# $6^{\text{th}}$ International Seminar on Numerical Mathematics NAday08

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**Edited by**
**Bojan Orel, Andrej Perne and Emil Žagar**

**Ljubljana, June 2008**

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# List of Abstracts

**Subspace gap residuals for Rayleigh-Ritz approximations**

Nela Bosner*, Zlatko Drmač
University of Zagreb
Croatia

Large scale eigenvalue and singular value computations are usually based on extracting information from a compression of the matrix to suitably chosen low dimensional subspaces. In this presentation we introduce a new posteriori relative error bounds based on a residual expressed using the largest principal angle (gap) between relevant subspaces. The eigenvector approximations are estimated using subspace gaps and relative separation of the eigenvalues.

**Stability analysis of the Gurtin-MacCamy model**

Dimitri Breda*, Mimmo Iannelli, Stefano Maset, Rossana Vermiglio
University of Udine
University of Trieste
Italy

In this talk we propose a numerical scheme to investigate the stability of steady states of the nonlinear Gurtin-MacCamy system which is a basic model in population dynamics. In fact the analysis of stability is usually performed by the study of transcendental characteristic equations that are too difficult to approach by analytical methods. The method is based on the discretization of the infinitesimal generator associated to the semigroup of the solution operator by using pseudospectral differencing techniques. The method computes the rightmost characteristic roots and it is shown to converge with spectral accuracy behavior.

## A Chebyshev Series Expansion Method with Break-point Location for State-dependent Delay Differential Equation Initial Data Problems

Paule Ečimović
York University
Canada

A method for approximating solutions to intial data problems of state-dependent delay differential equations will be presented based on Chebyshev series expansion combined with discontinuity location. The performance of this method will be compared to that of some codes based on implicit Runge-Kutta integration schemes on an initial data problem test set. Various approaches to performance enhancement of this method will also be presented.

## Highly oscillatory Fredholm operators: from spectral methods to modified Fourier expansions

Arieh Iserles
University of Cambridge
United Kingdom

In this talk we report recent advances in the calculation of spectra of complex-valued highly oscillatory Fredholm operators by the finite section method. Standard considerations based on spectral methods seem to indicate that expansions in Legendre polynomials are likely to lead to rapid convergence, hence to small matrices. However, calculation of matrix coefficients is expensive. On the other hand, modified Fourier expansions come with rapid algorithms for the calculation of coefficients. Moreover, their slower convergence is offset by the technique of hyperbolic cross. So far, all is intuitive – but numerical results seem to indicate that, surprisingly, the 'slowly convergent' modified Fourier basis actually leads to smaller matrices. Careful asymptotic analysis reveals the truth: numerical results are right and intuition wrong!

## Interpolation by Planar Cubic $G^2$ Pythagorean-hodograph Spline Curves

Gašper Jaklič*, Jernej Kozak, Marjetka Krajnc, Vito Vitrih, Emil Žagar
Instiute of Mathematics, Physics and Mechanics
University of Ljubljana
University of Primorska
Slovenia

In this talk, the geometric interpolation of planar data points and two boundary tangent directions by a cubic $G^2$ Pythagorean-hodograph (PH) spline curve will be considered. It is well known that any cubic PH curve is a segment of a Tschirnhausen curve, which does not have any inflection points. Thus it is expected that such a curve can not be used to interpolate arbitrary chosen planar data points. But it will be shown that under some restrictions on data points such an interpolant exists.

An algorithm for the construction of the spline will be presented and numerical examples given which indicate that the resulting spline curve has nice shape properties. At the end some heuristic preprocessing methods for data points which do not guarantee the existence of the spline curve will be described.

## Graph-Theoretical Approach for Protein Binding-Sites Prediction

Dušanka Janežič
National Institute of Chemistry
Slovenia

A new algorithm for finding a maximum clique in an undirected graph is described. An approximate coloring algorithm has been improved and used to provide bounds to the size of the maximum clique in a basic algorithm which finds a maximum clique. This basic algorithm was then extended to include dynamically varying bound and later used for protein binding-sites prediction. The algorithm uses the conservation of 3D structure of protein surfaces, as opposed to their sequences, to detect protein-protein binding sites. The protein in which protein-protein binding sites are sought is compared with structures of multiple structurally related proteins and the surface that is conserved at least once is considered to be a part of the binding site. The binding site predictions obtained in this way for a set of protein-protein complexes correspond well with the actual protein-protein binding sites.

