8th NAI Workshop on

Numerical Analysis of Evolution Equations

October 14 – 17, 2014

Innsbruck, Austria

Welcome

We wish you a warm welcome to Innsbruck, and we are looking forward to an interesting *8th NAI Workshop on Numerical Analysis of Evolution Equations*.

The intention of the workshop is to provide a platform for exchanging new ideas and results in the development of innovative integrators for evolution equations. 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 2012.

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, Alfredo Bellen, Katharina Schratz and Peter Kandolf

Accommodation

The workshop will take place in Vill at the Bildungsinstitut Grillhof. The address is

Tiroler Bildungsinstitut - Grillhof
Grillhofweg 100
6080 Vill, Austria
Phone: +43-512-38380
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The workshop starts in the evening of October 14, 2014 with an informal dinner and will end on October 17, 2014 after lunch.

The conference fee (330 Euro before 31st August, 380 Euro from 1st September) includes the accommodation in a double room at Grillhof, full board (breakfast, lunch, dinner, coffee breaks), and the excursion. The surcharge for single occupation is 50 Euro.

Scientific Program

Contributions

All communications will be given in plenary sessions. Each contribution is scheduled for 25 minutes including a brief discussion.

The conference language is English.

Equipment

The seminary room is equipped with a data projector. A Windows computer with Adobe Acrobat Reader will be provided as well as a presenter. Talks can be transferred to the conference computer through USB sticks or CD/DVD. We recommend you not to use your own laptop. However, if you need to use your own laptop, be sure it provides a VGA or HDMI connection. In addition, the room is equipped with a blackboard and an overhead projector.

Schedule

	Tuesday, 14 October 2014
17.00 – 19.00	**Registration at Grillhof**
19.00	**Dinner**
	Wednesday, 15 October 2014
08.40 – 08.45	**Opening**
08.45 – 09.30	Pauline Lafitte Time-subcycling & splitting schemes: some results on the asymptotic behavior
09.30 – 09.55	David Hipp An exponential integrator for non-autonomous parabolic problems
09.55 – 10.20	Denis Kolesnikov From low-rank approximation to an efficient rational Krylov subspace method for the Lyapunov equation
10.20 – 11.00	**Coffee break**
11.00 – 11.25	Marcel Mikl Strang splitting for a NLS with damping and forcing
11.25 – 11.50	Petra Csomós Numerical stability for nonlinear evolution equations
12.15 – 14.00	**Lunch break**
14.00 – 14.45	Tobias Jahnke Adiabatic integrators for the dispersion-managed nonlinear Schrödinger equation
14.45 – 15.10	Marino Zennaro Most unstable trajectories of linear switched systems
15.10 – 15.35	Georg Spielberger Analysis of underdamped linear systems driven by Brownian motion with the help of ARMA processes
15.35 – 16.00	**Coffee break**
16.00 – 16.25	Thomas Kassebacher Adaptive time splitting for nonlinear Schrödinger equations in the semiclassical regime
16.25 – 16.50	Tony Stillfjord Splitting the differential Riccati equation
16.50 – 17.15	Tobias Hell Modification of dimension splitting methods for two dimensional parabolic problems and its limitations in higher dimensions
17.15 – 17.40	Ekaterina Muravleva Operator-splitting method for numerical modeling of unsteady viscoplastic Bingham medium flows
18.30	**Dinner**
20.00	**Evening programme**

Thursday, 16 October 2014

08.30 – 08.55	Helmut Podhaisky On positive explicit peer methods of high order
08.55 – 09.20	Lukas Einkemmer A numerical investigation of error propagation for semi-Lagrangian methods
09.20 – 09.45	Roberto Garrappa Exponential integrators for fractional differential equations
09.45 – 10.10	Andreas Sturm Locally implicit time integration for linear Maxwell's equations
10.10 – 10.35	**Coffee break**
10.35 – 11.00	Winfried Auzinger Representation and estimation of local errors for splitting methods involving two or three parts
11.00 – 11.25	Robert Altmann Convergence of the Rothe method applied to operator DAEs
11.25 – 11.50	Tomislav Pažur Time integration of quasilinear Maxwell's equations
11.50 – 12.15	Hermann Mena Numerical solution of the infinite dimensional SLQR problem
12.30 – 14.00	**Lunch**
14.00 – 17.00	**Excursion to Hall Mint Museum,** `http://www.muenze-hall.at`
17.00 – 19.00	**Unsupervised strolling through the center of Innsbruck**
19.00	**Conference Dinner, Weißes Rössl, Innsbruck**

Friday, 17 October 2014

08.30 – 08.55	Marlis Hochbruck On the convergence of Lawson methods for semilinear stiff problems
08.55 – 09.20	Greg Rainwater On the similarities and differences between classes of exponential integrators
09.20 – 09.45	Stefano Maset An abstract framework in the numerical solution of boundary value problems for neutral functional differential equations
09.45 – 10.10	Peter Kandolf A backward error analysis for the Leja method
10.10 – 10.35	**Coffee break**
10.35 – 11.00	Ivan Oseledets Time integration of tensor trains

11.00 – 11.25	Martina Prugger Baseline performance studies of a hydrodynamics code with adaptive mesh refinement
11.25 – 11.50	Patrick Krämer Efficient time integration of the Klein–Gordon equation in the non-relativistic limit regime
11.50 – 12.15	István Faragó On a spatial epidemic propagation model
12.15 – 12.20	**Closing**
12.30	**Lunch**

Abstracts of Talks

In alphabetical order

Convergence of the Rothe Method Applied to Operator DAEs

Robert Altmann (TU Berlin, Germany)

