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BOOK OF ABSTRACTS

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Galerkin and Runge–Kutta methods: Unified formulation and a posteriori error analysis

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AMS subject classification: 65M15, 65M50

Key words: Parabolic equations, single-step methods, a posteriori error analysis, superconvergence.

We consider the time discretization of initial value problems for linear parabolic equations in an abstract Hilbert space setting,

$$\begin{cases} u'(t) + Au(t) = f(t), \quad 0 < t < T, \\ u(0) = u^0, \end{cases} \tag{1}$$

by single-step schemes.

We cast Galerkin and Runge–Kutta methods into a unified formulation; the approximate solutions U are piecewise polynomials in partitions of $[0, T]$. The residual R of U, i.e., the amount by which U misses being exact solution, is in general of suboptimal order. Therefore, the straightforward approach leads to suboptimal a posteriori error estimates.

Using suitable reconstructions $\hat{U}$ of U, we derive optimal order, residual based a posteriori error estimates.

These methods yield, under appropriate compatibility conditions, nodal approximations of order higher than the global order. We derive analogous a posteriori nodal superconvergence estimates.

Solving the Boltzmann equation

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While the analytical study of the solutions of the Boltzmann equation made nice progress, precisely this year, its numerical solution remains a challenge staying beyond current computational capabilities. We shall review in this talk the methods that have been developed recently to solve its linear version (that applies a.o. to neutron and photon transport). We shall restrict to its monoenergetic (monochomatic) version for simplicity. We shall also focus on the developments in which our department took an active part, trying to put them within the framework of a broad historical perpective.

This will cover a.o. the development of mixed hybrid discretization methods taylored to the linear transport equation. Such methods have been actively developed in the recent years for many PDEs and their transport version is based on the even and odd (angular) parity flux decomposition that had been introduced by Vladimirov in the late nineteen fifties.

This decomposition allows us to define primal and dual and thus also mixed variational formulations while the hybrid methods are characterized by the introduction of Lagrange multipliers to enforce interface continuity properties weakly rather than imposing them in a strong sense.

On the other hand, this will also cover the use of spectral expansion methods initiated for 1D geometries by the spectral analyses of Case and Mika and applied in the nineteen sixties to the solution of 1D piecewise uniform media such as cell problems in neutronics, later generalized to multidimensional geometries through the development of transverse integration based nodal codes (which transform multi-dimensional problems into sets of one-dimensional problems coupled by transverse leakage terms).

Present developments under progress concern their direct application to multidimensional geometries and we shall indicate how such generalizations are planned.

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Bypassing tedious computations via numerics guided by targeted experiments: The case of a saturation mechanism investigation

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Abstract

The illumination of mechanisms of wetting of conducting liquids on dielectric solids, due the interaction of electric fields and interfacial tensions, usually requires realistic computations in scales ranging from a few millimetres to hundreds of nanometres or less and particularly in regions where electric field singularities are present. The effect of the field singularities on the dielectric properties of solids is critical since they are connected to physical limitations of electrostatic enhancement of wetting. Direct and securely realistic simulation of the dependence of dielectric properties on high electric field is computationally prohibitive due to the demanding molecular scale computations. However, simple phenomenological relations arising from the interplay between targeted experimentation and continuum computations provide the required accuracy and realism. The core computations involve the solution of the nonlinear partial differential equations of capillary electrohydrostatics with the Galerkin/finite element method. As an example, the illumination of the contact angle saturation in electrowetting is presented and its connection with dielectric breakdown is discussed.

References

A.I. Drygiannakis, A. G. Papathanasiou and A. G. Boudouvis "On the connection between dielectric breakdown strength, trapping of charge and contact angle saturation in electrowetting."*Langmuir* 25, 147 (2009).

A. G. Papathanasiou and A. G. Boudouvis "On the connection between dielectric breakdown strength, trapping of charge and contact angle saturation in electrowetting."*Applied Physics Letters* 86, 164102 (2005).

Impact of Architecture and Technology for Extreme Scale on Software and Algorithm Design

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In this talk we examine how high performance computing has changed over the last 10-year and look toward the future in terms of trends. These changes have had and will continue to have a major impact on our software. Some of the software and algorithm challenges have already been encountered, such as management of communication and memory hierarchies through a combination of compile–time and run–time techniques, but the increased scale of computation, depth of memory hierarchies, range of latencies, and increased run–time environment variability will make these problems much harder.

We will look at five areas of research that will have an importance impact in the development of software and algorithms.
We will focus on following themes:

- Redesign of software to fit multicore architectures
- Automatically tuned application software
- Exploiting mixed precision for performance
- The importance of fault tolerance
- Communication avoiding algorithms

Adaptive methods for time-dependent PDEs

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Self adjusted meshes have important benefits approximating PDEs with solutions that exhibit nontrivial characteristics. When appropriately chosen, they lead to efficient, accurate and robust algorithms. Error control is also important, since appropriate analysis can provide guarantees on how accurate the approximate solution is through a posteriori estimates. Error control may lead to appropriate adaptive algorithms by identifying areas of large errors and adjusting the mesh accordingly. Successful error control and associated adaptive algorithms for important equations in Mathematical Physics is an open problem. In this talk we consider the main structure of an algorithm which permits mesh redistribution with time and the nontrivial characteristics associated with it. We present improved algorithms and we discuss successful approaches towards error control for model problems (linear and nonlinear) of parabolic or hyperbolic type.

Combined Reconstruction and Segmentation in Compressive Spectral Imaging

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A spectral imager captures the power spectral density of light as a function of wavelength w and spatial location (x, y). In other words, it acquires a 3D data cube (tensor) of information, (x, y; w), about the scene being imaged. Knowledge of the spectral content at various spatial locations is invaluable for identifying the composition and structure of objects in the scene being observed. This talk describes our numerical methods for the joint reconstruction and segmentation of spectral images taken by coded aperture snapshot spectral imagers (CASSI). In a snapshot, a CASSI captures a two-dimensional (2D) array of measurements that is an encoded representation of both spectral information and 2D spatial information of a scene, resulting in significant savings in acquisition time and data storage. The reconstruction process decodes the 2D measurements to render a three-dimensional spatio-spectral estimate of the scene, and is therefore an indispensable component of the spectral imager. A two-step iterative shrinkage/thresholding method with total variation regularization is used for reconstructing the spectral datacube. This processes is combined with a variational fuzzy segmentation method to form a joint reconstruction/segmentation model. The advantages of this joint model are illustrated with numerical tests on both simulated and real compressive sensing data.

[1]The presentation represents joint work with David Brady, David Kittle, Fang Li, Michael Ng, Sudhakar Prasad, Ashwin Wagadarikar, and Peter Zhang.

Bergman Orthogonal Polynomials: Asymptotics, Zeros and Shape Reconstruction

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Key words: Bergman orthogonal polynomials, zeros of polynomials, strong asymptotics, equilibrium measure, shape reconstruction, geometric tomography.

Let $G := \cup_{j=1}^{N} G_j$ be the union of N mutually exterior, bounded Jordan domains G_j in the complex plane and let $\{P_n\}_{n=0}^{\infty}$ denote the sequence of *Bergman polynomials* of G. This is defined as the sequence

$$P_n(z) = \lambda_n z^n + \cdots, \quad \lambda_n > 0, \quad n = 0, 1, 2, \ldots,$$

of polynomials that are orthonormal with respect to the inner product

$$\langle f, g \rangle := \int_G f(z)\overline{g(z)} dA(z),$$

where dA stands for the area measure. (In the case when $N > 1$ we call G an *archipelago*.)

The purpose of the talk is to present some very recent developments regarding the theory and applications of Bergman polynomials.

These developments include: (i) Strong asymptotics for the Bergman polynomials, in the single component case $N = 1$, over domains with corners. (ii) Distribution of zeros and estimates of $P_n(z)$, in the archipelago case. (iii) An reconstruction algorithm for recovering the shape of an archipelago G from a finite section of its complex moment matrix:

$$\mu_{mn} := \int_G z^m \overline{z}^n dA(z), \;\; 0 \leq m, n \leq k.$$

The importance of this algorithm in the general shape-reconstruction-problem in 2D geometric tomography, is underlined by the fact that suitable tomographic data (for example, parallel ray measurements) of the uniformly distributed area measure on G, can be transformed into a finite section of the moment matrix.

The construction of second derivative general linear methods for numerical solution of ODEs

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Key words: Ordinary differential equation, General linear methods, Runge–Kutta stability.