**Runge–Kutta methods for stochastic differential- and differential–algebraic equations**

Anne Kværnø*, Kristian Debrabant, Dominique Küpper
University of Trondheim
TU Darmstadt
Norway

The first part of this talk is devoted to a unified order theory for Runge-Kutta methods applied to stochastic differential equations. In the second part of the talk, these ideas are used to derive methods for differential-algebraic equations, with emphasis on applications from electrical circuit theory.

**Numerical approximation of characteristic values of Partial Retarded Functional Differential Equations: part II**

Dimitri Breda, Stefano Maset*, Rossana Vermiglio
University of Udine
University of Trieste
Italy

The stability of an equilibrium point of a dynamical system is determined by the position in the complex plane of the so-called characteristic values of a linearization around the equilibrium.

In this talk we extend the results given for Retarded Functional Differential Equations in the first part and we present an approach for the numerical computation of characteristic values of semi-linear partial differential equations of evolution involving time delay, restated as abstract linear retarded functional differential equations

$$\frac{dv(t)}{dt} = A_T v(t) + L v_t,\ t \geq 0,$$

where $v(t)$ belongs to a Banach space $X$, $A_T$ is the infinitesimal generator of a $C_0$-semigroup on $X$, $v_t$ is the function

$$v_t(\theta) = v(t+\theta),\ \theta \in [-r, 0],$$

belonging to the space $\mathcal{C}$ of the continuous functions $[-r, 0] \to X$ and $L : \mathcal{C} \to X$ is a linear bounded functional.

The numerical approach is a combination of a pseudospectral method for the discretization of functions defined in $[-r, 0]$ with a spectral method for the discretization of $X$. The convergence of the approximated characteristic values to the exact ones is of infinite order with respect to the pseudospectral discretization and only of finite order with respect to the spectral discretization. However, for one dimensional reaction diffusion equations, the finite order of the spectral discretization is so high that the convergence turns out to be as fast as one of infinite order.

## Progressive lens design

Jernej Krmelj, Bojan Orel*, Boris Turk
University of Ljubljana
Slovenia

The common option in treatment of presbyopia is by progressive optical lenses. In the upper part of the lens (the distant vision area) the powwer is less then in the lower part (the near vision area). Between this two parts (the intermidiate vision area) the power is smoothly changing. The unplesant consequece of the changing power of the lens is astigmatism. For the overall quality of the progressive lens it is very important to reduce the astigmatism. We will present a novel approach to solve this problem.

## Numerical approximation of characteristic values of Partial Retarded Functional Differential Equations: part I

Dimitri Breda, Stefano Maset, Rossana Vermiglio*
University of Udine
University of Trieste
Italy

The stability analysis of equilibrium points plays a main role in the study of Partial Retarded Functional Differential Equations (PRFDEs). The stability of an equilibrium point of the dynamical system is determined by the position in the complex plane of the infinite characteristic values of the linearization around the equilibrium. We present a numerical approach for the computation of characteristic values for linear PRFDEs and we organize it into two parts.

In the first part, we consider linear autonomous Retarded Functional Differential Equations (RFDEs)

$$\frac{dv(t)}{dt} = Lv_t,\ t \geq 0,$$

where $v_t$ is the function

$$v_t(\theta) = v(t+\theta),\ \theta \in [-r, 0],$$

belonging to the space $\mathcal{C}$ of the continuous functions $[-r, 0] \to \mathbb{R}^d$ and $L : \mathcal{C} \to \mathbb{R}^d$ is a linear bounded functional. We present in particular the Infinitesimal Generator method, which is based on the discretization of the infinitesimal generator by pseudospectral techniques into a finite dimensional linear operator whose eigenvalues provide approximations of the characteristic values. The convergence of infinite order represents, for sufficiently small error tolerance, the outstanding advantage of this technique.

## The joint spectral radius of a matrix family: applications and computational aspects

Marino Zennaro
University of Trieste
Italy

The study of a linear discrete dynamical system of the form $x^{(k+1)} = A^{(k)}x^{(k)}$, $k \geq 0$, is important for a large number of applications. Of particular interest is the asymptotic behaviour of its solutions, which is related to the so-called joint spectral radius $\rho$ of its associated family $\mathcal{F} = \{A^{(k)}\}_{k\geq 0}$. More precisely, a system is stable if $\rho < 1$ or if $\rho \leq 1$ and there exists an extremal norm.

