First Congress of Greek Mathematicians
Special Session in Numerical Analysis and Scientific Computing
June 27-28, 2018

Organizers

Georgios Akrivis – Konstantinos Chrysafinos – Manolis Georgoulis
Chrysoula Tsogka – Georgios Zouraris

Time Schedule of Talks

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Speakers

Georgios Akrivis (University of Ioannina)

On the stability of implicit–explicit multistep methods

We study the stability of implicit–explicit multistep methods, with particular emphasis on the popular implicit–explicit BDF methods, applied to Dahlquist’s test problem.
Joint work with E. Katsoprinakis (U. of Crete).

George Anastassiou (University of Memphis)

Approximation by Choquet integrals

Here we present the quantitative approximation of positive sublinear operators to the unit operator. These are given a precise Choquet integral interpretation. Initially we start with the study of the rate of the convergence of the well-known Bernstein-Kantorovich-Choquet and Bernstein-Durrweyer-Choquet polynomial Choquet-integral operators. Then we study the very general comonotonic positive sublinear operators based on the representation theorem of Schmeidler (1986). We finish with the approximation by the very general direct Choquet-integral form positive sublinear operators. All approximations are given via inequalities involving the modulus of continuity of the approximated function or its higher order derivative.

Dimitra Antonopoulou (University of Chester)

Finite elements for stochastic PDEs from phase separation

We consider a class of \( \varepsilon \)-dependent nonlinear stochastic PDEs of Cahn-Hilliard and Allen-Cahn type, with additive noise. The positive parameter \( \varepsilon \) models the width of the
layers that may develop during the phase separation of a binary alloy. We construct finite element schemes proper for our models, and derive optimal a priori error estimates.

**Agis Athanassoulis** (University of Dundee)

*Error control for the nonlinear Heisenberg-von Neumann equation*

The nonlinear Heisenberg-Von Neumann equation (NLHvN) appears in many applications, including for example quantum chemistry, ocean waves (where it is called Alber equation) and recently in cosmology (as the quantised Vlasov-Poisson equation). Despite its wide use, no rigorous numerical analysis for the NLHvN exists in the literature. Thus developing practical methods for the NLHvN, with good stability and convergence properties, is a natural goal.

The main difficulty in proposing and analysing efficient numerical methods for the NLHvN is that the trace of the approximation (i.e. the approximate position density) will appear in the definition of the method, leading to effective reduction of smoothness and making standard techniques not applicable. However, the appearance of the trace is in agreement with the continuous problem, and it should be implemented appropriately for an efficient numerical method.

Having all this in mind, we considered two numerical schemes for the numerical solution of the NLHvN. More precisely, we propose a first order implicit-explicit Euler method and a second order relaxation Crank-Nicolson scheme. For both methods, we are able to prove that the approximations satisfy a discrete analogue of the mass invariance that the continuous problem satisfies. We also prove stability and consistency estimates. The Wiener algebra norm is used to effectively control the trace.

Joint work with G. Akrivis (Ioannina) and I. Kyza (Dundee).

**George Biros** (University of Texas, Austin)

*N-body algorithms in computational science and machine learning*

*N*-body algorithms are the computational cornerstone for many problems in computational science and engineering. In this talk, I will present (1) a brief history of *N*-body algorithms and their application to multiscale problems; (2) give a brief overview of the most basic *N*-body algorithm, the Barnes-Hut method; (3) expand the notion of *N*-body problems to high-dimensional problems and statistical inference; (4) conclude with applications of *N*-body algorithms to physics (fluid mechanics) and statistics (supervised learning).

**Konstantinos Chrysafinos** (National Technical University of Athens)

*Stability analysis and error estimates of fully-discrete schemes for the Brusselator equations*

The Brusselator system consists of two coupled nonlinear parabolic reaction-diffusion PDEs with different diffusion constants. This type of system arises in chemical kinetics, and in pattern formation theory. In this talk, we discuss several results regarding stability and error estimates of suitable fully-discrete schemes of arbitrary order. In particular, fully-discrete schemes based on a discontinuous (in time) Galerkin approach, combined with standard conforming finite elements in space, are analyzed and various stability properties are presented under minimal regularity assumptions on the given data. Using properties of the discrete additive dynamics of the system, and a bootstrap argument, we establish stability bounds in the natural energy norm, with bounds depending polynomially upon the inverse of the diffusion constants. Special care is exercised to avoid any restriction between the temporal and spacial discretization parameters. In addition, a-priori error estimates are presented in the energy norm under a smallness assumption on
the size of the temporal discretization parameter. The error analysis also includes higher order schemes.