Second derivative general linear methods (SGLMs) are an extension of general linear methods (GLMs) that are used for the numerical solution of autonomous system of ordinary differential equations

$$y' = f(y(x)), \qquad y : \mathbb{R} \to \mathbb{R}^m, \qquad f : \mathbb{R}^m \to \mathbb{R}^m. \tag{1}$$

An SGLM makes use of r input and output values and s first and second derivatives stage values. These methods are characterized by six matrices denoted by $A, \overline{A} \in \mathbb{R}^{s\times s}$, $U \in \mathbb{R}^{s\times r}$, $B, \overline{B} \in \mathbb{R}^{r\times s}$ and $V \in \mathbb{R}^{r\times r}$. In an SGLM, these quantities are related by the formula

$$Y_i^{[n]} = \sum_{j=1}^{s} h a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{s} h^2 \overline{a}_{ij} g(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, 2, \cdots, s, \tag{2}$$

$$y_i^{[n]} = \sum_{j=1}^{s} h b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{s} h^2 \overline{b}_{ij} g(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \cdots, r, \tag{3}$$

where $g(\cdot) = f'(\cdot)f(\cdot)$ for function f introduced in (1)

We will divide SGLMs into four types, depending on the nature of the differential system to be solved and the computer architecture that is used to implement these methods. For type 1, matrices A and $\overline{A}$ are lower triangular with the same element 0 on the diagonal and for type 2, matrices A and $\overline{A}$ are lower triangular with the same element $\lambda > 0$, $\mu < 0$ on the diagonal, respectively. Such methods are appropriate for nonstiff or stiff differential systems in a sequential computing environment. For type 3 or 4 methods, matrices A and $\overline{A}$ take the form

$$A = diag(\lambda, \lambda, \cdots, \lambda) = \lambda I, \tag{4}$$

$$\overline{A} = diag(\mu, \mu, \cdots, \mu) = \mu I, \tag{5}$$

where $\lambda = \mu = 0$ and $\lambda > 0$, $\mu < 0$, respectively. Such methods are appropriate for nonstiff or stiff differential systems in a parallel computing environment.

Since Runge–Kutta methods have excellent stability properties, it is desirable that SGLMs to be equipped by Runge–Kutta stability property. In this paper, we will construct some methods in type 4 which have Runge–Kutta stability property.

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A stabilized GPBiCG method with a strategy to remedy accuracy of Bi-CG coefficients for solving linear systems

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Key words: linear systems, Krylov subspace method, generalized product-type method, Bi-CG, hybrid Bi-CG, Lanczos-type method.

Bi-conjugate gradient (Bi-CG) is a well-known method for solving linear systems $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$ for $\boldsymbol{x}$, where $\mathbf{A}$ is a given n-by-n matrix, and $\boldsymbol{b}$ a given n-vector. A number of hybrid Bi-CG methods such as conjugate gradient squared (CGS), Bi-CG STABilized (Bi-CGSTAB), BiCGStab2, BiCGstab(ℓ), Generalized Product-type Bi-CG (GPBiCG), and BiCG×MR2 have been developed to improve the convergence of Bi-CG and to avoid multiplication by the transpose conjugate $\mathbf{A}^*$ of $\mathbf{A}$.

The residual polynomials of hybrid Bi-CG methods can be expressed as the product of the bi-Lanczos polynomial and other, so-called *stabilizing polynomials*, say P_k, with $P_k(0) = 1$ and degree k. In GPBiCG and BiCG×MR2, these stabilizing polynomials can be generated by a three-term recurrence similar to the Lanczos polynomials but with different recurrence coefficients. As the Lanczos polynomials, they can also be obtained by coupled two-term recurrences. GPBiCG exploits the coupled two-term version, while BiCG×MR2 exploits the three-term variant. A third variant of GPBiCG, which is referred to as the RG variant of GPBiCG, has been proposed by Röllin and Gutknecht to improve the stability of the original GPBiCG method. The stabilizing polynomials of this variant also rely on the coupled two-term recurrences.

As in BiCG×MR2, we propose to redesign the recurrences of GPBiCG by coupling the coupled two-term recurrences of Bi-CG with the three-term recurrence for the stabilizing. However, the coupled two-term recurrences of Bi-CG that we use differ slightly from the standard ones. This modification appears to lead to slightly more accurate Bi-CG coefficients and allows a more elegant derivation of GPBiCG. We consider two combinations. The recurrences of the resulting two algorithms are different from those of the original GPBiCG, BiCG×MR2, and the RG variant of GPBiCG. The better accuracy of the Bi-CG coefficients in our new variants appears to be important specifically in cases of a long stagnation phase. We therefore propose a strategy to remedy accuracy of BiCG coefficients in our variants. Our numerical experiments show that our new variants are less affected by rounding errors than the original GPBiCG, the RG variant of GPBiCG and BiCG×MR2, and the stabilized GPBiCG method with the strategy is effective.

Algorithms $\mathbb{AH}$ and $\mathbb{AH}2$: On the identification of an H-matrix

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Key words: H-matrices, strictly diagonally dominant matrices

A matrix $A \in \mathbb{C}^{n,n}$ is considered to be an $H-$matrix if and only if there exists a positive diagonal matrix $D \in \mathbb{R}^{n,n}$ so that AD is *(row-wise) strictly diagonally dominant*, that is

$$|a_{ii}|d_i > \sum_{j=1,\ j\neq i}^{n} |a_{ij}|d_j,\ i = 1(1)n.$$

The class of $H-$matrices is of great importance for the numerical solution of linear systems of algebraic equations arising in various applications, for instance, in the Linear Complementarity Problem (LPC) in Optimization Theory, in the Free Boundary Value Problems in Fluid Analysis, etc. This lead to wide study and proposals of criteria, the majority of which are iterative ones, for the identification of the H-matrix character of a given matrix $A \in \mathbb{C}^{n,n}$. In that direction, the present authors proposed two criteria, Algorithm $\mathbb{AH}$ and its extension, Algorithm $\mathbb{AH}2$, to completely identify the H-matrix property of both, an *irreducible* and *reducible* matrix.

References

[1] M. Alanelli and A. Hadjidimos. *A New Iterative Criterion for $H-$Matrices*. SIAM J. Matrix Anal. Appl., 29 (2006/07), no. 1, 160–176.

[2] M. Alanelli and A. Hadjidimos. *A New Iterative Criterion for $H-$Matrices: The Reducible Case.* Linear Algebra Appl. 428 (2008), no. 11-12, 2761–2777.

[3] B. Li, L. Li, M. Harada, H. Niki and M.J. Tsatsomeros. *An Iterative Criterion for $H-$Matrices*. Linear Algebra Appl., 271 (1998), 179–190.

[4] L. Li. *On the Iterative Criterion for Generalized Diagonally Dominant Matrices*. SIAM J. Matrix Anal. Appl., 24 (2002), 17–24.

A technique for entrapping a time series' future optima

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Key words: Backtrack, Future optima, Time series.

In statistics and mathematical finance, a time series is a sequence of data points, measured typically at successive times spaced at uniform time intervals. Time series forecasting is described as the usage of a model to forecast future events based on known, past events; that is to predict future data points before they actually occur.

Recently was implied the usage of non-value oriented future approximations, approached as time-oriented ones, referring to the future point a time series would be locally optimized by exploiting the usage of unconstrained optimization iterative schemes. The revolutionary characteristic of those techniques, named *backtrack* techniques is accommodating time-oriented forecasts, through their usage that enables the forward step with quite accuracy. Such applications focus on the selection of some past points that affect the time series' evolution instead of exploiting all past data that may carry misleading information. A major inconsistency of the backtrack methods is that the estimated future point deriving from their application is either an optimum or a point that eventually would lead to an optimum one; hence the forecast is not strictly accurate. On the other hand as the method approximates the optimum, it is most possible that the application of any optimization technique would finally converge to a steplength that leads to the closest local optimum. Thus, if the simultaneous application of two different optimization methods results to an interval amongst forecasts that is relatively narrow, it is rather possible that the future optimum woould be entrapped in-between these two forecasts, that is the double-technique interval.

The basic idea of this paper is the usage of two different optimization methods for the future step of the backtrack methodology, with completely different convergence characteristics, in order to entrap the future optima in a time range. The interval is estimated through the joint exploitation of two different optimization methods, however based on the same past dataset. Different convergence characteristics of the methods result to the interval that is eligible to envelop the local optima; for the same reason the interval's width tends to decrease as the time series approaches its critical value. Moreover, this interval's width may be used as an approximation of the error in the accuracy of future optimum convergence. The advantage of the new methodology is that the convergence of the two different optimization techniques to the same future optimum is proved. The new methodology was applied to various time series and the results are quite satisfactory. Moreover, numerical results confirm that in most cases the time interval resulting from application of the new methodology is narrow and sufficiently precise in identifying the future optimum.

The Schrödinger Equation in time-dependent domains: Continuous and Discontinuous Galerkin Methods

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Key words: Schrödinger Equation, Galerkin methods, time-dependent domains.

We analyze Galerkin-finite element methods that approximate the solutions of initial-boundary-value problems for Schrödinger evolution equations in time-dependent domains. Error estimates of optimal rates of convergence in L^2 and H^1 are proved for the associated semidiscrete and fully discrete Crank-Nicolson-Galerkin approximations. For the Dirichlet problem we construct Discontinuous in time space-time Galerkin methods. We establish the existence and uniqueness of numerical solution and as well as an abstract error estimate.

A Variational method for stress fields calculation in nonhomogeneous cracked materials

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Key words: Fracture mechanics, Elasticity equations, Singular geometries, Finite element method, Variational method.