The talk is devoted to the convergence analysis of the implicit Euler method to a special class of operator differential-algebraic equations (DAEs). Such an operator DAE can be seen as a DAE in an abstract setting as well as a standard operator equation with an additional constraint. Note that this constraint may again contain a differential operator. We consider semi-explicit systems of the form

$$\dot{u} + \mathcal{K}u + \mathcal{B}^* p = \mathcal{F}, \qquad \mathcal{B}u = \mathcal{G}, \qquad u(0) = u_0. \tag{*}$$

A well-known example is given by the Navier-Stokes equations for which $\mathcal{B}$ equals the divergence operator and $\mathcal{G} \equiv 0$. In the analysis of fluid flows, one considers the equations in the space of divergence-free functions such that the system reduces to an ODE in the abstract setting.
If we consider perturbations of the right-hand side or applications with $\mathcal{G} \not\equiv 0$ (e.g. optimal control problems constrained by a fluid flow), then instabilities occur as expected from the theory of DAEs. We consider a regularized formulation of (*) as introduced in [1] which essentially plays the role of an index reduction in the finite-dimensional case. This then allows to perform the convergence analysis similar as for operator ODEs.

References

[1] Altmann, R. and Heiland, J., 2014. Regularization of constrained PDEs of semi-explicit structure. Preprint 2014–05, Technische Universität Berlin, Germany.

Representation and estimation of local errors for splitting methods involving two or three parts

Winfried Auzinger * (Vienna University of Technology, Austria)
Harald Hofstätter (Vienna University of Technology)
Othmar Koch (Vienna University of Technology)
Mechthild Thalhammer (University of Innsbruck)

We consider higher-order splitting methods for evolution equations

$$\tfrac{\partial}{\partial t}u = H(u) = A(u) + B(u)\ [\,+C(u)\,], \quad u = u(t,\,\cdot\,), \tag{1}$$

realized via composition of the subflows φ_A, φ_B, and φ_C approximating the exact flow φ_H. For a splitting step $v \mapsto \mathcal{S}(h,v)$ with stepsize h, the local error $\mathcal{L}(h,v) = \mathcal{S}(h,v) - \varphi_H(h,v)$ can be analyzed in the following way:

- For a scheme of asymptotic order p, the leading term in the Taylor expansion of $\mathcal{L}(t,v)$ is of the form $\mathcal{C}\,t^{p+1}$, where $\mathcal{C}$ is a linear combination of higher-order commutators of the operators A, B, and C applied to the current numerical approximation v. This is well-defined under appropriate regularity assumptions on v.
- An exact analytical representation of the local error is more challenging. We describe how to derive a multiple variation of constants representation based on the defect of $\mathcal{S}(t,v)$ expanded into higher-order defect terms. For higher-order schemes a complete theory is available for the case of linear evolution equations. Compared to splitting into two operators ($C = 0$), the general case is significantly more involved, see [2]. Rigorous results for the general nonlinear case with $C = 0$ and for standard lower-orders schemes, see [1], are also briefly discussed. This general representation forms the basis for the local error analysis in concrete applications.

Furthermore, we consider a posteriori estimators for the local error whose asymptotic behavior can be studied via an extension of the local error analysis. These estimators are based on a general, natural approximation principle involving evaluation of the defect of $\mathcal{S}(t,v)$ with respect to (1), and for this purpose a representation for the defect is derived which can be used for practical computation. Numerical examples presented include equations of Schrödinger type, as well as other types of nonlinear wave equations. It is demonstrated that for these types of problems evaluation of the error estimator can be realized with reasonable effort and leads to reliable adaptive time integration methods.

References

[1] Auzinger, W., Hofstätter, H., Koch, O., Thalhammer, M., 2014. Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part III: The nonlinear case. J. Comput. Appl. Math. 273, 182–204.

[2] Auzinger, W., Koch, O., Thalhammer, M., 2014. Defect-based local error estimators for high-order splitting methods involving three linear operators. ASC Report No. 22/2014, Institute for Analysis and Scientific Computing, Vienna University of Technology.

Numerical Stability for Nonlinear Evolution Equations

Petra Csomós * (Hungarian Academy of Sciences, Hungary)
István Faragó (Eötvös Loránd University, Hungary)
Imre Fekete (Eötvös Loránd University, Hungary)

The talk deals with the usual N-stability notion for such nonlinear problems which can be formulated as evolution equations. We present the stability analysis of the generalisation of rational approximations to nonlinear operators as well.
In order to analyse N-stability, we consider the problem $F(u) = 0$ between the normed spaces X and Y, and discretise it as $F_n(u_n) = 0$, between certain spaces X_n and Y_n, for all index n from an index set. Then the scheme is called N-stable if there exists a constant $S > 0$ such that the estimate

$$\|v_n - z_n\|_{X_n} \leq S\|F_n(v_n) - F_n(z_n)\|_{Y_n}$$

holds for all $v_n, z_n \in X_n$ and the stability constant S is independent of n (see e.g. in López-Marcos and Sanz-Serna [3]).
In the present talk we consider the special map

$$\big(F(u)\big)(t,\cdot) = \tfrac{\mathrm{d}}{\mathrm{d}t}u(t,\cdot) - A\big(u(t,\cdot)\big)$$

for all $t \geq 0$ with the nonlinear m-dissipative operator $A : D(A) \subset \mathcal{X} \to \mathcal{X}$ on some Banach space $\mathcal{X}$. The results of Crandall and Liggett [2] and Brezis and Pazy [1] imply that the operator A generates a nonlinear semigroup which yields the solution to the problem above. By using another result in Brezis and Pazy [1], one can define a suitable approximation to the generator as well. The combination of the approximations of the generator and that of the corresponding semigroup serves as the full discretisation method in space and time.
After proving the N-stability of that combined method, we present a way how to generalise the rational approximations for nonlinear semigroups, and we analyse their stability as well.

References

[1] Brezis, H., Pazy, A., 1972. Convergence and approximation of semigroups of nonlinear operators in Banach spaces. Journal of Functional Analysis 9, 63–74.