**Vassilios A. Dougalis** (National and Kapodistrian University of Athens and Institute of Applied and Computational Mathematics, FORTH)

*Numerical solution of long-wave models in surface water-wave theory*

Considered in this talk will be long-wave (shallow-water) nonlinear pde systems that model propagation of surface water waves, approximating solutions of the 2d Euler equations. These will include the nonlinear hyperbolic system of shallow water equations, the weakly nonlinear dispersive Boussinesq systems, the fully nonlinear dispersive Serre equations, and the Camassa-Holm equation. A review will be given of issues such as modelling, well-posedness, and the numerical analysis of such systems. Results of numerical experiments simulating properties of solitary-wave solutions of the dispersive systems will also be shown.

**Emmanuil H. Georgoulis** (University of Leicester / National Technical University of Athens / IACM-FORTH)

*Discontinuous Galerkin methods on polygonal and polyhedral elements*

Numerical methods defined on computational meshes comprising of polygonal and/or polyhedral (henceforth collectively termed “polytopic”) elements, with, potentially, many faces, have gained substantial traction recently for a number of important reasons. A key underlying issue is the design of a suitable computational mesh upon which the underlying PDE problem will be discretized. The task of generating the mesh must address two competing issues. The mesh should provide a good representation of the given computational geometry with sufficient resolution for the accurate approximations. On the other hand, the mesh should not be so fine that computational complexity becomes prohibitive, due to the high number of numerical degrees of freedom. Standard mesh generators generate grids consisting of triangular/quadrilateral elements in 2D and tetrahedral/hexahedral/prismatic/pyramidal elements in 3D. In the presence of essentially lower-dimensional solution features, for example, boundary/internal layers, anisotropic meshing may be exploited. However, in regions of high curvature, the use of such highly-stretched elements may lead to element self-intersection, unless the curvature of the geometry is carefully propagated into the interior of the mesh through the use of (computationally expensive) isoparametric element mappings. These issues are particularly pertinent in the context of high-order methods, since in this setting, accuracy is often achieved by exploiting coarse meshes in combination with local high-order polynomial basis functions. I will argue that, by dramatically increasing the flexibility in terms of the set of admissible element shapes present in the computational mesh, the resulting, possibly discontinuous, FEMs can potentially deliver dramatic savings in computational costs. Moreover, I will present some recent theoretical developments in the error analysis of such methods.

**Mohammad Javidi** (University of Tabriz, Iran)

*A numerical solution for fractional differential equations*

In this work, the predictor-corrector (PC) approach is used to propose an algorithm for the numerical solution of non-linear fractional differential equations (FDEs). The properties of the Caputo derivative are used to reduce the fractional differential equation into a Volterra integral equation. Then polynomial approximation is used to approximate integral and achieve new schemes for numerical solution of the FDEs. The error and stability analysis of each of the methods is carried out. The proposed scheme is compared with the PC schemes of literature for illustrating the effectiveness of the algorithm.

Joint work with Mohammad Shahbazi Asl.
Fotini Karakatsani (University of Chester)

On the error control for fully discrete approximations of the time-dependent Stokes equation

We consider fully discrete finite element approximations to the time-dependent Stokes system. The space discretization is based on popular stable spaces, including Crouzeix-Raviart and Taylor-Hood finite element methods. Implicit Euler is applied for the time discretization. The finite element spaces are allowed to change with time steps and the projection steps include alternatives that are hoped to cope with possible numerical artifices and the loss of the discrete incompressibility of the schemes. The final estimates are of optimal order in $L^\infty(L^2)$ for the velocity error.

Joint work with Eberhard Bänisch (University of Erlangen, Germany), Charalambos Makridakis (University of Crete & IACM FORTH, Greece).

Stelios Kotsios (National and Kapodistrian University of Athens, Department of Economics)

Invariants Of A Planar Point Cloud Undergoing A Linear Transformation

The goal of this paper is to present invariants of planar point clouds, that is functions which take the same value before and after a linear transformation of a planar point cloud via a $2 \times 2$ invertible matrix. In the approach we adopt here, these invariants are functions of two variables derived from the least squares straight line of the planar point cloud under consideration. A linear transformation of a point cloud induces a nonlinear transformation of these variables. The said invariants are solutions to certain Partial Differential Equations, which are obtained by employing Lie theory. We find cloud invariants in the general case of a fourparameter transformation matrix, as well as, cloud invariants of various oneparameter sets of transformations which can be practically implemented. Case studies and simulations which verify our findings are also given. The invariants we find lend itself to practical implementation. By practical implementation we mean that these invariants can be used as a tool for studying changes of planar figures and for creating proper software which monitors and displays these changes in real time. This would have many applications in optical character recognition, as well as, in image analysis and computer graphics techniques; icons created by the same “source” will be readily identified. Joint work with Evangelos Melas.