Fracture mechanics deals with the study of the formation of cracks in materials, using methods of analytical mechanics to calculate the force on a crack and the material's resistance to fracture. It applies the physics of stress and strain, the theories of elasticity and plasticity, to the microscopic defects found in real materials in order to predict the mechanical failure of bodies, and a crack propagation. However, the classical methods of calculating are not generally valid in domains with complicated geometry with non homogeneous materials.

This work deals with the crack problem simulation on such non homogeneous stratified materials. It proposes a new numerical approach based on a variational formulation of the Navier-Lame equations in a two dimensional domain. We present the variational method which provides the solution in terms of displacements field in the case of a crack existence in a two dimensional plate domain Ω made of k different layers characterized by different known material properties.

The problem definition is obtained from the equilibrium equations for a plane stress and formulated in terms of stress tensors S_i in each layer Ω_i of the domain Ω. The presented problem implements the mode I deformation of the elastic non homogeneous plate with cracks, which is perfectly jointed on the interface between two consecutive layers. The plate is loaded by the opposed surface forces on the external boundary Γ_{L_i} (top and bottom) , clamped on the surface Γ_{C_i} (on the right) and free on Γ_{F_i} (on the left). The system to solve is written:

$$\left\{\begin{array}{rcl} -\mathrm{div}\,\mathrm{S_i} = \mathbf{F_i} & \text{in} & \Omega_i,\ 1 \le i \le k \\ \mathbf{u_i} = 0 & \text{on} & \Gamma_{C_i},\ 1 \le i \le k \\ S_i = 0 & \text{on} & \Gamma_{F_i},\ 1 \le i \le k \\ S_i \cdot \mathbf{n} = \mathbf{G_i} & \text{on} & \Gamma_{L_1},\ \ i = 1,\ i = k \end{array}\right. \tag{1}$$

In the talk, details will be given and numerical results will be shown for $k = 2$ to prove the efficiency of the method.

Improved Transparent Boundary Conditions for Pricing American Options

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Key words: Black-Scholes equation, American option pricing, Free boundary value problem, Transparent boundary conditions, Chebyshev polynomials, Finite difference method.

In this paper, we present a new method for the approximation of transparent boundary conditions, when solving the American option pricing problem in financial mathematics. Using the standard change of variables cited in [1], the free boundary value problem for pricing American options is equivalent to the following problem:

$$\begin{cases} \frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2}, \quad a < x < x_f(\tau), \quad 0 < \tau \leq \tau^*, \\ u(x,\tau) = g(x,0), \quad a < x < x_f(0), \\ u(x_f(\tau),\tau) = g(x_f(\tau),\tau), \quad 0 < \tau \leq \tau^*, \\ e^{(\alpha-1)x_f(\tau)+\beta\tau}\left(\frac{\partial u(x_f(\tau),\tau)}{\partial x} + \alpha u(x_f(\tau),\tau)\right) = 1, \quad 0 < \tau \leq \tau^*, \\ u(x,\tau) \to 0 \text{ as } x \to -\infty. \end{cases} \tag{1}$$

where $g(x,\tau) = e^{-\alpha x - \beta\tau}\max(e^x - 1, 0)$ and the free boundary has changed to $x_f(\tau) = \ln(S_f(t)/E)$. Using this transformation, the free boundary value problem for an American call option which pays dividend and has an unbounded domain, is reduced to a problem in a bounded domain (see §3 in [1]). Hence, the last equation of (1) is changed to:

$$\left.\frac{\partial u}{\partial x}\right|_{x=a} = \frac{1}{\sqrt{\pi}}\int_0^\tau \frac{\partial u(a,\lambda)}{\partial \lambda}\frac{d\lambda}{\sqrt{\tau-\lambda}}. \tag{2}$$

We call this equation as the transparent boundary condition (TBC) [2]. In this paper, we have proposed some new improvements in Han and Wu's approach [1] via explicit form of transparent boundary condition by expanding it in a Taylor series:

$$\phi(\lambda) = \sum_{k=0}^{+\infty} \frac{(\lambda-\tau)^k \phi^{(k)}(\tau)}{k!}. \tag{3}$$

Obviously, $\phi(\tau) = u(a,\tau)$ is defined and differentiable on $[0,\tau^*]$ (for some τ^*) so our Taylor expansion is meaningful. We prove then that the transparent boundary condition (3) is equivalent to the following equation:

$$\frac{\partial u}{\partial x}|_{x=a} = \frac{1}{\sqrt{\pi}}\sum_{k=0}^{+\infty}\frac{(-1)^{k+1}4^k}{k!(2k-1)}\phi^{(k)}(\tau)\cdot\tau^{k-\frac{1}{2}} \tag{4}$$

and by this we obtain:

$$\frac{u(a,\tau)}{\sqrt{\tau}} \to 0 \text{ when } \tau \to 0^+. \tag{5}$$

Based on this approximation, we calculate the price of the corresponding American call option with high precision. By using the third-kind Chebyshev polynomials in the context of implicit Crank-Nicolson and explicit Dufort-Frankel techniques for solving the Black-Scholes equation, we will arrive at a high order of accuracy in price approximations. We illustrate the efficiency of the proposed method on two examples and compare it with perviously published results from the literature.

References

[1] H. Han and X. Wu, A fast numerical method for the Black–Scholes equation of American options, *SIAM J. Numer. Anal.,* **41** (2003), pp. 2081-2095.

[2] M. Ehrhardt, R. E. Mickens, A fast, stable and accurate numerical method for the Black-Scholes equation of American options, *Inter. J. Theoretical and Applied Finance,* **11** (2008), pp. 471-501.

LAPACK WS: Offering Lapack over the Web

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Key words: LAPACK, Web services, Scientific computing.

Software-as-a-service has been recognized as the next step in the software industry and already fundamentally alters the economics of software. At almost the same time internet and the World Wide Web in general and Web Services and Cloud in particular offer the promise of virtually unlimited processing and storage power as well as applications running on widely-dispersed computers as though they are on our own desktops.

This paper presents a summary of our efforts to provide a foundation for a service-based paradigm, in which scientific computing resources and services are transparently provisioned and managed on an on-demand basis, at run-time if needed at competitive costs. We envision that web services[1] will alow us to effectively merge existing high quality scientific computing software and high performance computing infrastructure into effective and value added web computational systems.

To prove the above concept, we have implemented a set of commonly used LAPACK routines (all subroutines whose name ends with SV) as web services by

- describing them with the Web Services Description Language (WSDL),
- using messages that follow the Simple Object Access Protocol (SOAP) standard
- exploiting the features and capabilities of the Electronic Business using XML (ebXML) Registry.

Our services can be accessed in several different ways, through most of the widely used programming languages and under diverse usage scenarios (see `http://lapack.ws`) ranging from humans using Web-based graphical user interfaces to automatic invocation at run-time. We currently offering (while we are still beta-testing) our web services on a desktop computer, on a DELL cluster of total of 48 cores and on the Amazon Elastic Compute Cloud (EC2) and the Amazon Simple Storage Service (S3).

[1] A web service is according to W3C a software system designed to support interoperable machine-to-machine interaction over a network.

An numerical approximation to the solution of an Fredholm integro-differential equation

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Key words: Nonlinear Fredholm integro-differential equation, numerical methods, Schauder bases.

Several numerical methods for approximating integro-differential equations are known. These methods often transform an integro-differential equation to a linear or nonlinear system of algebraic equations which can be solved by direct or iterative methods. This work considers the specific case of the nonlinear Fredholm integro-differential equation of second kind:

$$y'(x) = g(x) + \int_a^b G(x,t,y(t))dt$$

where $g : [a,b] \to \mathbb{R}$ and $G : [a,b] \times [a,b] \times \mathbb{R} \to \mathbb{R}$ are continuous functions.

We present a method of numerical approximation for solving the above equation that uses strongly the properties of certain classical Schauder bases in the respective of Banach spaces $\mathcal{C}([a,b])$ and $\mathcal{C}([a,b] \times [a,b])$ of continuos and real-valued functions. The method is computationally attractive and some numerical examples are provided to illustrate the high accuracy of the method.

Biorthogonal systems and numerical solution of the nonlinear Volterra integro-differential equations

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Key words: Numerical methods, Volterra integro-differential equation, biorthogonal systems in a Banach space.

