefficients and can not be used for
solving these problems. In this work we consider the case in which the system is separable and non-autonomous

\[ \frac{du}{dt} = A(t, u) + B(t, u), \]

where we suppose both subproblems, when the explicit time-dependency is frozen,

\[ \frac{du}{dt} = A(\bar{t}, u), \quad \frac{du}{dt} = B(\bar{t}, u), \]

are exactly solvable (or can be numerically solved to high accuracy). To solve this non-autonomous problem using splitting methods with complex coefficients requires to compute the operators \( A(t, u), B(t, u) \) at complex values of \( t \).

We show that if the splitting methods are such that one set of the coefficients is real, say \( a_i \in \mathbb{R}^+, b_i \in \mathbb{C}^+ \), one can build high order methods where both operators are evaluated at real times. This requires to solve the non-autonomous equation

\[ \frac{du}{dt} = A(t, u), \]

either exactly or up to high accuracy (e.g. using a Magnus integrator). This procedure also extends to perturbed problems, i.e. \( \|B\| \ll \|A\| \), as far as the real coefficients are used to advance the dominant part. We illustrate the performance of the methods on several numerical examples.

High order splitting methods which involve real and complex coefficients can also be useful for other problems and are also being investigated at this moment by Bader, Blanes, Casas, Chartier, Makazaga and Murua.
6 Campus Map: ICMAT & Bus Stop 714 + 827

Campus Cantoblanco - UAM - Bus Stop 714 - ICMAT