[2] Crandall, M. G., Liggett, T. M., 1971. Generation of semi-groups of nonlinear transformations on general Banach spaces. American Journal of Mathematics 93, 265–298.

[3] López-Marcos, J. C., Sanz-Serna, J. M., 1988. A definition of stability for nonlinear problems. Numerical treatment of differential equations 104, 216–226.

A numerical investigation of error propagation for semi-Lagrangian methods

Lukas Einkemmer * (University of Innsbruck, Austria)
Alexander Ostermann (University of Innsbruck)

Semi-Lagrangian methods are a class of numerical solvers that follow the characteristic curves backward in time. Due to the low computational cost such methods are employed in applications ranging from plasma physics (Vlasov equation) to fluid dynamics (dissipative effects are often handled by a splitting approach in this context). The necessary reconstruction of the function values is usually carried out by polynomial interpolation, a discontinuous Galerkin approximation, or fast Fourier techniques. An interesting property of such schemes is that they mix the time and space discretization errors.
In this presentation we consider the error propagation of semi-Lagrangian methods for the advection equation in the case where high precision is desired. We demonstrate that the worst case error estimates given in the literature provide a good explanation for the error propagation of the interpolation-based semi-Lagrangian methods. For the discontinuous Galerkin approximation, however, we find that the characteristic property of semi-Lagrangian error estimates (namely the fact that the error increases proportionally to the number of time steps) is not observed. The method based on the fast Fourier transform is exact but, due to round-off errors, susceptible to a linear increase of the error in the number of time steps. We show how to modify the Cooley–Tukey algorithm in order to obtain an error growth that is proportional to the square root of the number of time steps.

References

[1] L. Einkemmer, A. Ostermann, 2014. On the error propagation of semi-Lagrange and Fourier methods for advection problems. arXiv:1406.1933.

On a spatial epidemic propagation model

István Faragó * (Eötvös Loránd University and MTA-ELTE "Numerical Analysis and Large Networks" Research Group, Hungary)
Róbert Horváth (Budapest Technical University and MTA-ELTE "Numerical Analysis and Large Networks" Research Group)

Most of the models of epidemic propagations do not take into the account the spatial distribution of the individuals. They give only the temporal change of the number of the infected, susceptible and recovered patients. In our presentation we present a spatial epidemic propagation model and give some of its qualitative properties both in the continuous and the finite difference numerical case: boundedness, nonnegativity preservation, the condition of forming epidemic waves. Some of the results are demonstrated on numerical tests.

Exponential integrators for fractional differential equations

Roberto Garrappa (Department of Mathematics - University of Bari, Italy)

Differential equations of fractional (i.e. non integer) order are nowadays frequently used for modeling real–life phenomena with anomalous properties in several fields, ranging from biology to engineering, finance, physics and so on.
Numerical methods for solving fractional differential equations (FDEs) and fractional partial differential equations (FPDEs) are therefore studied with an increasing interest.
In this talk we discuss the generalization of exponential integrators [1] to systems of fractional–order.
The main theoretical and numerical aspects are presented; in particular we discuss the derivation of a suitable variation–of–constant formula for problems of non integer order, the evaluation of a generalization of the exponential function (namely the Mittag–Leffler function [3, 4]), the development of ad-hoc difference schemes [2] and the analysis of the convergence properties.
We also present some results related to convergence properties of Krylov subspace methods for the evaluation of the Mittag–Leffler function with matrix arguments and we illustrate an example of a recent application to the solution of a class of time–fractional Schrödinger equations [5].

References

[1] Hochbruck, M., Ostermann, A., 2010. Exponential integrators, Acta Numer. 19, 209–286.

[2] Garrappa, R., Popolizio, M., 2011, Generalized exponential time differencing methods for fractional order problems, Comput. Math. Appl. 62 (3), 876–890.

[3] Moret, I., Novati, P., 2011. On the convergence of Krylov subspace methods for matrix Mittag–Leffler functions, SIAM J. Numer. Anal. 49 (5), 2144–2164.

[4] Garrappa, R., Popolizio, M., 2013. Evaluation of generalized Mittag–Leffler functions on the real line, Adv. Comput. Math. 39 (1), 205–225.

[5] Garrappa, R., Moret, I., Popolizio, M., 2014. Solving the time-fractional Schrödinger equation by Krylov projection methods. *submitted*.

Modification of dimension splitting methods for two dimensional parabolic problems and its limitations in higher dimensions

Tobias Hell * (University of Innsbruck, Austria)
Alexander Ostermann (University of Innsbruck)
Bertram Tschiderer (University of Innsbruck)

A *dimension splitting method* may suffer from a severe order reduction when applied to an inhomogeneous evolution equation of the form

$$u'(t) = \mathcal{L}u(t) + g(t)\,, \quad u(0) = u_0$$

on $L^2(\Omega)$, where $\Omega = (0,1)^2$ and $\mathcal{L} = \partial_x(a\partial_x) + \partial_y(b\partial_y)$ is an uniformly strongly elliptic operator with $a, b \in \mathcal{C}^2(\overline{\Omega})$ and $D(\mathcal{L}) = H^2(\Omega) \cap H_0^1(\Omega)$. For instance, the *Lie resolvent splitting* involving the split operators $\mathcal{A} = \partial_x(a\partial_x)$ and $\mathcal{B} = \partial_y(b\partial_y)$ converges, in general, with order of $1/4-\varepsilon$ in time for arbitrarily small $\varepsilon > 0$ due to arising corner singularities in the derivatives of the solution, see [1]. By applying the modification described in [2], the full convergence order of 1 is achieved.
Recently established regularity results for the corresponding stationary problem on $(0,1)^d$ with $d > 2$ might however lead to the conclusion that such an approach is limited to two dimensions.