Let us consider the nonlinear Volterra integro–differential equation

$$\begin{cases} y'(t) = f(t, y(t)) + \displaystyle\int_0^t K(t, s, y(s))\, ds \qquad (t \in [0,1]) \\ y(0) = y_0 \end{cases},$$

where $y_0 \in \mathbb{R}$ and $K : [0,1] \times [0,1] \times \mathbb{R} \to \mathbb{R}$ and $f : [0,1] \times \mathbb{R} \to \mathbb{R}$ are continuous functions satisfying a Lipschitz condition at their last variables: there exist $L_f, L_K \geq 0$ such that for all $y_1, y_2 \in \mathbb{R}$ we have

$$\max_{0 \leq t \leq 1} |f(t, y_1) - f(t, y_2)| \leq L_f |y_1 - y_2|$$

and

$$\max_{0 \leq t,s \leq 1} |K(t, s, y_1) - K(t, s, y_2)| \leq L_K |y_1 - y_2|.$$

Volterra's integro-differential equations are usually difficult to solve in an analytical way. Many authors have paid attention to their numerical treatment. This work deals with obtaining a numerical method in order to approximate the solution of the nonlinear Volterra integro-differential equation. We define, following a fixed-point approach, a sequence of functions which approximate the solution of this type of equation, thanks to some properties of certain biorthogonal systems for the Banach spaces $C[0,1]$ and $C[0,1]^2$. Among the main advantages of our numerical method as opposed to the classical ones, such as collocation or quadrature, we can point out that it is not necessary to solve algebraic equation systems; furthermore, the integrals involved are immediate and therefore we do not have to require any quadrature method to calculate them. On the other hand, the method presented generalizes one developed by the authors for the linear case in a previous work. The behaviour of the method introduced will be illustrated with some examples.

A numerical scheme for the modified Burgers' equation

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Key words: Burgers' equation; Modified Burgers' equation, Finite-difference method

A finite-difference method based on third order rational approximants to the matrix-exponential term in a two-time level recurrence relation is proposed for the numerical solution of the modified Burgers' equation (MBE) given by

$$u_t + u^\mu \, u_x - \nu \, u_{xx} = 0 \,; \;\; L_0 < x < L_1 \,, \;\; t > t_0, \tag{1}$$

where μ is a positive integer with $\mu \geq 2$ - the case $\mu = 1$ corresponds to the classical Burgers' equation, $u = u\,(x,t)$ is a sufficiently often differentiable function and ν is a constant, which can be interpreted as viscosity, controlling the balance between convection and diffusion. The cases $\mu = 2$ and $\mu = 3$ will be examined. The MBE equation has the strong nonlinear aspects of the governing equation in many practical transport problems such as nonlinear waves in a medium with low-frequency pumping or absorption, ion reflection at quasi-perpendicular shocks, turbulence transport, wave processes in thermoelastic medium, transport and dispersion of pollutants in rivers and sediment transport, etc. Numerical solutions of the MBE equation can be found among others in [1, 2], etc.

The resulting nonlinear system, which is analysed for stability, is solved using an already known modified predictor-corrector scheme (see [3] and the references therein). The results arising from the experiments are compared with the relevant ones known in the bibliography.

References

[1] Ramadan, M. A., El-Danaf, T. S., Alaal, F., A numerical solution of the Burgers' equation using septic B–splines, Chaos, Solitons & Fractals 26 (2005) 795-804.

[2] Bratsos, A. G. and Petrakis, L. A., An explicit numerical scheme for the modified Burgers' equation, to be appeared in Communications in Numerical Methods in Engineering (DOI: 10.1002/cnm.1294).

[3] Bratsos, A. G., A numerical method for the one-dimensional sine-Gordon equation, Numer Methods Partial Differential Eq 24 (2008) 833–844.

Nonlinear functional equations satisfied by orthogonal polynomials

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Key words: Orthogonal polynomials, nonlinear functional equations.

Let c be a linear functional defined by its moments $c(x^i) = c_i$ for $i = 0, 1, \ldots$. We proved that the nonlinear functional equations $P(t) = c(P(x)P(x+t))$ and $P(t) = c(P(x)P(xt))$ admit polynomial solutions which are the polynomials belonging to the family of formal orthogonal polynomials with respect to a linear functional related to c. Other types of nonlinear functional equations whose solutions are formal orthogonal polynomials are also presented. Then, orthogonality with respect to a definite inner product is studied. When c is an integral functional with respect to a weight function, the preceding functional equations are nonlinear integral equations, and these results lead to new characterizations of orthogonal polynomials on the real line, on the unit circle, and, more generally, on an algebraic curve.

On correct boundary conditions in numerical schemes for the gravity wave equations

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Key words: gravity waves, shallow water equations, initial-boundary value problems, well-posed problems

In the atmosphere-ocean regional models, the initial conditions are supplied by data assimilation schemes and the boundary conditions are usually provided by a global model. Therefore, the values of almost all the prognostic fields are usually available on the domain boundary and there are many options for specification of the boundary conditions. The main difficulties for the formulation of the differential conditions at artificial boundaries are usually related to the necessity to mimic the physical medium, which surrounds the problem domain, and to specify physically reasonable conditions, which produce a well-posed mathematical problem. In discrete problems, besides keeping the well-posedness of differential problems, other important issues are the accuracy of approximation and the numerical stability, which connect differential and discrete problems. Different approaches to solution of these problems in atmosphere-ocean modeling can be found in a number of sources.

In this study we consider a non-physical growth of solutions leading to numerical blow-up in the cases when the choice of the boundary conditions appears to be physically justifiable and the initial-boundary value problem for the primitive differential system is well posed. This growth can be observed in both conditionally and absolutely stable numerical schemes and it can not be eliminated by reducing the time step. Since the corresponding numerical problem with the periodic boundary conditions is conditionally or absolutely stable, such instability is related to the specific non-periodic boundary conditions. We study this problem in a simplified model of one-dimensional gravity waves, which allows us to perform complete theoretical analysis and reveal the causes of such instability. Based on the performed analysis and numerical experiments, some recommendations for choosing the boundary conditions are given to avoid this non-physical behavior of numerical solutions.

A semi-implicit time-splitting scheme for a regional atmospheric model

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Key words: atmospheric model, Euler equations, semi-implicit scheme, time-splitting scheme

The atmosphere is a complex system supporting complex processes of different space and time scales. Accordingly, the complete 3D mathematical models of the atmosphere (Navier-Stokes or Euler equations) contain multi-scale solutions with fast and slow components. It is well-known that the fastest atmospheric waves are the acoustic ones, which do not contain any significant part of the atmospheric energy. The slower gravity waves are more energy valuable, while relatively slow advective processes and Rossby waves carry the main part of the atmospheric energy. Since differential approximations, which filter out fast waves, introduce distortions to the main physical modes, the problem of stiffness of the complete mathematical models of atmospheric dynamics should be addressed in design of numerical scheme.

In this study, a semi-implicit finite difference scheme is proposed for the nonhydrostatic atmospheric model based on Euler equations. The fast acoustic and gravity waves are approximated implicitly, while slow advective terms and Rossby modes are treated explicitly. Such time approximation requires solution of 3D elliptic equations at each time step. Efficient elliptic solver is based on decoupling in the vertical direction and then splitting in the horizontal directions. Stability analysis of the scheme shows that the time step is restricted only by the maximum velocity of advection and does not depend on speed propagation of the fast waves. The performed numerical experiments show computational efficiency of the designed scheme and accuracy of the predicted atmospheric fields.

Towards the development of high performance scientific software for simulating 3D fluid-dynamic processes in a viscoelastic fluid

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Key words: parallel computing, mathematical software, partial differential equations

To understand the onset and the evolution of rheological behavior of materials realized by adding solid fillers to viscoelastic fluids, a collaboration between computing scientists and chemical engineers was established to develop scientific software to simulate such processes on high end computing infrastructures. The results of this activity will be used as starting point of future applications in industrial processes such as flow intubation and injection molding.

The specific application that we consider consists of a single sphere in a sheared viscoelastic fluid. Assuming incompressibility, negligible inertia, and buoyancy free conditions the governing equations are the continuity (mass balance) and momentum balance equations, plus a constitutive equation depending on the nature of the suspending liquid [2].

Governing equations (non linear evolutionary PDEs) are discretized by using finite elements, while linearization is based on a semi implicit scheme which gives rise to a linear systems to solve at evolution step whose matrices are large (i.e. $O(10^6)$ unknowns), symmetric and sparse.

Taking into account that the underlying mathematical model is described by partial differential equations and to guarantee code *maintainability, portability, reusability and efficiency*, the parallel computing environment that supports the simulation software relies on PETSc (Portable, Extensible Toolkit for Scientific Computation) components [1] integrated with the TFEM (Toolkit for Finite Element Method) software toolkit [3], already employed to discretize and solve 2D problems.

We discuss computational efforts towards the development of high performance software tools needed to perform such computational expensive simulations. We also address the *validation* of numerical results and *performance* gain on the basis of same case studies.

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References

[1] S. Balay, K. Buschelman, V. Eijkhout, W. Gropp, D. Kaushik, M. Knepley, L. Curfman McInnes, B. Smith, H. Zhang, *PETSc Users Manual*, Technical Report ANL-95/11 - Revision 2.1.5, Argonne National Laboratory, 2004.

[2] G. D'Avino, M.A. Hulsen, F. Snijkers, J. Vermant, F. Greco, P.L. Maffettone, *Rotation of a sphere in a viscoelastic liquid subjected to shear flow. Part I: Numerical results*, J. Rheol. 52(6), 2008.

[3] M.A. Hulsen, *TFEM: A toolkit for the finite element method*, Userguide, 2009.

Some error estimates for the lumped mass finite element method for a parabolic problem

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Key words: Lumped mass method, parabolic pde's, nonsmooth initial data, error estimates.