Irene Kyza (University of Dundee)

A posteriori error control for evolution nonlinear Schrödinger equations

We provide a posteriori error estimates for fully discrete approximations for a class of evolution Schrödinger equations, including nonlinear Schrödinger equations up to the critical exponent. The estimates are obtained in the $L^\infty(L^2)$-norm and are of optimal order. For the discretisation in time we use a relaxation Crank-Nikolson scheme which is a generalisation to variable time steps of the relaxation scheme introduced earlier in [Ch. Besse, A relaxation scheme for the nonlinear Schr"{o}dinger equation, SIAM J. Numer. Anal. 42 (2004), 934-952] for constant time steps. For the spatial discretisation we use finite element spaces that are allowed to change from one time-step to another.

For the derivation of the estimates we use the reconstruction technique and nonlinear stability arguments as in the continuous problem. More precisely, key ingredients for our analysis include the time-space reconstruction for the relaxation Crank-Nicolson finite element scheme; the conservation laws available for the continuous problem; and appropriate bounds of the $L^\infty(L^2)$-norm of the gradient of the exact solution of the continuous problem.

Various numerical experiments verify and complement our theoretical results.

This is joint work with Th. Katsaounis (KAUST & University of Crete).
Dimitrios Mitsoudis (University of West Attica)

*Imaging Extended Reflectors in a Terminating Waveguide*

We consider the problem of imaging extended reflectors in a terminating waveguide $\Omega \subset \mathbb{R}^2$ that consists of two subdomains: a semi-infinite strip $\Omega_{L-} = (-\infty, L) \times (0, D)$ and a bounded domain $\Omega_{L+}$. We assume that the medium is homogeneous in $\Omega_{L-}$, while it can be inhomogeneous in $\Omega_{L+}$, which may also contain the reflector to be imaged.

We introduce an imaging functional that relies on the back-propagation of a modal projection of the array response matrix. The projection is adequately defined for any array aperture size that covers fully or partially the waveguide’s vertical cross-section. A resolution analysis of the proposed imaging method shows that the resolution of the image is determined by the central frequency, while the signal-to-noise ratio improves as the bandwidth increases.

The resulting images provide reconstructions that allow us to recover the reflector’s location, size and shape with very good accuracy. Moreover, as one may intuitively expect, in the terminating waveguide we benefit from the reflections (multiple-scattering paths) that bounce off the terminating boundary of the waveguide, thus providing views of the reflector that are not available in an infinite waveguide.

The robustness of the imaging method is assessed with fully non-linear scattering data in terminating waveguides with complex geometries.

Joint work with Chrysoula Tsogka and Symeon Papadimitropoulos.

Dimitrios Noutsos (University of Ioannina)

*Preconditioned GMRES Method for the Solution of Non-Symmetric Real Toeplitz Systems*

Preconditioned conjugate gradient (PCG) methods are widely used to solve ill-conditioned real symmetric and positive definite Toeplitz linear systems $T_n(f)x = b$. This case has been entirely studied while the case of real non-symmetric and non-definite Toeplitz systems is still open. Toeplitz matrices have the same entries along their diagonals. Such systems appear in various Mathematical Topics: differential and integral equations, Mechanics, Fluid Mechanics and in applications: signal processing, image processing and restoration, time series and queueing networks.

The PCG method, fails to solve non-symmetric systems. We focus on finding fast and efficient methods, based on Krylov subspaces, to solve large real non-symmetric Toeplitz systems. Especially, we concentrate on Preconditioned Generalized Minimum Residual (PGMRES) method. Real nonsymmetric Toeplitz systems are generated by complex symbols $f = f_1 + if_2$, where $f_1$ and $f_2$ are $2\pi$-periodic even and odd, respectively functions. If $f_1$ and $f_2$ have roots in $[-\pi, \pi]$, then the problem becomes illconditioned and some kind of preconditioning is necessary.

We propose efficient band Toeplitz preconditioners generated by symbols being trigonometric polynomials, which aim to raise the roots and to give some kind of approximation of $f_1$ and $f_2$. We achieve good clustering of the singular values of the preconditioned matrix in a small interval around 1. We also show the efficiency of the proposed technique by various numerical experiments.