References

[1] T. Hell, A. Ostermann, 2014. Compatibility conditions for Dirichlet and Neumann problems of Poisson's equation on a rectangle. J. Math. Anal. Appl. 420, 1005–1023.

[2] T. Hell, A. Ostermann, M. Sandbichler. Modification of dimension splitting methods – overcoming the order reduction due to corner singularities. To appear in IMA J. Numer. Anal.

An exponential integrator for non-autonomous parabolic problems

David Hipp * (Karlsruhe Institute of Technology, Germany)
Marlis Hochbruck (Karlsruhe Insitute of Technology)
Alexander Ostermann (Universität Innsbruck)

In this talk we discuss an exponential integrator for non-autonomous parabolic problems of the form

$$u'(t) + A(t)u(t) = 0, \qquad u(0) = u_0.$$

which we first presented in [1] and analyzed in [3]. The construction of this integrator is closely related to general construction principles of the continuous evolution system in an abstract framework. In contrast to the often used Magnus integrators, the proximity of our scheme to the continuous problem allows one to obtain a third-order method that does not suffer from order reduction.
A discussion of the efficient implementation of the integrator will be a central part of this talk. To illustrate the theoretical results we consider a finite element discretization of a diffusion equation on an evolving domain. This yields a stiff system of ordinary differential equations. We show that our scheme converges with the expected rate and obeys an error bound which is independent of the spatial mesh width. Moreover, we comment on some implementation aspects of rational Krylov subspace methods for the evaluation of products of matrix functions with vectors combined with multigrid preconditioning for evolving meshes, cf. [2].

References

[1] Hipp, D., Hochbruck, M. and Ostermann, A., 2012. Exponential integrators for parabolic problems with time dependent coefficients. Oberwolfach Reports 9(4), 3602–3606.

[2] Hipp, D. and Hochbruck, M., 2014. A preconditioned Krylov method for an exponential integrator for non-autonomous parabolic problems. Oberwolfach Reports 14.

[3] Hipp, D., Hochbruck, M. and Ostermann, A., 2014. An exponential integrator for non-autonomous parabolic problems, to appear in ETNA.

On the convergence of Lawson methods for semilinear stiff problems

Marlis Hochbruck * (Karlsruhe Institute of Technology, Germany)
Alexander Ostermann (University of Innsbruck, Austria)

In this talk we consider semilinear stiff problems of the form

$$u'(t) = Au(t) + g\big(u(t)\big), \qquad u(0) = u_0,$$

where the stiffness is contained in the linear part. To overcome the stability restriction of explicit methods, the idea of Lawson [3] was to use the transformation $w(t) = \mathrm{e}^{-tA}u(t)$ involving the exact flow of the homogeneous, linear problem. Solving the differential equation for w with an explicit Runge–Kutta method and transforming back to the original u-variable yields the so-called Lawson methods. These methods can be interpreted as a special form of exponential integrators involving matrix exponentials only. The convergence theory of explicit exponential integrators [2] shows that, in general, the stiff order of Lawson methods does not exceed one, since no φ-functions occur.
In the recent paper [1], Cano and González-Pachón showed excellent numerical results of Lawson methods applied to the nonlinear Schrödinger equation. The aim of this talk is to explain this behavior theoretically.

References

[1] B. Cano and A. González-Pachón, 2014. Projected explicit Lawson methods for the integration of Schrödinger equation. *Numerical Methods for Partial Differential Equations*.

[2] M. Hochbruck and A. Ostermann, 2005. Explicit exponential Runge–Kutta methods for semilinear parabolic problems. *SIAM J. Numer. Anal.*, 43(3):1069–1090.

[3] J. D. Lawson, 1967. Generalized Runge–Kutta processes for stable systems with large Lipschitz constants. *SIAM J. Numer. Anal.*, 4(3):372–380.

Adiabatic integrators for the dispersion-managed nonlinear Schrödinger equation

Tobias Jahnke * (Karlsruhe Institute of Technology, Germany)
Marcel Mikl (Karlsruhe Institute of Technology)

Data transmission through a dispersion-managed optical fiber is described by the one-dimensional nonlinear Schrödinger equation

$$\partial_t u = \frac{i}{\varepsilon}\gamma\left(\tfrac{t}{\varepsilon}\right)\partial_x^2 u + i|u|^2 u, \qquad t \in [0, t_{\text{end}}], \quad x \in \mathbb{T}, \tag{1}$$

with a small parameter $0 < \varepsilon \ll 1$. The function $\gamma(t) := d(t) + \varepsilon\alpha$ is the sum of the mean dispersion $\varepsilon\alpha$ and a piecewise constant function

$$d(t) = \begin{cases} -\delta & \text{if} \quad t \in [2m, 2m+1) \qquad \text{for some } m \in \mathbb{N} \\ \delta & \text{if} \quad t \in [2m+1, 2m+2) \quad \text{for some } m \in \mathbb{N}, \end{cases}$$

with parameters $\alpha \geq 0$ and $\delta > \varepsilon\alpha$. Solving (1) numerically is nontrivial because of the discontinuous, ε-dependent prefactor $(i/\epsilon)\gamma(t/\varepsilon)$ which grows larger and larger and changes faster and faster when ε decreases. As a consequence, traditional methods (e.g. Runge-Kutta methods, multistep methods, splitting methods etc.) require a very small step-size $\tau < \varepsilon$ to produce acceptable approximations.
In this talk, we will present an adiabatic integrator of order 2 which is not affected by such a step-size restriction. This method is based on a transformation of (1) to adiabatic variables and the observation that certain highly oscillatory functions can be integrated exactly.