We consider the model initial–boundary value problem

$$u_t - \Delta u = 0, \quad \text{in } \Omega, \quad u = 0, \quad \text{on } \partial\Omega, \quad \text{for } t \geq 0, \quad u(0) = v, \quad \text{in } \Omega, \tag{1}$$

where Ω is a bounded convex polygonal domain in $\mathbb{R}^2$. We study the spatially semidiscrete lumped mass method for (1), where we seek an approximation $\bar{u}_h(t) \in S_h$ of $u(t)$, with $S_h = \{\chi \in \mathcal{C}(\Omega) : \chi|_\tau \text{ linear}, \forall\, \tau \in \mathcal{T}_h;\ \chi|_{\partial\Omega} = 0\}$, $\{\mathcal{T}_h\}_{0<h<1}$ a family of regular triangulations of Ω, with h denoting the maximum diameter of the triangles $\tau \in \mathcal{T}_h$. The lumped mass solution $\bar{u}_h(t)$ is obtained by

$$(\bar{u}_{h,t}, \chi)_h + (\nabla \bar{u}_h, \nabla \chi) = 0, \quad \forall \chi \in S_h, \quad \text{for } t \geq 0, \quad \text{with } \bar{u}_h(0) = v_h, \quad (v, w) = \int_\Omega vw\, dx,$$

where $(v, w)_h$ is a given quadrature approximation of (v, w) and $v_h \in S_h$ an approximation of v. Improving earlier results, our aim is to show that

$$\|\bar{u}_h(t) - u(t)\| \leq Ch^2 t^{-1+q/2} |v|_q, \quad \text{for } t > 0, \quad q = 0, 1, 2, \tag{2}$$

with $|v|_0 = \|v\| = (v, v)^{1/2}$ the norm in $L_2(\Omega)$, $|v|_1$ the norm in $H_0^1(\Omega)$ and $|v|_2 = \|\Delta v\|$. We show (2) for $q = 2$, and for $q = 1$ under an inverse assumption on S_h. However, for $q = 0$, we are only able to show (2) under an additional hypothesis on $\mathcal{T}_h$, which is satisfied for symmetric triangulations. If this hypothesis on $\mathcal{T}_h$ is not satisfied, we are only able to show the nonoptimal order error estimate,

$$\|\bar{u}_h(t) - u(t)\| \leq Cht^{-1/2} \|v\|, \quad \text{for } t > 0.$$

In addition, we give examples of nonsymmetric partitions in one space dimension, where this assumption is not valid. We also discuss the application to time discretization by the backward Euler and Crank-Nicolson methods.

A fixed point iteration method for multiscale modeling of Chemical Vapor Deposition processes.

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Key words: multiscale modeling, CVD, level-set method, parallel processing, MPI.

A fixed point iteration method for coupling multiple length scales in Chemical Vapor Deposition (CVD) processes is presented. A Reactor Scale Model (RSM), used for the description of the macro-scale in the bulk, is coupled with a Feature Scale Model (FSM), used for the description of the topography evolution of the micro-scale features on the wafer. The RSM is implemented with a commercial software for computational fluid dynamics, namely FLUENT, and the FSM combines [1] a ballistic model for the species' transport inside features (e.g. trenches), a surface chemistry model, and a profile evolution algorithm based on the level set method. The coupling of the RSM with the FSM is performed through the correction of the boundary condition for the species consumption along the wafer. The pre-exponential factor for the expression of the surface reaction rate is corrected [2] in order for the RMS to take into account the existence of the features in the micro-scale, wihout including them in the computational domain of the macro-scale. The correction is performed through a fixed point iteration method. In the present work the boundness and the stability of the iteration method is studied. Furthermore, the time consuming computations in the micro-scale are sufficiently treated by using parallel processing and Message Passing Interface (MPI) [3].

References

[1] G. Kokkoris, A. Tserepi, A. G. Boudouvis and E. Gogolides, *Journal of Vacuum Science and Technology A* 22, 1896 (2004).

[2] N.Cheimarios, G.Kokkoris and A.G. Boudouvis,*Chemical Engineering Science*, under review process (2010).

[3] G.E. Karniadakis and R.M.Kirby II, (2003), Parallel Scientific Computing in C++ and MPI, Cambridge University Press, Cambridge.

Some Generalized Iterative Methods

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Key words: Arnoldi Process, SYMMLQ/SYMMQR methods, Generalized and Modified SYMMLQ method, double linear system, Lanczos/SYMMLQ algorithm

For the numerical solution of partial differential equations, we have to obtain the solution of systems of linear algebraic equation of the form $Ax = b$. The most well-known direct method for solving

$$Ax = b$$

is Gaussian elimination. However, the method requires expensive computer storage and computer time, especially for problems arising from partial differential equations in three dimension.

We consider the use of iterative methods in this thesis. For linear systems involving symmetric and positive definite (SPD) matrices, the conjugate gradient (CG) method works fairly well.

For solving the linear system $Ax = b$, where the matrix A is indefinite symmetric, the methods SYMMLQ and MINRES (Paige and Saunder (1975)) work very well. Saad and Schultz generalized the method MINRES to GMRES for the nonsymmetric matrix A.

We describe the methods LQ-MINRES and QR-MINRES and show that the two methods are the same while using two different ways to factorize the tridiagonal matrix in Paige and Saunders's paper. We generalize the method QR-MINRES method for the nonsymmetric linear systems and show that the method is equivalent to the method GMRES. We also define the methods MMINRES and MSYMMQR. The difference between the method MGMRES and MMINRES is indicated. We apply the methods MMINRES and MSYMMQR to double linear system to obtain the methods LAN/MINRES and LAN/SYMMQR for nonsymmetric linear systems.

A method for the inverse numerical range problem

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Key words: Numerical range, Inverse problem, Field of values, Generating vector.

The *numerical range* (also known as the *field of values*) of a square matrix $A \in \mathbf{C}^{n\times n}$ is the compact and convex set $F(A) = \{x^*Ax \in \mathbf{C} : x \in \mathbf{C}^n,\ x^*x = 1\}$. The compactness follows readily from the fact that $F(A)$ is the image of the compact unit sphere of $\mathbf{C}^n$ under the continuous mapping $x \longmapsto x^*Ax,$ and the convexity of $F(A)$ is the celebrated Hausdorff-Toeplitz Theorem. The concept of the numerical range and related notions has been studied extensively for many decades. It is quite useful in studying and understanding matrices and operators, and has applications in numerical analysis, differential equations, systems theory etc.

In this work, we propose a simple geometric algorithm for solving the inverse numerical range problem: *given an interior point μ of $F(A)$, determine a unit vector $x_\mu \in \mathbf{C}^n$ such that $\mu = x_\mu^*Ax_\mu$*. The new algorithm is fast and gives numerically accurate results where known methods often fail, such as when μ lies in very close distance from the actual numerical range boundary $\partial F(A)$, both if $\mu \in F(A)$ and $\mu \notin F(A)$.

The Singular Function Boundary Integral Method for 3-D Laplacian Problems with a Boundary Straight-Edge Singularity

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Key words: Laplace problem, edge singularity, boundary integral method.

We consider the Laplace problem in a three-dimensional domain with a straight-edge singularity caused by two intersecting flat planes. The solution in the neighbourhood of such edge can be expressed as an asymptotic expansion involving the eigenpairs of the analogous two-dimensional problem in polar coordinates, which have as coefficients the so-called edge flux stress intensity functions (EFIFs). The EFIFs are functions of the axial coordinate the higher derivatives of which appear in an infinite series in the expansion.

The objective of this work is to extend the singular function boundary integral method (SFBIM) for solving the above problem and directly extracting the EFIFs. Approximating the latter by either piecewise constant or linear elements eliminates the second infinite series and allows the straightforward extension of the SFBIM. As in the case of two-dimensional problems, the solution is approximated by the leading terms of the local asymptotic solution expansion, simplified in the axial direction as explained above. These terms are also used to weight the governing harmonic equation in the Galerkin sense. The resulting discretized equations are reduced to boundary integrals by means of the divergence theorem. The Dirichlet boundary conditions are then weakly enforced by means of Lagrange multipliers. The values of the latter are calculated together with the coefficients of the EFIFs. The SFBIM appears to converge fast with the number of EFIFs, the number of the Lagrange multipliers, and the number of elements in the axial direction, leading to very accurate results.

Reduced averaging of directional derivatives in vertices of unstructured triangulations

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AMS subject classification: 65D25, 65N30

Key words: Conforming shape-regular triangulation, reduced averaging, superapproximation of the partial derivatives, recovery operator.

