Workshop on

Innovative Time Integration




May 13 – 16, 2012

Innsbruck, Austria

Welcome

We wish you a warm welcome to Innsbruck, and we are looking forward to an interesting *Workshop on Innovative Time Integration*.

The intention of the workshop is to provide a platform for exchanging new ideas and results in the development of innovative time integrators. The workshop covers both theoretical and practical aspects, and wants to bring together numerical analysts working in the field as well as PhD students, who intend to start in this area. The present workshop continues a series of conferences that were held in Innsbruck from 2004 to 2010.

We wish you a scientifically inspiring and enjoyable time in Innsbruck. If you have any questions, please do not hesitate to contact us.

Alexander Ostermann and Petra Csomós

General Information

The workshop takes place from 13th till 16th May 2012 at the SOS-Kinderdorf, Hermann-Gmeiner-Akademie. The address is

SOS-Kinderdorf, Hermann-Gmeiner-Akademie

Hermann-Gmeiner-Straße 51
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The workshop starts in the evening of 13th May with an informal dinner and will end on 16th May after lunch.

The conference fee (320 Euro before 31rd March, 370 Euro from 1st April) includes the accommodation in a double room at the SOS-Kinderdorf, Hermann-Gmeiner-Akademie, full board (breakfast, lunch, dinner, coffee breaks), and the excursion. The surcharge for single occupation is 50 Euro.

Scientific Programme

Contributions

All communications will be given in plenary sessions. Each contribution is scheduled to last 30 minutes, including a brief discussion.

The conference language is English.

Equipment

The seminary room is equipped with an overhead projector and a data projector. A Windows computer with Microsoft Powerpoint and Acrobat Reader will be provided. We recommend you not to use your own laptop. Talks can be transferred to the conference computer through CDs or USB sticks.

Schedule

Sunday, May 13, 2012

17.00 – 19.00	*Registration at the SOS-Kinderdorf, Hermann-Gmeiner-Akademie*
19.00	*Dinner*

Monday, May 14, 2012

8.30 – 8.40	*Opening*
8.40 – 9.25	MARTIN ARNOLD Second order convergence of a Lie group time integration method for constrained mechanical systems
9.25 – 9.55	BERND BRUMM Heterogeneous multiscale methods for highly-oscillatory mechanical systems with solution-dependent frequencies
9.55 – 10.15	*Coffee break*
10.15 – 10.45	GUILLAUME LEBOUCHER Stroboscopic method for wave equation
10.45 – 11.15	STEVEN VANDEKERCKHOVE Higher order time integration of wave equations
11.15 – 11.45	DHIA MANSOUR Numerical solution of linear wave equations on evolving surfaces
11.45 – 12.15	CHRISTIAN LUBICH Backward difference time discretization of parabolic differential equations on evolving surfaces
12.30 – 14.00	*Lunch break*
14.00 – 14.30	ISTVÁN FARAGÓ Convergence of diagonally implicit Runge–Kutta methods combined with Richardson extrapolation
14:30 – 15.00	MARINO ZENNARO Stability criteria for functional continuous Runge–Kutta methods
15.00 – 15.30	STEFANO MASET The collocation method and the truncation of Fourier series method in the numerical solution of boundary value problems for functional differential equations
15.30 – 16.00	*Coffee break*
16.00 – 16.30	VU THAI LUAN Higher-order exponential Rosenbrock-type methods
16.30 – 17.00	JOHN LOFFELD Tailoring exponential integrators for computational efficiency
17.00 – 17.30	WINFRIED AUZINGER Krylov subspace approximation of rational matrix functions
17.30 – 18.00	PETER KANDOLF Leja interpolation for matrix functions
18.30	*Dinner and social programme*

Tuesday, May 15, 2012

8.30 – 9.15	PHILIPPE CHARTIER Averaging in Banach spaces
9.15 – 9.45	TOBIAS HELL Strong order convergence of splitting methods for stochastic differential equations with jumps
9.45 – 10.15	*Coffee break*
10.15 – 10.45	KATHARINA SCHRATZ Exponential splitting methods with boundary conditions
10.45 – 11.15	PETRA CSOMÓS Operator splitting for delay equations, part I
11.15 – 11.45	BÁLINT FARKAS Operator splitting for delay equations, part II
11.45 – 12.15	LUKAS EINKEMMER Convergence analysis of Strang splitting for Vlasov-type equations
12.30	*Lunch and social programme*