A backward error analysis for the Leja method

Marco Caliari (Università di Verona)
Peter Kandolf * (University of Innsbruck, Austria)
Alexander Ostermann (University of Innsbruck)
Stefan Rainer (University of Innsbruck)

The Leja method is a well established scheme for computing the action of the matrix exponential. We present a new backward error analysis that allows us to make the method more efficient. From the scalar computation in high precision we predict the necessary number of scaling steps based only on the norm of the matrix and the desired backward error tolerance. Some preprocessing steps are applied to allow a more stable and more efficient computation, but the overall cost of the algorithm are dominated by the matrix vector products.
In numerical experiments we show that the method saves matrix vector products for a large class of matrices with regards to the truncated Taylor series method presented in [1]. The numerical experiments include spatial discretization of time dependent partial differential equations and various prototypical test cases.

References

[1] Al-Mohy, A.H., Higham, N.J., 2011. Computing the action of the matrix exponential, with an application to exponential integrators. SIAM J. Sci. Comput. 33 (2), 488-511.

[2] Caliari, M., Kandolf, P., Ostermann, A., Rainer, S., 2014. Comparison of software for computing the action of the matrix exponential. BIT Numerical Mathematics, 54 (1), 113-128.

Adaptive time splitting for nonlinear Schrödinger equations in the semiclassical regime

Winfried Auzinger (Vienna University of Technology)
Thomas Kassebacher * (University of Innsbruck, Austria)
Othmar Koch (Vienna University of Technology)
Mechthild Thalhammer (University of Innsbruck)

We study the convergence of exponential operator splitting methods for cubic Schrödinger equations in the semiclassical regime in dependence on the parameter ε. By deriving an integral representation of the local error $\mathcal{L}(h)$ for the Lie and Strang splitting methods (based on [1]), an error bound depending on the stepsize and on the semiclassical parameter ε is proven. For $\varepsilon \ll 1$, the dominant terms show the following behavior.

Lie Splitting: The local error is of basic order $\mathcal{O}(h^2)$, but more precisely we have

$$\|\mathcal{L}_{\mathrm{Lie}}(h,u)\|_{L^2} \leq C\left(h^2 + h^3\left(\tfrac{1}{\varepsilon}+\varepsilon\right) + h^4\left(\tfrac{1}{\varepsilon^2}+1\right)\right) + \mathcal{O}(h^5)\,,$$

with a constant C dominated by the H^2-norm of the initial value u. For $h > \varepsilon$, $C_2\, h^3 \frac{1}{\varepsilon}$ dominates the error such that an order of $\mathcal{O}(h^3)$ is observed, but for $h < \varepsilon$ this passes over to the classical $\mathcal{O}(h^2)$ behavior.

Strang Splitting: The dominant terms behave as

$$\|\mathcal{L}_{\mathrm{Strang}}(h,u)\|_{L^2} \leq h^3\left(C_1\,\tfrac{1}{\varepsilon} + C_2\,\varepsilon\right) + h^4\left(C_3\,\tfrac{1}{\varepsilon^2} + C_4\right) + \mathcal{O}(h^5)\,,$$

with constants C_1, C_3 depending on the H^2-norm of the initial value u and constants C_2, C_4 depending on its H^4-norm. Hence, the local error is dominated by $C\,h^3$ due to the coefficient $\frac{1}{\varepsilon}$ for $\varepsilon \ll h$, while it behaves as $C\,h^2$ for $h \approx \varepsilon$, which has already been observed numerically in [2].

All these effects are illustrated by numerical examples. Moreover, the performance of a defect-based a posteriori error estimator studied in [3] is discussed as to its dependence on ε and tested numerically.

References

[1] Auzinger, W., Hofstätter, H., Koch, O., Thalhammer, M., 2014. Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part III: The nonlinear case. J. Comput. Appl. Math. 273, 182–204.

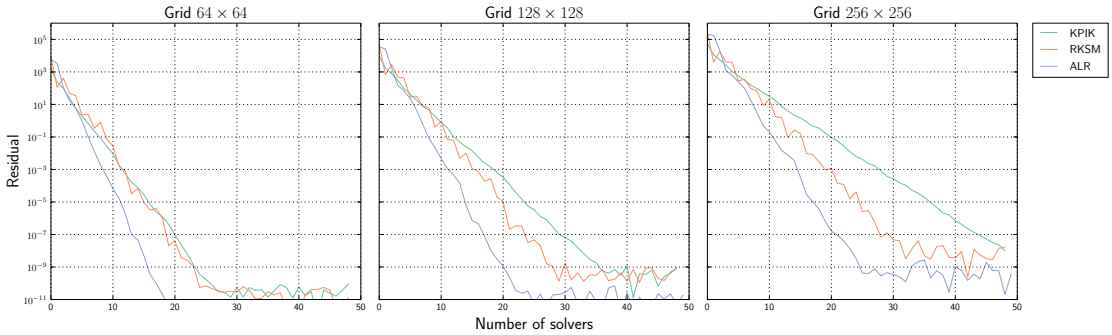
[2] Descombes, S., Thalhammer, M., 2012. The Lie-Trotter splitting for nonlinear evolutionary problems with critical parameters. A compact local error representation and application to nonlinear Schrödinger equations in the semi-classical regime. IMA J. Numer. Anal. 33, 722–745.

[3] Auzinger, W., Kassebacher, T., Koch, O., Thalhammer, M., 2014. Adaptive splitting methods for nonlinear Schrödinger equations in the semiclassical regime. ASC Report No. 27/2014, Institute for Analysis and Scientific Computing, Vienna University of Technology.