Let us consider a unit vector z, a conforming shape-regular triangulation $\mathcal{T}_h$ without obtuse angles of a planar domain Ω with polygonal boundary and a smooth function $u = u(x, y)$ on Ω. In many situations, the values of u are known in the vertices of $\mathcal{T}_h$ only. These values may be the results of some measurements or, more often, of numerical solutions of the second-order differential boundary-value problems. These known values can be naturally extended to the piecewise linear and globally continuous interpolant $\Pi_h(u)$ of u on Ω. In some cases it is important to know accurate approximations of the values $\partial u/\partial z(a)$ in the vertices a of $\mathcal{T}_h$. As the approximations $\partial \Pi_h(u)/\partial z$, defined inside of the triangles from $\mathcal{T}_h$, have an error of the size $O(h)$ only, the following classical problem appeared: For a unit vector z and for the triangles $T_1, \dots, T_n$ from $\mathcal{T}_h$ with a common vertex a, find coefficients $f_1, \dots, f_n$ such that the linear combination

$$f_1 \partial(\Pi_h(u)|_{T_1})/\partial z + \ldots + f_n \partial\left(\Pi_h(u)|_{T_n}\right)/\partial z$$

approximates $\partial u/\partial z(a)$ with an error $O(h^2)$.

In the case $n \geq 5$, we present an elementary construction of a selection $r = (b^1, \dots, b^5)$ from the set of vertices of the triangles $T_1, \dots, T_n$ different from a such that the triangles $U_1 = \overline{ab^5b^1}, \dots,$ $U_5 = \overline{ab^4b^5}$ are equally oriented and $\angle(b^5ab^1) + \ldots + \angle(b^4ab^5) = 2\pi$ and denote by $\Pi_i(u)$ the linear interpolant of a function u in the vertices of U_i for $i = 1, \dots, 4$. We derive a matrix $N(r)$ of size four, a vector d and show that $N(r)$ is non-singular and that the value

$$\mathrm{RA}_{h,z}[u](a) = g_1 \partial\Pi_1(u)/\partial z + \ldots + g_4 \partial\Pi_4(u)/\partial z$$

of the *reduced averaging operator* RA, related to the solution $g = [g_1, \dots, g_4]^\top$ of the equations $N(r)g = d$, is a second-order approximation of $\partial u/\partial z(a)$ for any function $u \in C^3(\overline{\Omega})$. We show that this operator is more effective and more accurate than any other known operator approximating $\partial u/\partial z(a)$ locally. We discuss the problem of effective approximation of the values of the gradient ∇u in the vertices of $\mathcal{T}_h$ and show that the piecewise linear extension of these approximations to Ω is a recovery operator in the sense of Ainsworth, Craig.

A Multithreaded Finite Element Algorithm with Element-by-Element Preconditioning

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Key words: Finite elements, conjugate gradients, preconditioning, multithreaded computations, Graphics Processing Units (GPUs), multicore CPUs.

A natural approach to parallelizing the finite element method stems from the concept of the "element" as a building block in the whole methodology. Elements are treated as disjoint and decoupled in many stages of the finite element computations (namely the formation of element level characteristics, such as element stiffness, strains and stresses) which are therefore inherently parallel in nature. In addition, when an iterative solver is employed, the explicit formation of the global stiffness matrix can be avoided by inducing the element connectivity information to the solver vectors. An elegant way to achieve this is by grouping them into two types: "Force type" vectors for each element are those derived from the RHS vector and should add up to the global external "force" contribution for each node. "Displacement type" vectors, on the other hand, are those related to the solution vector and should guarantee the compatibility of the "displacements" around each node.

Under such an element distribution the conjugate gradient algorithm can be implemented with perfectly parallel matrix-vector multiplications and linked triad operations on the *element level*. The only communication involved is related to the two inner products and a single vector update among neighbouring element in order to maintain the "force/displacement type" distribution across all iterations. The bottleneck in the above procedure is the preconditioning of the *unassembled* stiffness matrix. Ideally, one would also like to use some kind of element level preconditioner that would follow this natural distribution. Apart from the trivial diagonal scaling, the options for such a preconditioner found in the literature are quite limited.

In this work, an SSOR type element-by-element preconditioner is proposed which is derived entirely from element stiffness matrices. Suitable modifications are enforced to ensure positive definiteness and to guarantee that its application conforms with the compatibility requirement for the "displacement-type" vectors. The preconditioner is analysed and evaluated in comparison with existing methods. The parallel implementation of the above finite element algorithm is based on multithreading which is particularly efficient on today's multicore CPUs and/or GPUs (Graphics Processing Units which can also be used for general purpose computations). This approach scales well as each thread can deal with as little as just a single element. Numerical results from structural analysis problems are given, tested on quad-core processors and NVIDIA GPUs.

Numerical Solution of Boussinesq Systems Modeling Two-Way Water Wave Propagation

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Key words: Water waves, Boussinesq Systems, Solitary Waves.

We review recent progress on the theory and numerical analysis of Boussinesq systems of water wave theory. These systems model two-way propagation of nonlinear dispersive waves in two and three spatial dimensions. Emphasis will be given on the interactions of their solitary-wave solutions and on initial-boundary- value problems for these systems.

Modeling and simulation of compressible two-phase flows

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Key words: two-phase flows, compressible flows, conservation laws, finite volumes, wave impacts, powder-snow avalanches.

Two-phase flows are very present in industry and nature. Typical examples go from pressurized water reactors [3] to the wave breaking [1] and powder-snow avalanches [2]. However, the mathematical modeling of two-phase flows is challenging and still represents several substantial difficulties. We can also mention that currently there is no consensus on these questions among specialists in this field.

We begin our exposition by presenting the six-equations model [3] (a compressible two-phase model with two velocities and two energies, one for each phase). However, this model is quite complex and its advection operator may become non-hyperbolic. Through the velocity relaxation procedure and the Chapman-Enskog expansion [4], we derive a compressible single velocity single energy model [1] (the so-called four-equations model). This formulation is more accessible for efficient numerical simulations. Nevertheless, if one wants to simplify further this model, we can perform the low Mach number asymptotic expansion to filter out acoustic effects [4].

Finally, we will discuss the discretization of the four-equations model in the framework of finite volumes method. We will also present a few numerical applications concerning the wave impact problem and powder-snow avalanches flows.

References

[1] DIAS, F., DUTYKH, D. & GHIDAGLIA, J.-M. 2010. A two-fluid model for violent aerated flows. *Comput. & Fluids*. **39(2)**, 283–293.

[2] DUTYKH, D., ACARY-ROBERT, C. & BRESCH, D. 2010. Numerical simulation of powder-snow avalanche interaction with an obstacle. *Submitted*.

[3] ISHII, M. & HIBIKI, T., 2006. Thermo-fluid dynamics of two-phase flow. *Birkhäuser*

[4] MEYAPIN, Y., DUTYKH, D. & GISCLON, M., 2010. Velocity and energy relaxation in two-phase flows. *Stud. Appl. Maths*. Accepted.

Application of variational iteration method and homotopy perturbation method to the Klein-Gordon-Schrödinger equation

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Key words: variational iteration method, homotopy perturbation method, Klein-Gordon-Schrödinger equation.

In this paper, we shall consider the coupled nonlinear Klein-Gordon-Schrödinger (K-G-S) equations in the form:

$$u_{tt} - c^2 u_{xx} + u + |v|^2 = 0,$$
$$iv_t + v_{xx} + uv = 0.$$

Here, u represents a complex scalar nucleon field and v a real scalar meson field.

Homotopy Perturbation Method (HPM) and Variational Iteration Method (VIM) are implemented for solving the K-G-S equation. The results were compared with results of Adomian decomposition Method (ADM). The results reveal that the HPM and VIM are very effective, convenient and quite accurate to systems of nonlinear partial differential equations.

Basic idea of the VIM: To illustrate the basic concepts of the VIM, we consider

$$Lu + Nu = g(x) \tag{1}$$

where L is a linear differential operator, N a nonlinear analytic operator, and $g(x)$ an inhomogeneous term. According to the VIM, we can construct a correction functional as follows:
$u_{n+1} = u_n + \int_0^x \lambda u_n(s) + N\widetilde{u}_n(s) - g(s)ds,$
where λ is a general Lagrange multiplier, which can be identify optimally via the variational theory, $\widetilde{u}_n$ is considered as a restricted variation , i.e.,$\delta\widetilde{u}_n 0$.

Basic idea of the HPM: for solving eq. (1) by HPM we can constract a homotopy in the form

$$H(v,p) = (1-p)(L(v) - L(u_0)) + p[Lv + Nv - g(x)] = 0, \quad p \in [0,\ 1] \tag{2}$$

where p is an embedding parameter, u_0 is an initial approximation of the Eq. (1). In HPM, one can use the embedding parameter as a small parameter. Therefore, the solution of Eq. (2) can be written as a power series of p in the form, $v = v_0 + pv_1 + p^2 v_2 + ...$ By setting $p = 1$, one can get an approximate solution of the Eq. (1) as, $u = \lim_{p\to 1} v_0 + v_1 + v_2 + ...$

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The SOR as a Benchmarking Tool for Single- Multi- and Many-core Systems

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Dedicated to the memory and work of Prof. David M. Young

Analyzing and bechmarking modern computing systems with several levels of cache, multiple cores, many cores such as GPUs, and distributed memory is becoming increasingly challenging. In this paper, we show how a flexible implementation of the SOR method as can be used as a benchmarking tools for such systems. The SOR method for solving linear equations, which Dr. David M. Young introduced in his doctoral work at Harvard in 1950, has had a major impact on many scientific fields. With red-black ordering the method parallelizes well on both vector and disptributed memory computing systems leding to renewed interest in it since the 1980s.