Wednesday, May 16, 2012

8.45 – 9.15	MARIE KOPEC Weak backward error analysis for a family of stochastic differential equations
9.15 – 9.45	DANG QUANG A Method of infinite system of equations for problems in unbounded domains
9.45 – 10.15	ANDRÁS BÁTKAI Shape preservation of evolution equations
10.15 – 10.45	*Coffee break*
10.45 – 11.15	OTHMAR KOCH Adaptive full discretization of Gross–Pitaevskii equations with rotation term
11.15 – 11.45	HARALD HOFSTÄTTER Convergence analysis of a generalized Laguerre–Fourier–Hermite method for the Gross–Pitaevskii equation with rotation term
11.45 – 12.15	ANTTI KOSKELA Exponential Taylor methods – Analysis and implementation
12.30	*Lunch*

Participants

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Abstracts of Talks

In alphabetical order

SECOND ORDER CONVERGENCE OF A LIE GROUP TIME INTEGRATION METHOD FOR CONSTRAINED MECHANICAL SYSTEMS

Martin Arnold

MARTIN LUTHER UNIVERSITY HALLE-WITTENBERG

Classical ODE and DAE time integration methods have been applied successfully for more than two decades to constrained systems in technical mechanics. For large scale systems, Newmark type integrators are considered to be an interesting alternative in terms of numerical effort and stability. In the present paper we study the time integration of constrained systems

$$\mathbf{M}(\mathbf{q})\ddot{\mathbf{q}} = -\mathbf{g}(\mathbf{q},\dot{\mathbf{q}},t) - \mathbf{B}^\top(\mathbf{q})\lambda\,, \quad \Phi(\mathbf{q}) = \mathbf{0}$$

by a generalized-α time integration method

$$\begin{aligned} \mathbf{q}_{n+1} &= \mathbf{q}_n + h\dot{\mathbf{q}}_n + (0.5-\beta)h^2\mathbf{a}_n + \beta h^2\mathbf{a}_{n+1} \\ \dot{\mathbf{q}}_{n+1} &= \dot{\mathbf{q}}_n + (1-\gamma)h\mathbf{a}_n + \gamma h\mathbf{a}_{n+1} \end{aligned}$$

with

$$(1-\alpha_m)\mathbf{a}_{n+1} + \alpha_m\mathbf{a}_n = (1-\alpha_f)\ddot{\mathbf{q}}_{n+1} + \alpha_f\ddot{\mathbf{q}}_n\,,$$

$$\mathbf{M}(\mathbf{q}_n)\ddot{\mathbf{q}}_n = -\mathbf{g}(\mathbf{q}_n,\dot{\mathbf{q}}_n,t_n) - \mathbf{B}^\top(\mathbf{q}_n)\lambda_n\,, \quad \Phi(\mathbf{q}_n) = \mathbf{0}$$

and appropriate parameters α_f, α_m, β, γ, see [1] and the recent extension to constrained systems in a Lie group setting [2]. The order condition $\gamma = 0.5 + \alpha_f - \alpha_m$ guarantees second order convergence in the classical case as well as for the Lie group integrator [3].

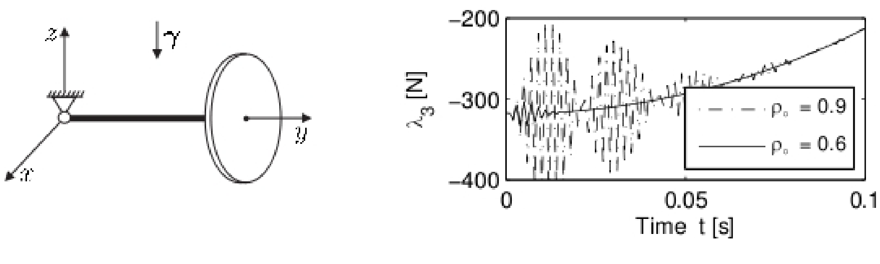

Fig. 1: Spurious transient oscillations: Generalized-α method applied to benchmark Heavy top.

A potential drawback of the methods are spurious transient oscillations of the constrained forces that result from an order reduction in the transient phase, see Fig. 1. We present a strict mathematical analysis of this phenomenon and show how to avoid the spurious oscillations by perturbed starting values $\dot{\mathbf{q}}_0$, $\mathbf{a}_0$.