In order to compute or approximate the joint spectral radius, in the literature of the last decades some algorithms have been proposed in order to find real extremal norms of polytope type in the case of finite families $\mathcal{F}$. Anyway, recently it has been observed that it is sometimes necessary to enlarge the class of norms to that of complex polytope norms.

In this talk, I review some of the last results obtained jointly with N. Guglielmi in this direction. In particular, I present an existence result of extremal complex polytope norms and a related constructive algorithm.

**Geometric Lagrange Interpolation by Planar Cubic Pythagorean-hodograph Curves**

Gašper Jaklič, Jernej Kozak, Marjetka Krajnc, Vito Vitrih, Emil Žagar*
Instiute of Mathematics, Physics and Mechanics
University of Ljubljana
University of Primorska
Slovenia

Planar Pythagorean-hodograph (PH) curves are a subclass of polynomial parametric curves which have some specific properties. In particular, the norm of their hodograph (the vector of derivatives of components) is a polynomial and their offset is a rational function. This makes them very useful in various practical applications, such as CAGD, CAD/CAM systems, robotics, animation,...

The parametric and geometric Hermite interpolation by PH curves are nowadays well established approaches for an approximation of discrete data but there are no results on *geometric* Lagrange interpolation methods. In this talk a geometric Lagrange interpolation by planar cubic PH curves will be considered. It will be shown that such an interpolatory curve can interpolate 4 data points provided that a data polygon, formed by the interpolation points, is convex, and satisfies an additional restriction on its angles. This gives rise to a conjecture that a PH curve of degree $n$ can, under some natural restrictions on data points, interpolate up to $n + 1$ points.

# List of Participants


Alfredo Bellen
University of Trieste
Italy
bellen@units.it

Zvonimir Bohte
University of Ljubljana
Slovenia
zvonimir.bohte@fmf.uni-lj.si

Iztok Bajc
University of Nova Gorica
Slovenija
iztok.bajc@libero.it

Nela Bosner
University of Zagreb
Croatia
nela@math.hr

Dimitri Breda
University of Udine
Italy
dimitri.breda@dimi.uniud.it

Paule Ečimović
York University
Canada
paule@certrex.net

Arieh Iserles
University of Cambridge
United Kingdom
ai@damtp.com.ac.uk

Gašper Jaklič
University of Ljubljana
Slovenia
gasper.jaklic@fmf.uni-lj.si

Dušanka Janežič
National Institute of Chemistry
Slovenia
dusa@cmm.ki.si

Maja Karaga
University of Zagreb
Croatia
karaga@math.hr

Andrej Kmet
University of Ljubljana
Slovenia
andrej.kmet@fmf.uni-lj.si

Jernej Kozak
University of Ljubljana
Slovenia
jernej.kozak@fmf.uni-lj.si

Marjetka Krajnc
University of Ljubljana
Slovenia
marjetka.krajnc@fmf.uni-lj.si

Anne Kværnø
University of Trondheim
Norway
anne@math.ntnu.no

Stefano Maset
University of Trieste
Italy
maset@univ.trieste.it

Brendon McQueen
University of Technology, Sydney
Australia
brendon.mcqueen@uts.edu.au

Andrej Muhič
University of Ljubljana
Slovenia
andrej.muhic@fmf.uni-lj.si

Bojan Orel
University of Ljubljana
Slovenia
bojan@gollum.fri.uni-lj.si

Andrej Perne
University of Ljubljana
Slovenia
andrej.perne@fe.uni-lj.si

Bor Plestenjak
University of Ljubljana
Slovenia
bor.plestenjak@fmf.uni-lj.si

Mladen Rogina
University of Zagreb
Croatia
rogina@math.hr

Lucio Torelli
University of Trieste
Italy
torelli@units.it

Roman Trobec
Institute Jožef Stefan
Slovenia
roman.trobec@ijs.si

Rossana Vermiglio
University of Udine
Italy
vermiglio@dimi.uniud.it

Vito Vitrih
University of Ljubljana
Slovenia
vito.vitrih@pef.upr.si

Martin Vuk
University of Ljubljana
Slovenia
martin.vuk@fri.uni-lj.si

Marino Zennaro
University of Trieste
Italy
zennaro@units.it

Emil Žagar
University of Ljubljana
Slovenia
emil.zagar@fmf.uni-lj.si