As processors become faster, the impact of memory latency and bandwidth on performance is increasing. To combat this problem, processors are continuously getting larger and more aggressive caches. If the problem does not fit in cache, blocking is needed (e.g. row bands). For the multi-CPU case, it pays off to parallelize across the rows. By having each CPU start in the middle of its assigned domain and spread out toward the edges in both directions, you effectively end up with two bands per CPU. The computation on each CPU would be the same as for the multicore single-CPU, parallelizing across the columns for each core

We have previouly shown (Elster & Holtet (2002)) that increasing the boarder sizes and doing redundant computations is an effective techique to overcome the latency factor on SMP clusters with dedicated communications links. By computing not only the border cells, but a border n cells wide, we can allow the neighbor node to compute n iterations before a new exchange is necessary. While this does increase bandwidth cost by a factor n, this will give a good speedup if latency dominates the bandwidth. I.e. if one benefits from wide boarders, one is hiding a lot of latency.

With Spampinato (Parco2009) we tested the NVIDIA s1070 sytem with 4 GPus each with 240 cores, Here, boarder bands of 1 were sufficient for good SOR performanance, but varying the dimensions up to 11GB, the application became I/O bound.

The SOR's stencil based structure can be found in many parallel applications, thus testing a system with a flexible test-implementation of a paralellized SOR, will uncover many of the system parameters one can expect will affect performance. Note also that the optimization techniques developed in our test suite can be applied to several applications with similar structure.

[1] This presentation represents joint work with Thorvald Natvig as well as Robin Holtet and Daniele Spampinato

Numerical modelling of tsunami waves: Application to the simulation of specific earthquake generated tsunamis

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Key words: Long waves, Tsunami, Numerical Modelling, Shallow Water Equations.

Tsunami waves (long waves) are effectively modelled by the nonlinear shallow water equations. These are often solved numerically by appropriate finite difference or finite volume techniques. For the applications presented herein, a splitting direction based, finite difference method is applied for the construction of an approximate solution. All three phases of the evolution of the tsunami wave, the generation, propagation and runup are reproduced, providing a complete simulation capability of the tsunami wave.

Historical descriptions of earthquakes in the sea, as well as geological/ seismological literature references, are used for the construction of appropriate initial conditions for the simulation of the tsunamis that followed. Detailed bathymetric and topographic data are used for accurate representation of the coastal areas under consideration. Inundation maps, focusing on selected coastal areas, are shown.

A proposal of GS-based preconditioning applicable to restarted GMRES(k) method

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As known well, preconditioning is a technique to improve convergence rate of Krylov subspace methods. ILU(0)-decomposition preconditioning without extra fill-in is a major preconditioning for nonsymmetric linear system. ILU(0) preconditioning, however, pays high cost to build preconditioner matrix and needs extra forward and backward substitutions. In this paper, we propose GS(Gauss-Seidel)-based preconditioning without forward and backward substitutions. Furthermore, GS-based preconditioning pays very low cost to build preconditioner matrix. Through numerical experiments, effectiveness of GS-based preconditioning for restarted GMRES(k) method will be demonstrated.

By Krylov subspace methods, we consider to solve a large non-singular linear system of equations,

$$A\boldsymbol{x} = \boldsymbol{b} \tag{1}$$

where A is a given nonsymmetric coefficient $(n \times n)$-matrix, and $\boldsymbol{x}$, $\boldsymbol{b}$ are a solution vector and right-hand side vector of order n, respectively. Krylov subspace of order m is spaned by

$$K_m(A; \boldsymbol{r}_0) \quad := \quad \mathrm{span}\{\boldsymbol{r}_0, A\boldsymbol{r}_0, \ldots, A^{m-1}\boldsymbol{r}_0\}, \tag{2}$$

where $\boldsymbol{r}_0 (= \boldsymbol{b} - A\boldsymbol{x}_0)$ is an initial residual vector. As known well, Krylov subspace methods are effective iterative methods for solving large linear systems of equations, e.g., restarted GMRES(k) method is often used. In addition, preconditioning is well known as a technique to improve convergence rate of Krylov subspace methods. In fact, I(Incomplete)LU(0)-decomposition preconditioning is often used for solving many realistic problems. ILU(0) preconditioning can improve convergence rate of Krylov subspace methods. On the other hand, computational cost of building of preconditioner matrix in ILU(0) preconditioning is very expensive, and it needs extra forward and backward substitution. In this article, we propose GS(Gauss-Seidel)-based preconditioning without extra forward and backward substitution.

We present performance of restarted GMRES(k) method without preconditioning and with ILU(0) and GS-based preconditionings in Table 1. "TRR" means the true relative residual of the approximate solution $\boldsymbol{x}_{n+1}$. Matrix "xenon1" is derived from Florida sparse matrix collection.

From Table 1, we can see that GS-based preconditioned GMRES(k) method outperforms compared with other preconditioned GMRES(k) methods in view of convergence rate and robustness.

Table 1: Performance of restarted GMRES(k) without preconditioning, and with ILU(0) and GS-based preconditionings.

matrix	method	k	ω	itr.	pre-t [sec.]	itr-t [sec.]	total-t [sec.]	$\log_{10}$ (TRR)	memory [Mb]	ratio
xenon1	GMRES	20	-	8053	0.00	30.28	30.28	-8.00	23.3	
		100	-	1934	0.01	15.54	**15.55**	-8.00	53.1	1.00
		500	-	1072	0.01	25.78	25.79	-8.00	203.2	
		1000	-	949	0.01	42.20	42.21	-8.00	394.4	
		5000	-	949	0.01	41.16	41.17	-8.00	2060.8	
	ILU(0)-GMRES	20	-	max	-	-	-	-2.32	37.8	
		100	-	max	-	-	-	-2.83	67.5	
		500	-	4183	0.10	110.41	110.51	-8.00	217.7	
		1000	-	1450	0.11	60.85	60.96	-8.00	408.8	
		5000	-	1055	0.10	53.70	**53.80**	-8.02	2075.2	3.83
	GS-GMRES	20	1.0	1841	0.01	7.03	7.04	-8.00	24.1	
		100	1.0	764	0.01	5.43	**5.44**	-8.00	53.8	0.39
		500	1.0	568	0.01	12.86	12.87	-8.01	204.0	
		1000	1.0	558	0.01	15.07	15.08	-8.00	395.1	
		5000	1.0	558	0.01	15.14	15.15	-8.00	2061.5	

On the use of Product Integration in Fractional Differential Equations

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Key words: Fractional differential equations, product integration, convergence.

Fractional differential equations are used in several areas, such as probability theory, biology, economics, control theory and physics for modeling systems exhibiting anomalous dynamics, usually characterized by an ultraslow diffusion.

The topic of this work concerns with the numerical solution of linear FDEs in the form

$$\begin{cases} D^{\alpha}_{t_0} y(t) + \lambda y(t) = f(t) \\ y(t_0) = y_0, \end{cases} \tag{1}$$

where $\alpha \in \mathbb{R}$ is the fractional order, $\lambda \in \mathbb{R}$, $y(t) : [t_0, T] \to \mathbb{R}$ and the forcing term $f(t)$ is assumed sufficiently smooth. With $D^{\alpha}_{t_0}$ we denote the fractional derivative operator, with respect to the origin t_0, according to the Caputo's definition

$$D^{\alpha}_{t_0} y(t) \equiv \frac{1}{\Gamma(1-\alpha)} \int_{t_0}^{t} \frac{y'(s)}{(t-s)^{\alpha}} ds,$$

where $\Gamma(\cdot)$ is the Euler's gamma function.

We present some results on a class of competitive and highly accurate Product Integration rules derived from an equivalent formulation of (1) in terms of a Volterra integral equation with a generalized Mittag–Leffler function in the kernel.

By means of the error analysis we show that the proposed rules allow to overcome the order barrier of classical PI rules and we discuss the way in which rules of higher order can be developed.

Some aspects related to the computational complexity are furthermore discussed.

Finally, some numerical tests are presented in order to confirm the theoretical findings .

Extrapolation of symmetrized Runge–Kutta methods

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Key words: extrapolation, order reduction, Gauss methods, stiff problems, symmetrizer

The *extrapolation* of symmetric methods of order 2 in accelerating the convergence of numerical solutions of stiff initial value problems has been investigated by Lindberg [1], Bader and Deuflhard [2]. In this paper we extend the investigation to symmetric Runge-Kutta methods of higher order. We show how to construct *symmetrizers* for arbitrary symmetric Runge-Kutta methods (see Chan [3]) that preserve the h^2-asymptotic error expansions while providing the necessary damping for stiff problems. We investigate the resulting suppression of order reduction that symmetric methods experience, thereby enabling extrapolation to be applied.