REFERENCES

[1] J. Chung and G. Hulbert. A time integration algorithm for structural dynamics with improved numerical dissipation: The generalized-α method. *ASME Journal of Applied Mechanics*, 60:371–375, 1993.

[2] O. Brüls and A. Cardona. On the use of Lie group time integrators in multibody dynamics. *J. Comput. Nonlinear Dynam.*, 5:031002, 2010.

[3] O. Brüls, A. Cardona, and M. Arnold. Lie group generalized-α time integration of constrained flexible multibody systems. *Mechanism and Machine Theory*, 48:121–137, 2012.

KRYLOV SUBSPACE APPROXIMATION OF RATIONAL MATRIX FUNCTIONS

Winfried Auzinger

VIENNA UNIVERSITY OF TECHNOLOGY

In a recent paper, P. Botchev showed how the so-called generalized residual $r_k \in \operatorname{span}\{v_{k+1}\}$ of a Krylov approximation $y_k = V_k u_k \approx y(h) = \exp(hA)v$ of FOM type can be interpreted in a natural way as the pointwise defect, at $t = h$, of a continuously interpreted approximation $y_k(t) \approx y(t) = \exp(tA)v$. This leads to natural techniques for estimating the error $e_k = y_k - y$ by approximating the differential equation satisfied by $e_k(t)$.

Here we consider the case where, for a rational function $R(z) = P(z)/Q(z)$, $y_k = V_k u_k$ is a Krylov approximation for $y = R(hA) = Q^{-1}(hA)P(hA)v$ (e.g., a rational approximation of $\exp(hA)$). There is no well-defined 'defect' in the above sense, and the residual $r_k = Q(hA)y_k - P(hA)v$ is usually not a reasonable measure of accuracy. However, we show that the error $e_k = y_k - y$ can be written in the form $e_k = R_k(hA)v_{k+1}$ with $R_k(z) = Q^{-1}(z)P_k(z)$, where the coefficients of the polynomial $P_k(z)$ can be explicitly determined in terms of u_k. This provides the basis for estimating e_k, following usual heuristics, via an appropriate Krylov approximation of the rational expression $R_k(hA)v_{m+1}$ for the error.

SHAPE PRESERVATION OF EVOLUTION EQUATIONS

András Bátkai

EÖTVÖS LORÁND UNIVERSITY, BUDAPEST

Motivated by positivity-, monotonicity-, and convexity preserving differential equations, we introduce a definition of shape preserving operator semigroups and analyze their fundamental properties. In particular, we prove that the class of shape preserving semigroups is preserved by perturbations and taking limits. These results are applied, among others, to partial delay differential equations.

HETEROGENEOUS MULTISCALE METHODS FOR HIGHLY-OSCILLATORY MECHANICAL SYSTEMS WITH SOLUTION-DEPENDENT FREQUENCIES

Bernd Brumm

UNIVERSITY OF TÜBINGEN

The framework of Heterogeneous Multiscale Methods (HMM) was originally proposed for the efficient computation of multiple time-scale problems. Briefly, HMM deals with systems of differential equations whose exact dynamics can be viewed as a superposition of an underlying averaged macroscale dynamics, which it approximates, and a fast microscale dynamics driving the actual motion. HMM does so without explicit knowledge of the macroscale forces and provides the missing data via a micro-simulation in each step.

The talk examines an application of HMM to mechanical systems with varying high frequencies. It is shown that a correct initialization of the micro-simulation depends crucially on the adiabatic invariance of the actions. This almost-invariance property guarantees the existence of an underlying averaged system and provides the initial values for the micro-simulation. However, the initialization of the micro-simulation is computationally costly – even, more expensive than solving transformed averaged differential equations, which are explicitly known for this class of problems. Using the example of a stiff spring double pendulum, an HMM including RATTLE as a macro-integrator is formulated and the convergence of this algorithm is proved. The analysis is done by using canonical transformations proposed by K. Lorenz and Ch. Lubich.

REFERENCES

[1] B. Brumm / D. Weiss, *Heterogeneous Multiscale Methods for Highly-Oscillatory Mechanical Systems with Solution-Dependent Frequencies*, preprint 2012; submitted, see `http://na.uni-tuebingen.de/pub/weiss/Brumm_Weiss_March2012.pdf`.