Joint work with Grigorios Tachyridis.

Evangelos Papoutselis (Université d’Orléans)

*Spatiotemporal PET reconstruction using total variation based priors*

In this talk, we discuss spatiotemporal reconstruction in the Positron Emission Tomography (PET) framework. We consider regularizers on total variation priors adapted to problems related to Poisson noise degradation. In particular, we consider spatiotemporal total variation and total generalized variation and their corresponding extensions to the
infimal convolution regularization. The numerical solutions of the corresponding variational problems are performed using Primal-Dual Hybrid Gradient optimization methods under a diagonal preconditioning. Our numerical experiments performed on human brain phantoms with different radiotracers, indicate that the infimal convolution approaches provide better reconstructions compared to the state of the art MLEM reconstructions.

Joint work with M. Bergounioux, S. Stute and C. Tauber.

Panayiotis Psarrakos (National Technical University of Athens)

*Gershgorin type sets for polynomial eigenvalue problems*

New localization results for polynomial eigenvalue problems are obtained, by extending the notions of the Gershgorin set, the generalized Gershgorin set (known also as the $\mathcal{A}$-Ostrowski set), the Brauer set, and the Dashnic-Zusmanovich set, to the case of matrix polynomials. For each eigenvalues inclusion set, basic topological and geometrical properties are presented, and illustrative examples are given. Joint work with Christina Michailidou.

Sotirios Sabanis (University of Edinburgh)

*At the crossroads of Numerical and Stochastic Analysis, Computational Statistics and Data Science: The Tamed Unadjusted Langevin Algorithm*

We will consider a typical problem in computational statistics and Baysian inference of sampling from a probability measure $\pi$ having a density on $\mathbb{R}^d$ proportional to $e^{-U(x)}$. The Euler discretization of the associated Langevin stochastic differential equation (SDE) is known to be unstable, when the potential $U$ is superlinear. Based on recent progress of explicit numerical methods for SDEs with superlinear coefficients, the Tamed Unadjusted Langevin Algorithm (TULA) is introduced. Non-asymptotic bounds in $V$-total variation norm and Wasserstein distance of order 2 are obtained between the iterates of TULA and $\pi$.

Nikos Stylianopoulos (University of Cyprus)

*The old Grunsky Matrix in Recent Applications*

We review well-known results regarding the Grunsky coefficients - matrix - inequalities, that played (till the early 80's) a central role in Geometric Function Theory and use them in order to improve recent results in Orthogonal Polynomials and in Quasi-conformal Mappings.

Michael Tsatsomeros (Washington State University)

*Detection and construction of matrices with positive principal minors*

There are several classes of matrices that feature prominently in many mathematical fields and whose numerical detection is quite challenging. One of these classes comprises the matrices all of whose principal minors are positive, known as $P$-matrices. We will discuss a method to detect whether or not a given matrix is a $P$-matrix, as well as the related problem of constructing generic $P$-matrices.

Paris Vassalos (Athens University of Economics and Business)

*A general tool for determining asymptotic spectral distribution of Hermitian matrix sequences*

The approximation theory for sequences of matrices with increasing dimension is a topic having both theoretical and practical interest. In this talk, we consider sequences
of Hermitian matrices with increasing dimension, and we provide a general tool for determining the asymptotic spectral distribution of a “difficult” sequence $A_{nn}$ from the one of “simpler” sequences $B_{n,mn}$ that approximate $A_{nn}$ when $m \to \infty$. The tool is based on the notion of an approximating class of sequences (a.c.s.), and it is applied in a more general setting. As an application we illustrate how it can be used in order to derive the famous Szego theorem on the spectral distribution of Toeplitz matrices.

Joint work with S. Serra Capizzano and C. Garoni.

**Georgios Zouraris** (University of Crete)

*Crank-Nicolson/Finite Element Approximations for a linear 4th order SPDE with additive space-time white noise*

We consider a model initial and Dirichlet boundary value problem for a fourth order linear stochastic parabolic equation in one space dimension, forced by an additive space-time white noise. First, we approximate its solution by the solution of an auxiliary fourth order stochastic parabolic problem with additive, finite dimensional, spectral-type stochastic load. Then, fully discrete approximations of the solution to the approximate problem are constructed by using, for the discretization in space, a standard Galerkin finite element method based on $H^2$-piecewise polynomials and, for time-stepping, the Crank–Nicolson method. Analyzing the proposed discretization approach, we derive strong error estimates that establish optimal rate of convergence without imposing CFL conditions on the discretization parameters.