From low-rank approximation to an efficient rational Krylov subspace method for the Lyapunov equation

Ivan Oseledets (Skolkovo Institute of Science and Technology, Institute of Numerical Mathematics of Russian Academy of Sciences, Russia)
Denis Kolesnikov * (Skolkovo Institute of Science and Technology, Russia)

Many approaches for solving large scale algebraic Lyapunov equations with low-rank right-hand sides are based on rational Krylov subspaces. In this article we propose a new method for the construction of a rational Krylov subspace and compare its efficiency to other approaches. We start from the connection between the approximation of the solution of the Lyapunov equation of the form $AX + XA^\top = -y_0 y_0^\top$, and the solution of a system of linear ODEs of the form $\frac{dy}{dt} = Ay, \quad y(0) = y_0$. Based on this we propose a new functional which minimization can be used to find low-rank approximation in non-symmetric case and compute its gradient. Using the gradient representation we propose a basis extension method that uses solution of an auxiliary Sylvester equation, and a rank-1 approximation to the solution of the Sylvester equation gives a very cheap and efficient method to compute the shifts for the rational Krylov subspace. We compare the new method (ALR) to two other approaches [1], [2] on several model problems and find that the new method has considerably fewer number of iterations (see Figure). The results will be presented in a forthcoming paper [3].



References

[1] V. Simoncini, 2007. A new iterative method for solving large-scale Lyapunov matrix equations. *SIAM J. Sci. Comput.*, 29(3):1268–1288.

[2] V. Simoncini and V. Druskin, 2009. Convergence analysis of projection methods for the numerical solution of large Lyapunov equations. *SIAM J. Numer. Anal.*, 47(2):828–843.

[3] D. Kolesnikov and I. Oseledets. From low-rank approximation to an efficient rational Krylov subspace method for the Lyapunov equation. *Paper in preparation.*

Efficient Time Integration of the Klein-Gordon Equation in the Non-Relativistic Limit Regime

Patrick Krämer * (Karlsruhe Institute of Technology, Germany)
Katharina Schratz (Karlsruhe Institute of Technology)

Solving the Klein-Gordon equation

$$\partial_{tt} z + c^2 \left(-\Delta + c^2\right) z + \left(-\phi^2 + 2i\phi\partial_t\right) z = 0, \quad z(0) = \varphi,\ \partial_t z(0) = c^2\gamma$$

in the non-relativistic limit regime $c \gg 1$ is numerically very delicate as we have to deal with a highly oscillatory problem. This problem manifests in **time step restrictions** if we apply standard integrators. We have to choose time step sizes of order c^{-2} in order to get a feasible approximation to the exact solution.
The idea to overcome this numerical challenge is to approximate the exact solution $z(t,x)$ by

$$\tilde{z}_0(t,x) := \frac{1}{2}\left(u_0(t,x)\mathrm{e}^{ic^2t} + \overline{v}_0(t,x)\mathrm{e}^{-ic^2t}\right),$$

such that $z(t,x) = \tilde{z}_0(t,x) + \mathcal{O}\left(c^{-2}\right)$, i.e. we **filter out the high frequencies** explicitly. Here u_0 and v_0 satisfy the so called *limit equations*

$$\begin{aligned}
\partial_t u_0 &= -i\frac{1}{2}\Delta u_0 - i\phi u_0, \qquad & u_0(0) &= \varphi - i\gamma,\\
\partial_t v_0 &= -i\frac{1}{2}\Delta v_0 + i\phi v_0, \qquad & v_0(0) &= \overline{\varphi} - i\overline{\gamma},
\end{aligned}$$

which are Schrdinger equations **independent** of the large parameter c and can be solved **very efficiently** by using splitting methods without any time step restriction.
In my talk I want to demonstrate how these equations can be derived and how we can prove an error bound for this approximation.

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Time-subcycling & splitting schemes : some results on the asymptotic behavior

Guillaume Dujardin (INRIA Lille Nord-Europe)
Pauline Lafitte * (Ecole Centrale Paris, France)

This talk addresses the numerical integration of well-posed multiscale systems of ODEs or evolutionary PDEs by means of time-subcycling techniques. These methods rely on a decomposition of the vector field in a fast part and a slow part and take advantage of that decomposition. This way, one can integrate the fast equations with a much smaller time step than that of the slow equations, instead of having to integrate the whole system with a very small time step to ensure stability. We will present a study of the long-time behavior of sub-cycled schemes built using standard decomposition methods, that are known to be convergent in short-time to the solution of the original problem. In particular, when the solutions of the systems converge in time to an asymptotic equilibrium state, the question of the accuracy of the numerical long-time limit of the schemes as well as that of the rate of convergence will be addressed.

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An abstract framework in the numerical solution of boundary value problems for neutral functional differential equations

Stefano Maset (Dipartimento di Matematica e Geoscienze, Università di Trieste, Italy)

In this talk, we consider the numerical solution of boundary value problems for general neutral functional differential equations

$$\begin{cases} y'(t) = F(t, y, y', p), \ t \in [a, b], \\ B(y, y', p) = 0, \end{cases}$$

where F and B are functionals and p is a vector of parameters to be determined along with the solution y.
These problems are restated in an abstract form and, then, a general discretization of the abstract form is introduced and a convergence analysis of this discretization is developed. The three most important types of discretization for differential equations, namely the Finite Element Method, the Spectral Element Method and the Spectral Method can be included in this general framework.

Numerical Solution of the Infinite Dimensional SLQR Problem

Hermann Mena (University of Innsbruck, Austria)

We consider an stochastic linear quadratic regulator (SLQR) optimal control problem on Hilbert spaces. For a well-posed SLQR problem, the optimal control is given in terms of an stochastic Riccati equation and a backward stochastic differential equation. Existence and uniqueness of the solutions to these equations are available only for certain special cases. We investigate the numerical treatment of the SLQR problem, in particular, the convergence of the Riccati operator. In addition, numerical methods for solving large-scale Riccati equations arising from the discretization are briefly introduced.