AVERAGING IN BANACH SPACES

Philippe Chartier

INRIA RENNES & ENS CACHAN BRETAGNE

In this talk, I will present a new simple proof of an averaging theorem for evolution equations posed in a Banach space (joint work with François Castella, Florian Méhats and Ander Murua). The technique relies on the derivation of a functional equation whose solution gives directly the averaged vector field. It allows to derive exponential error estimates in an easy way and to address geometric aspects such as symplecticity and conservation of invariants. The theorem being designed for Banach spaces, it can be used for the Schrödinger or the wave equations. I will conclude with some numerical experiments.

OPERATOR SPLITTING FOR DELAY EQUATIONS, PART I

Petra Csomós

UNIVERSITY OF INNSBRUCK

We investigate operator splitting methods for a class of partial differential equations with delay. By using a semigroup approach to delay equations, the convergence of the splitting methods is easily explained, and abstract semigroup results yield the convergence of these methods. We illustrate the efficiency of these procedures by numerical examples for nonautonomous and nonlinear delay equations.

The talk is based on joint works with András Bátkai (Budapest), Bálint Farkas (Budapest), and Gregor Nickel (Siegen).

CONVERGENCE ANALYSIS OF STRANG SPLITTING FOR VLASOV-TYPE EQUATIONS

Lukas Einkemmer

UNIVERSITY OF INNSBRUCK

A rigorous convergence analysis of the Strang splitting algorithm for Vlasov-type equations in the setting of abstract evolution equations is provided. It is shown that under suitable assumptions the convergence is of second order in the time step h. As an example, it is shown that the Vlasov–Poisson equation in 1+1 dimensions fits into the framework of this analysis. Also, some numerical experiments for the latter case are presented.

THE CONVERGENCE OF DIAGONALLY IMPLICIT RUNGE–KUTTA METHODS COMBINED WITH RICHARDSON EXTRAPOLATION

István Faragó

Eötvös Loránd University, Budapest

Runge–Kutta methods are widely used in the solution of systems of ordinary differential equations. Richardson extrapolation is an efficient tool to enhance the accuracy of time integration schemes. In this paper we investigate the convergence of the combination of any diagonally implicit (including also the explicit) Runge–Kutta method with active Richardson extrapolation and show that the obtained numerical solution converges under rather natural conditions.

This is a joint work with Ágnes Havasi (Budapest) and Zahari Zlatev (Roskilde).

OPERATOR SPLITTING FOR DELAY EQUATIONS, PART II

Bálint Farkas

EÖTVÖS LORÁND UNIVERSITY, BUDAPEST

We study the sequential splitting procedure for delay equations which are 1) nonautonomous or 2) nonlinear. Under relatively mild assumptions on the delay operator it is possible to prove the first order convergence of the sequential splitting for suitably nice initial values.

This is a joint work with Petra Csomós (Innsbruck) and András Bátkai (Budapest).

STRONG ORDER CONVERGENCE OF SPLITTING METHODS FOR STOCHASTIC DIFFERENTIAL EQUATIONS WITH JUMPS

Tobias Hell

UNIVERSITY OF INNSBRUCK

We investigate the strong order convergence of splitting methods for the jump-diffusion Itô stochastic differential equation (SDE)

$$\mathrm{d}u(t) = \mu\,(u(t))\,\mathrm{d}t + \sigma\,(u(t))\,\mathrm{d}W_t + \int_{\mathbb{R}^m\setminus\{0\}} \eta\,(u(t-),\xi)\,\mathrm{d}N(\xi,t)$$

on the time interval $[0,T]$ for a given initial value $u(0) = u_0 \in \mathbb{R}^d$, where $W = \{W_t\}_{t\in[0,T]}$ is a k-dimensional Brownian motion, N denotes the Poisson random measure corresponding to an m-dimensional compound Poisson process with intensity $\lambda > 0$ which is independent of W and

$$\mu\colon\ \mathbb{R}^d \to \mathbb{R}^d, \quad \sigma\colon\ \mathbb{R}^d \to \mathbb{R}^{d\times k} \quad \text{and} \quad \eta\colon\ \mathbb{R}^d \times \mathbb{R}^m \setminus \{0\} \to \mathbb{R}^d$$

are Borel measurable functions. Especially the case of a pure jump SDE, i. e. $\sigma = 0$, is discussed.

This talk is based on a joint work with Christel Geiss (Innsbruck).

CONVERGENCE ANALYSIS OF A GENERALIZED LAGUERRE–FOURIER–HERMITE METHOD FOR THE GROSS–PITAEVSKII EQUATION WITH ROTATION TERM

Harald Hofstätter

VIENNA UNIVERSITY OF TECHNOLOGY

For computing the dynamics of rotating Bose–Einstein condensates a time-splitting generalized Laguerre–Fourier–Hermite pseudospectral method was recently proposed by W. Bao, H. Li, and J. Shen. We give a detailed analysis of the linear part of the underlying Gross–Pitaevskii equation by examining properties of the eigenfunctions of A, which are defined in terms of scaled generalized Laguerre functions. We show how our obtained results can be utilized to give a convergence proof for the proposed time-splitting pseudospectral method. Higher-order time-splitting schemes are also covered by our results.

LEJA INTERPOLATION FOR MATRIX FUNCTIONS

Peter Kandolf

UNIVERSITY OF INNSBRUCK

This talk is going to address Leja interpolation. Stability and convergence result for Leja interpolation are investigated and extended to the matrix case. In particular we investigate the φ-functions needed for exponential integrators.

ADAPTIVE FULL DISCRETIZATION OF GROSS–PITAEVSKII EQUATIONS WITH ROTATION TERM

Othmar Koch

VIENNA UNIVERSITY OF TECHNOLOGY

We discuss the adaptive full discretization of Gross–Pitaevskii equations with rotation term. The model suggests to use a Laguerre–Hermite spatial discretization in a method of lines approach. The resulting ODE system is propagated with higher-order splitting methods. Based on theoretical error bounds for this full discretization, asymptotically correct local error estimates employing either embedding formulae or the defect correction principle enable adaptive time-stepping which correctly reflects the solution behavior. Numerical examples illustrate the theoretical bounds and demonstrate the practical performance of the methods.

This is a joint work with Winfried Auzinger (Vienna), Harald Hofstätter (Vienna), and Mechthild Thalhammer (Innsbruck).

WEAK BACKWARD ERROR ANALYSIS FOR A FAMILY OF STOCHASTIC DIFFERENTIAL EQUATIONS

Marie Kopec

ENS CACHAN BRETAGNE

I will deal with the long times numerical approximations of overdamped Langevin stochastic differential equations by implicit numerical methods. First, I will explain some probabilistic notions. Then, I will speak about a weak backward error analysis result in the sense that the generator associated with the numerical solution coincides with the solution of a modified Kolmogorov equation up to high order terms with respect to the step- size. This implies that every invariant measure of the numerical scheme is close to a modified invariant measure obtained by asymptotic expansion. Moreover, I have that, up to negligible terms, the dynamic associated with the numerical scheme is exponentially mixing.

EXPONENTIAL TAYLOR METHODS – ANALYSIS AND IMPLEMENTATION

Antti Koskela

UNIVERSITY OF INNSBRUCK

We consider a Taylor series based exponential integrator for the time integration of large stiff systems of ordinary differential equations, which result from semidiscretization of partial differential equations and which are of the form $u'(t) = Au(t) + g(u(t))$. The integrator can be obtained by Taylor series expansion of the nonlinear part $g(u(t))$ at each numerical approximation u_n, and is given by a sum of the form $\varphi_0(hA)u_n + \sum_{k=1}^{p} h^k \varphi_k(hA)w_k$. The matrix functions φ_k are related to the exponential function, and the coefficients w_k represent time derivatives of $g(u(t))$ at u_n. The computational attractiveness of this method comes from the fact that this sum can be expressed in terms of a single exponential of a matrix $\widetilde{A}$ built by augmenting A with p additional rows and columns. The integrator works well for small values of p. For $p \geq 4$, however, the method suffers from instabilities which are caused by the loss of smoothness in the numerical solution along the time integration. The accumulation of round-off errors is demonstrated. Moreover, we perform numerical comparisons for the case of a state-independent inhomogeneity $u'(t) = Au(t) + g(t)$, where these instabilities do not occur. For the case of a state-dependent inhomogeneity we shortly discuss the efficient computation of the Taylor coefficients using the principles of automatic differentiation. Numerical experiments supporting the theoretical analysis are given using MATLAB.

The talk is based on a joint work with Alexander Ostermann (Innsbruck).