Strang Splitting for a NLS with damping and forcing

Marcel Mikl * (Karlsruhe Institute of Technology, Germany)
Tobias Jahnke (Karlsruhe Institute of Technology)

Frequency combs are special solutions of a nonlinear Schrödinger equation with additional damping and forcing terms. It has been experimentally demonstrated that these frequency combs can be used for high-speed data transmission [1]. However, there is a lack of mathematical analysis for simulation techniques. In this talk I will discuss a Strang splitting approach, where the equation is partitioned into the non-linear part and the linear part together with the forcing term. It is well-known that the non-linear part can be solved exactly. The inhomogeneous linear part is propagated with the exponential trapezoidal rule. I will present a short sketch of the convergence proof, which is strongly related to the basic structure of [2]. Concluding, I will address some open questions regarding the simulation of frequency combs.

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Operator-splitting method for numerical modeling of unsteady viscoplastic Bingham medium flows

Ekaterina Muravleva * (Institute of Numerical Mathematics, Russian Academy of Sciences, Russia)
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The numerical simulation of viscoplastic fluid flow is difficult due to the non- differentiable form of the constitutive law and the inability to evaluate the stresses in regions where the material has not yielded. There are two main approaches that have been proposed in the literature in order to overcome the aforementioned mathematical difficulties in solving viscoplastic flows. The first one, known as regularization method, consists of approximating the constitutive equation by a smoother one. The second one is based on the theory of variational inequalities by means of which the problem is reduced to the minimization of a functional and requires the solution of the equivalent saddle-point problem. Regularization methods may offer an attractive alternative to the ideal Bingham model for engineering calculations, but may also mask interesting viscoplastic effects. It has been convincingly argued that variational inequalities are better suited for obtaining accurate results for the yielded/unyielded zones and finite stopping times when using the ideal Bingham model.
We use the generalization of the finite-difference scheme on staggered grids with auxiliary grids for discretization of the strain and stress tensors [1]. We have employed operator splitting method to simplify the computation. The system is decoupled into two subsystems by fractional step method: the Navier-Stokes problem and the plasticity problem. The Navier-Stokes problem is solved by the modified Van Kan scheme of the second order and the plasticity problem is solved by Uzawa-like algorithm. The numerical simulation of high Reynolds numbers flow requires in particular a good approximation of the convective terms. They are treated explicitly and approximated by third-order upwind scheme [3]. We have applied the suggested technique to the numerical modelling of the cavity flows: unsteady flows (start-up and cessation) and natural convection in a square cavity with differentially heated vertical sides.
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Time integration of tensor trains

Christian Lubich (University of Tubingen, Germany)
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Approximation of solution of high-dimensional evolution equations plays a crucial role in different application in chemistry and physics. The idea of dynamical low-rank approximation can be traced back to the work by Dirac and Frenkel in quantum physics. In quantum molecular dynamics it is actively used in the framework of multiconfigurational time-dependent Hartree-Fock method (MCTDH) pioneered by H.-D. Meyer and his coauthors [6]. Rigorous mathematical study of the dynamical low-rank approximation was started by C. Lubich and O. Koch [2]. Recently, extension of this approach to novel tensor decompositions, namely tensor-train (TT) and hierarchical Tucker (HT) formats was proposed [1, 3]. It allows for efficient reduction of dimensionality, but leads to a complicated system of nonlinear ODEs.
In [4, 5] we present a very robust and efficient time integrator for dynamical tensor approximation in the tensor train or matrix product state format is presented. The method is based on splitting the projector onto the tangent space of the tensor manifold. The algorithm can be used for updating time-dependent tensors in the given data-sparse tensor train / matrix product state format and for computing an approximate solution to high-dimensional tensor differential equations within this data-sparse format. The proposed integrator is studied both theoretically and numerically. For a 10-dimensional quantum molecular dynamics problem a 10x speed-up over the MCTDH package was obtained. The implementation is available as a part of the **ttpy** package, http://github.com/oseledets/ttpy.

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Time integration of quasilinear Maxwell's equations

Marlis Hochbruck (Karlsruhe Institute of Technology)
Tomislav Pažur * (Karlsruhe Institute of Technology, Germany)

In this talk we consider quasilinear Maxwell's equations in an abstract Hilbert space framework. We are interested in nonlinearities of the form

$$\Lambda(u(t))u'(t) = Au(t), \qquad u(0) = u_0,$$

where the operator A is skew-adjoint and Λ is symmetric and positive definite in some neighborhood of zero. In contrast to the linear case, the well-posedness of this equation is a nontrivial task. On the full space $\mathbb{R}^3$ existence and uniqueness of the solution has recently been proven in [1]
In this talk we present an error analysis for the implicit Euler method and the implicit midpoint rule applied to this abstract problem. Our error analysis is based on energy estimates discussed in [2]. Under appropriate regularity assumptions we establish optimal order a priori error bounds for both methods. We discuss the question of well-posedness of the methods as well.

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On positive explicit peer methods of high order

Helmut Podhaisky * (Martin Luther University Halle-Wittenberg, Germany)
Rüdiger Weiner (Martin Luther University Halle-Wittenberg, Germany)
Horváth Zoltán (Széchenyi István Egyetem Győr, Hungary)

We discuss the construction of explicit general linear methods which preserve the positivity of the solution of certain initial value problems for sufficiently small step sizes. We restrict ourselves to peer methods which are characterized by high stage order. The methods we found by applying numerical tools for constraint optimization (FMINCON and NMinimize) to the SSP condition exhibit an interesting sparsity pattern. We have found positive methods up to order 13.