STROBOSCOPIC METHOD FOR WAVE EQUATION

Guillaume Leboucher

UNIVERSITÉ RENNES 1 - INRIA

I am interested by long time numerical integration of highly oscillatory equations. Classical theory says that in order to make a good numerical approximation of the solution, the integration step must be significantly less than one period. This leads to two problems: The time of computation and the performance of computer to integrate this type of equation over millions of periods.

In the periodic case, a strategy is introduced in [1], [2] by M.P. Calvo, P. Chartier, A. Murua and J.M. Sanz-Serna and called stroboscopic method. The idea of this method is to follow the solution along another equation called averaged equation which has two interesting properties. It doesn't oscillate and coincides with the exact solution at the stroboscopic times,i.e., every multiple of the period.

Existence of this averaged equation in the ODE case has been rigorously proved for instance by L.M. Perko in [3]. The observations of P. Chartier & al. lead to a numerical method solving highly oscillatory ODEs over long time with a numerical cost independent of the ratio between the period and the final time of observation.

Perko's proof for ODE can be adapted to partial differential equation like the wave equation or the Schrödinger equation. I will explain how to adapt this proof to the semi-linear wave equation case and show some numerical results to illustrate the benefits of this method.

REFERENCES

[1] M.P. CALVO, P. CHARTIER, A. MURUA AND J.M. SANZ-SERNA, *A stroboscopic numerical method for highly oscillatory problems*, in Numerical Analysis and Multiscale Computations, B. Engquist, O. Runborg and R. Tsai, editors, Lect. Notes Comput. Sci. Eng., Vol. 82, Springer 2011, 73–87.

[2] P. CHARTIER, A. MURUA AND J.M. SANZ-SERNA, *Higher-order averaging, formal series and numerical integration I: B-series*, FOCM, Vol. 10, No. 6, 2010.

[3] L.M. PERKO, *Higher order averaging and related methods for perturbed periodic and quasi-periodic systems*, SIAM J. Appl. Math. 17, 1969, Pages 698–724.

[4] P. CHARTIER, G. LEBOUCHER, F. MÉHATS, *Stroboscopic Averaging of highly oscillatory nonlinear wave equations*, in preparation.

TAILORING EXPONENTIAL INTEGRATORS FOR COMPUTATIONAL EFFICIENCY

John Loffeld

UNIVERSITY OF CALIFORNIA, MERCED

Exponential integrators have received renewed interest in recent years as a means to solve stiff systems of ODEs, due to the development of Krylov projection techniques to efficiently approximate exponential functions of large matrices, While this has allowed Krylov-based exponential integrators to become potentially competitive with implicit methods, the cost of evaluating the Krylov iterations remains their dominant computational cost. To that extent, tailoring an exponential integrator specifically towards lowering the cost of the Krylov projections can achieve significant gains in efficiency. In this talk we discuss some aspects of exponential integrators that can be adapted for more efficient Krylov evaluation of the φ-functions of which they're composed. A fifth-order exponential Runge-Kutta method designed to take advantage of the Niesen-Wright adaptivity procedure for reducing the quadratic cost scaling of the Krylov iteration is described, and some performance comparisons are given. Implementation strategies are also discussed.

BACKWARD DIFFERENCE TIME DISCRETIZATION OF PARABOLIC DIFFERENTIAL EQUATIONS ON EVOLVING SURFACES

Christian Lubich

UNIVERSITY OF TÜBINGEN

A linear parabolic differential equation on a moving surface is discretized in space by evolving surface finite elements and in time by backward difference formulas (BDF). Using results from Dahlquist's G-stability theory and Nevanlinna & Odeh's multiplier technique together with properties of the spatial semi-discretization, stability of the full discretization is proven for the BDF methods up to order 5 and optimal-order convergence is shown. Numerical experiments illustrate the behaviour of the fully discrete method.

The talk is based on joint work with Dhia Mansour (Tübingen) and Chandrasekhar Venkataraman (Warwick).

NUMERICAL SOLUTION OF LINEAR WAVE EQUATIONS ON EVOLVING SURFACES

Dhia Mansour

UNIVERSITY OF TÜBINGEN

We introduce a linear wave equation on evolving surfaces driven via the Hamilton principle of stationary action. We present a numerical scheme to solve the equation using an evolving surface finite element preposed by Dziuk and Elliott and variational time integrators derived from the Hamilton principle. The stability and convergence of the full discretization are analysed. Numerical experiments illustrate the behaviour of the fully discrete method. The talk is based on joint work with Ch. Lubich (Tübingen).

THE COLLOCATION METHOD AND THE TRUNCATION OF FOURIER SERIES METHOD IN THE NUMERICAL SOLUTION OF BOUNDARY VALUE PROBLEMS FOR FUNCTIONAL DIFFERENTIAL EQUATIONS

Stefano Maset

UNIVERSITY OF TRIESTE

We analyze the numerical solution of boundary value problems for general neutral functional differential equations by the collocation Method and the truncation of Fourier series method. The results are applied to two particular types of neutral functional differential equations, namely differential equations with deviated arguments and integro-differential equations.

METHOD OF INFINITE SYSTEM OF EQUATIONS FOR PROBLEMS IN UNBOUNDED DOMAINS

Dang Quang A

INSTITUTE OF INFORMATION TECHNOLOGY, VAST, HANOI

Many problems of mechanics and physics are posed in unbounded (or infinite) domains. For solving these problems one typically limits them to bounded domains and finds ways to set appropriate conditions on artificial boundaries or use quasi-uniform grid that maps unbounded domains to bounded ones. Differently from the above methods we approach to problems in unbounded domains by infinite system of equations.

In this paper we present starting results in this approach for some one-dimensional problems. The problems are reduced to infinite system of linear equations. A method for obtaining approximate solution with a given accuracy is proposed. Numerical experiments for several examples show the effectiveness of the offered method.

EXPONENTIAL SPLITTING METHODS WITH BOUNDARY CONDITIONS

Katharina Schratz

UNIVERSITY OF INNSBRUCK, ENS CACHAN BRETAGNE & INRIA RENNES

It is generally known that inhomogeneous time-dependent Dirichlet boundary conditions lead to a severe order reduction of splitting methods. In this talk we analyze the convergence order of exponential splitting methods applied as a numerical time integration method to partial differential equations, where

$$\begin{aligned}
&\partial_t w(t,x,y) = \mathscr{L}(\partial_x,\partial_y)w(t,x,y), \quad (x,y)\in\Omega=(0,1)^2, t\in]0,T] \\
&w(0,x,y) = w_0(x,y) \\
&w(t,\cdot,\cdot)|_{\partial\Omega} = f(t,\cdot,\cdot)|_{\partial\Omega} \qquad \text{for all } t\in[0,T]
\end{aligned}$$

with a strongly elliptic differential operator

$$\mathscr{L}(\partial_x,\partial_y) = \partial_x\big(a(x,y)\partial_x\big) + \partial_y\big(b(x,y)\partial_y\big)$$

and smooth, positive coefficients a,b. The splitting ansatz is the so-called dimension-splitting, where the differential operator $\mathscr{L}(\partial_x,\partial_y)$ is split along its dimensions, i.e.

$$\begin{aligned}
&\mathscr{L}(\partial_x,\partial_y) = \mathscr{A}(\partial_x) + \mathscr{B}(\partial_y) \text{ with} \\
&\mathscr{A}(\partial_x) = \partial_x\big(a(x,y)\partial_x\big), \quad \mathscr{B}(\partial_y) = \partial_y\big(b(x,y)\partial_y\big).
\end{aligned}$$

We will prove full-order convergence of the exponential Lie splitting method, although its order of consistency reduces to $0.25-\varepsilon$ for arbitrary small positive ε. Furthermore we state a sharp result on the global order reduction to $1.25-\varepsilon$ for arbitrary small positive ε of the exponential Strang splitting applied to equations with general inhomogeneous time-dependent Dirichlet boundary conditions.

This is a joint work with E. Faou (ENS Cachan Bretagne & INRIA Rennes) and A. Ostermann (University Innsbruck).

HIGHER-ORDER EXPONENTIAL ROSENBROCK-TYPE METHODS

Vu Thai Luan

UNIVERSITY OF INNSBRUCK

In this talk, we will derive higher-order exponential Rosenbrock-type methods and analyze their convergence properties for the time discretization of large systems of stiff differential equations.

We present a new and simpler approach to derive stiff order conditions. This allows us to derive new pairs of embedded methods of high order. As an example, we present a fifth-order method with five stages. By relaxing order conditions we further give fifth-order methods with less stages, namely with four and three stages only. The error analysis is performed in a semigroup framework of semilinear evolution equations in Banach spaces. Convergence results are proved for variable step size methods. To demonstrate the efficiency of the new integrators, we give some numerical experiments in MATLAB. In particular, numerical comparisons for semilinear parabolic PDEs in one and two space dimensions are presented.