Baseline Performance Studies of a Hydrodynamics Code with Adaptive Mesh Refinement

Martina Prugger (University of Innsbruck, Austria)

Shock propagation, such as in high-speed flows and explosions, are an important class of problems that can be modeled using hyperbolic systems of PDEs. Since the occurrence of shocks is usually scarce compared with the domain, specialized algorithms, including Adaptive Mesh Refinement (AMR), have been developed to capture their behavior. Good parallel performance of these algorithms is critical, particularly for the next generation of supercomputers with millions of processing units and consequently increased occurrences of soft faults (errors that occur during the runtime of the code and are caused by temporary hardware flaws; e.g., cosmic or radioactive rays, which may lead to random bit flips). In order to focus the effort on areas for improvement, we must understand the current performance of our algorithms. To get some insight in the current state of the art, we investigate the baseline performance of an inviscid gas dynamics code provided by the Chombo AMR software infrastructure [1]. We performed both weak and strong scaling studies on a 2D shock propagation problem with and without adaptivity. Our results were consistent with the previously reported results in [2]. Furthermore, the response of these algorithms to soft faults has not been extensively investigated. To begin to understand the potential effects of those faults and their possible detection, we artificially injected faults by flipping random bits in the solution state vector and generated statistics on the effects of these bit flips on the integral metrics of the solution. Initial results indicate that the algorithm may survive such faults but unacceptable errors are introduced.

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On the similarities and differences between classes of exponential integrators

Mayya Tokman (University of California, Merced)
Greg Rainwater * (University of California, Merced, United States of America)

The idea of using an exponential-like function of a Jacobian to approximate the solution to $y' = f(y)$ led to development of a number of exponential integrators over the past decade. In particular, the most general classes of exponential methods of this type are the exponential Rosenbrock (EXPRB) integrators [1, 2, 5] and the exponential propagation iterative methods of Runge-Kutta type (EPIRK) [4, 3]. As we progress with the development and analysis of exponential methods, it is of interest to better understand the relationship between EXPRB and EPIRK schemes. We present some preliminary work on studying the differences and similarities of these classes of methods in the context of both classical and stiff order conditions. In addition to outlining the structural characteristics of these integrators, we pose some questions focused on how to construct a particularly efficient exponential method for a given problem.

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Analysis of underdamped linear systems driven by Brownian motion with the help of ARMA processes

Alexander Ostermann (University of Innsbruck)
Georg Spielberger * (University of Innsbruck, Austria)

In this talk we consider SDEs resulting from an underdamped linear system driven by Brownian motion. The solution of such an SDE is a weakly stationary stochastic process. The time series, which results from uniform sampling of the solution, is covariance equivalent to an ARMA process [1]. With the aim of applying this result to structural health monitoring we present measured data from a aluminium small-scale four-storey shear frame model and show how damage can be detected and different structural states can be distinguished. The possibility of damage location with ARMA processes is shortly discussed and experimental results are provided.

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Splitting the differential Riccati equation

Eskil Hansen (Lund University)
Tony Stillfjord * (Lund University, Sweden)

In this talk I will present recent results on the application of splitting methods to differential Riccati equations. Such equations arise in many different areas and are especially important within the field of optimal control. We analyse the proposed scheme in the setting of Hilbert-Schmidt operators and conclude that it converges with the same order as the implicit Euler method, under the same low regularity requirements. Further, I will show that the scheme preserves two structural properties of the initial condition. Firstly, the solution is positive semi-definite, like the exact solution. Secondly, the scheme preserves low rank in the finite-dimensional case, such as after a spatial discretization. The latter property is essential in large-scale problems, as otherwise both the storage and computational requirements become unfeasible. I will conclude by showing results from applying the method to the real-world application of optimal cooling of steel.

Locally implicit time integration for linear Maxwell's equations

Marlis Hochbruck (Karlsruhe Institute of Technology)
Andreas Sturm * (Karlsruhe Institute of Technology, Germany)

An attractive feature of discontinuous Galerkin (DG) spatial discretizations of the Maxwell equations is their ability to handle complex geometries by using unstructured, possibly locally-refined meshes. Furthermore, DG methods lead to block diagonal mass matrices which in combination with an explicit time integration method allow for a fully explicit scheme. However, such explicit approaches require a constraint on the time step size related to the smallest mesh element to ensure stability. This makes the simulation inefficient if the number of tiny elements is small compared to the total number of elements. A natural way to overcome this restriction is obtained by using implicit time integrators but at the expense of having to solve a large linear system each time step.
A more suitable approach consists in treating only the tiny mesh elements implicitly while retaining an explicit time integration for the remaining elements. This results in so called locally implicit methods which have been considered in [1, 2], for instance.
In this talk we will present an error analysis for the full discretization of locally implicit methods based on a variational formulation and energy techniques.

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Most unstable trajectories of linear switched systems

Nicola Guglielmi (University of L'Aquila)
Marino Zennaro * (University of Trieste, Italy)

We deal with discrete-time *linear switched system* of the form

$$x(n+1) = A_{\sigma(n)}\, x(n), \quad \sigma : \mathbf{N} \longrightarrow \{1, 2, \ldots, m\},$$

where $x(0) \in \mathbf{R}^k$ and $A_{\sigma(n)} \in \mathbf{R}^{k\times k}$ is an element of a finite family of matrices $\mathcal{F} = \{A_i\}_{1\le i\le m}$ associated to the system and σ denotes the *switching law*.
It is known that the *most unstable switching laws* are associated to the so-called *spectrum-maximizing products* of the family $\mathcal{F}$ and that, if $\mathcal{F}$ is normalized (i.e., its *joint spectral radius* $\rho(\mathcal{F})$ is equal to 1), for any initial value $x(0)$ the *most unstable trajectories* lie on the boundary of the unit ball of a so-called *invariant Barabanov norm*.
So far no general constructive method was proposed to determine such invariant Barabanov norms. In this talk (see also Guglielmi & Zennaro [2]) we show how, parallel to the constructive procedure for polytope extremal norms recently introduced by Guglielmi, Wirth & Zennaro [1], a canonical constructive procedure for invariant Barabanov norms can be automatically provided as well.

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