This is a joint work with A. Ostermann (Innsbruck).

HIGHER ORDER TIME INTEGRATION OF WAVE EQUATIONS

Steven Vandekerckhove

KU LEUVEN KULAK

We solve the semi-discrete system of first-order equations

$$\begin{pmatrix} \mathbf{M}_u & 0 \\ 0 & \mathbf{M}_v \end{pmatrix} \begin{pmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{v}} \end{pmatrix} = \begin{pmatrix} 0 & -\mathbf{K}^T \\ \mathbf{K} & -\mathbf{M}_\sigma \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{j} \end{pmatrix}, \tag{1}$$

using higher order time integrators. Equation (1) may represent a scalar (acoustic), vectorial (electromagnetic) or tensorial (elastodynamic) wave equations discretized by either the finite element method or finite integration technique. In this equation the vectors $\mathbf{u}$ and $\mathbf{v}$ contain the degrees of freedom for the unknown fields, $\mathbf{j}$ is a source term, $\mathbf{K}$ and $\mathbf{K}^T$ are topological operators and $\mathbf{M}_u$, $\mathbf{M}_v$ and $\mathbf{M}_\sigma$ denoted discrete Hodge operators.

The classical leapfrog scheme is used as reference method and is compared to related higher (4th, 6th and 8th) order composition methods [1, 2]. Also a typical fourth order Runge-Kutta method and Richardson extrapolation are included in the study. Some attention will be given to source term treatment, damping and error criteria.

This study indicates that higher order methods may be advantageous compared to the classical method, even in the case of low order spatial discretisation.

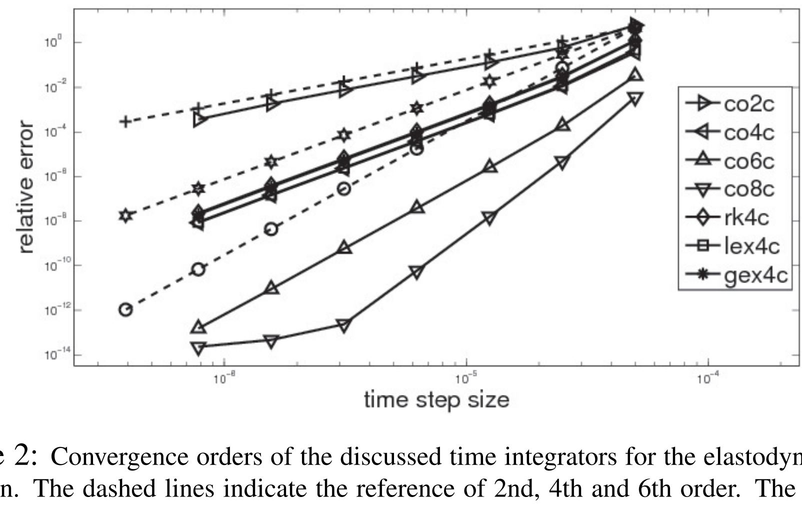

Figure 2: Convergence orders of the discussed time integrators for the elastodynamic wave equation. The dashed lines indicate the reference of 2nd, 4th and 6th order. The considered error is computed with the exact solution of equation (1) as reference.

REFERENCES

[1] M.A. Botchev and J.G. Verwer, *Numerical Integration of Damped Maxwell Equations*, SIAM J. Sci. Comput. , VOL 31(2), pp. 1322–1346, 2008.

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STABILITY CRITERIA FOR FUNCTIONAL CONTINUOUS RUNGE–KUTTA METHODS

Marino Zennaro

UNIVERSITY OF TRIESTE

We deal with the numerical integration of *Retarded Functional Differential Equations* of the type $y'(t) = f(t, y_t)$ by means of so called *Functional Continuous Runge-Kutta Methods*. Such methods are characterized by the fact that the entries of both the matrix A and the weight vector b are polynomial functions rather than numbers. In particular, in this talk we adapt the concept of *stiff order* (well established for Runge–Kutta methods in the ODE case) to such methods for an appropriate treatment of stiff problems.

This is a joint work with S. Maset (Trieste).

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