We construct symmetrizers for Gauss methods with 2 and 3 stages and study different ways of applying symmetrizers/extrapolation depending on how the numerical solution is propagated. In particular we analyse the error behaviour for the Prothero-Robinson problem in detail and report on some numerical experiments that show the merit of using symmetrizers.

References

[1] B. Lindberg, *On the smoothing and extrapolation for the trapezoidal rule*, BIT., **11**, 29 – 52, 1971.

[2] G. Bader and P. Deuflhard, *A semi-implicit midpoint rule for stiff systems of ordinary differential equations*, Numer. Math. **41**, 373 – 398, 1983.

[3] R. P. K. Chan, *Extrapolation of Runge–Kutta methods for stiff initial value problems*, Thesis submitted for the degree of Doctor of Philosophy at the University of Auckland, 1989.

Approximate Inverse Preconditioning using POSIX threads on multicore systems

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Key words: Sparse linear systems, parallel preconditioned conjugate gradient method, parallel computations, POSIX threads, multicore systems.

During the last decades, explicit approximate inverse preconditioning methods have been extensively used for efficiently solving sparse linear systems on multiprocessor systems. The effectiveness of explicit approximate inverse preconditioning schemes relies on the use of efficient preconditioners that are close approximants to the coefficient matrix and are fast to compute in parallel.
In this article, new parallel computational techniques are proposed for the parallelization of explicit preconditioned conjugate gradient type methods, based on Portable Operating System Interface for UniX (POSIX) Threads, for multicore systems. For parallelization purposes, a replication of the parallel explicit preconditioned bi-conjugate conjugate gradient - STAB (PEPBiCG-STAB) method was assigned on each created thread, with different index bands and with proper synchronization points on inner products and matrix-vector multiplications. The excessive overhead produced by the template-based parallel implementations was avoided by using POSIX Threads, maximizing the overall performance of the parallel implementation of the PEPBiCG-STAB method and throttling it close to the corresponding theoretical estimate.
Finally, numerical results for the performance of the PEPBiCG-STAB method for solving characteristic two dimensional boundary value problems on multicore computer systems are presented, which are favorably compared to corresponding results from multiprocessor systems. The implementation issues of the proposed method are also discussed using POSIX Threads on a multicore computer system.

On the convergence of the method of alternating projections for multivariate symmetric eigenvalue problem

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Key words: multivariate eigenvalue problem, method of alternating projections, linear convergence

Let Λ be a diagonal matrix of the form

$$\Lambda = diag\{\lambda_1 I^{[n_1]}, ..., \lambda_m I^{[n_m]}\}, \tag{1}$$

where $\sum_{i=1}^{m} n_i = n,\ \lambda_i \in R$ or $\lambda_i \in C$ for $i = 1, 2, ..., m$ and $I^{[n_i]}$ is the identity matrix of the size n_i. Let $x \in R^n$ be partotioned into blocks $x = [x_1^T, ..., x_m^T]^T$ with $x_i \in R^{n_i},\ i = 1, 2, ..., m$.

Definition. A multivariate eigenvalue problem (MEP) we define as: for a given symmetric matrix $A \in R^{n\times n}$ we should find the matrix Λ and vector x such that

$$Ax = \Lambda x,\ \|x_i\| = 1,\ i = 1, 2, ..., m, \tag{2}$$

where $\|x\|^2 = \sum_{i=1}^{k} x_i^2$ for $x \in R^k$.

Multivariare eigenvalue problems for symmetric and positive definite matrices appear in multivariate statistic theory where coefficients are to be determined so that the resulting linear combinations of sets of random variables are maximally correlated.

Algorithm. Let $x^0 \in R^n,\ \|x_i^0\| = 1,\ i = 1, 2, ..., m,$ be given. We define the method of alternative projections in the following way: let $k = 0$, here k denotes number of iteration. Given $x^k \in R^n$, solve the inhomogeneous symmetric eigenvalue problems for $i = 1, 2, ..., m$

$$A_{ii}x = \lambda_i x_i + b_i^k, \qquad \|x_i\| = 1 \tag{3}$$

where $b_i^k = -\sum_{j=1}^{i-1} A_{ij}x_j^{k+1} - \sum_{j=i+1}^{m} A_{ij}x_j^k$, and matrix A is partitioned into blocks, where $A_{ii} \in R^{n_i\times n_i},\ i = 1, 2, ..., m$. Denote the solution of the problem as $(\lambda_i^{k+1}, x_i^{k+1})$. In the k-th iteration we get the diagonal matrix Λ^{k+1} and the vector $x^{k+1} \in R^n,\ k := k + 1$.

If we take the maximum (minimum) solutions of the inhomogeneous problems, then the method is convergent to the maximum (minimum) solution (Λ^*, x^*) of the multivariate symmetric eigenvalue problem. Here we prove the quadratic convergence of the method on the subspace

$$Q = Q_1 \times Q_2 \times ... \times Q_m \tag{4}$$

where $Q_i = \{y \in R^{n_i} : y = \alpha_i x_i^*,\ \alpha_i \in R\},\ i = 1, 2, ..., m$.

In generally, we prove only q-linear convergence of the method. In practice, for some examples the method is superlinearly convergent to the solution.

Extrapolated Modulus Algorithms for the Solution of the Linear Complementarity Problem with an H_+-Matrix Coefficient

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AMS subject classification: Primary 65F10

Key words: LCP, $P-$matrices, real symmetric positive definite matrices, H_+-matrices, iterative schemes, extrapolation, (Block) Modulus Algorithm.

The numerous applications the *Linear Complementarity Problem* (LCP) has as, e.g., in the solution of Linear and Convex Quadratic Programming, in Free Boundary Value problems of Fluid Mechanics, etc, makes its efficient numerical solution a very imperative and interesting area of research. For the solution of LCP many methods have been proposed especially when its matrix coefficient is a real symmetric positive definite or an H_+-matrix. In this work we assume that the matrix coefficient $M \in \mathbf{R}^{n,n}$ of the LCP is an H_+-*matrix* and propose a *(non)stationary extrapolation* of the *(Block) Modulus Algorithm* for its solution. As will be shown by theory and illustrative numerical examples the *(Non)stationary Extrapolated Block Modulus Algorithm* is far better than all other previous similar Algorithms.

Compact Fourier Analysis for Multigrid Methods based on Block Generating Functions

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Key words: Multigrid, Fourier Analysis, generating function, block symbol.

A crucial point for the efficiency of a multigrid (MG) method is the appropriate choice of its components, which allows for an efficient interplay between smoother and coarse grid correction. In many cases, this coordination can be made by means of a Local Fourier Analysis (LFA), which is an important quantitative tool for the development of new efficient MG methods. Here we consider the notion of Compact Fourier Analysis (CFA) based on block generating functions which is connected with the LFA. However, the CFA offers a more elegant and easy to survey description and a clear overview on the MG components. The principal idea of CFA is to model the MG mechanisms by means of generating functions and block symbols. The block symbol captures the behavior of the full matrices and it is absolutely simple to handle, since it is a matrix of small order.

We present the formalism and framework of the CFA approach. An important goal is to utilize the CFA for deriving MG as a direct solver, i.e. an MG cycle that will converge in just one iteration step. We give necessary and sufficient conditions that have to be fulfilled by the MG components for deriving a direct solver. We introduce general and practicable MG components that lead to MG as a direct solver. The CFA is used for calculating smoothing factors and the combined smoothing and coarse grid correction total error reduction of a twogrid step. New highly efficient MG algorithms are derived by modifying appropriately the MG components that lead to the direct solver. Numerical experiments demonstrate the theoretical results.

Local Meshless Method for the Numerical Solution of the Two-Dimensional Nonlinear Burger's Equations

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Key words: Haar wavelets, System of coupled second-order ordinary differential equations, Boundary-value problems(BVPs), Numerical method.

Abstract

This paper examines the numerical solution of the nonlinear coupled Burger's equations with various values of viscosity by local meshless methods. The local radial basis functions collocation method (LRBFCM) belongs to the class of truly meshless methods which do not need any underlying mesh but work on a set of uniform or random nodes only, without any a priori node to node connectivity. The numerical solution obtained from the LRBFCM for different value of viscosity parameter are compared with analytical solution as well as other numerical methods. Time discretization is performed in explicit way and collocatio with the multiquadric radial basis functions (RBFs) are used to interpolate diffusion-convection variable and its spatial derivatives. Five nodded sub-domains are used in the local support. Accuracy of the method is assessed as a function of the time and space discretizations. It can be easily seen that the proposed method is efficient, accurate and stable for high Reynolds numbers.

Well-balanced shock-capturing hybrid finite volume - finite difference schemes for Boussinesq-type models

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Key words: finite volume method, Boussinesq-type equations, solitary waves, run-up, breaking waves

A numerical scheme for numerical solving a class of extended Boussinesq equations is presented. Both the extended Boussinesq formulations of Nwogou (1993) and Madsen and Sörensen (1992) are considered. The governing equations include the conservative form of the nonlineal shallow water equations for shock capturing. The numerical scheme combines a Godunov-type finite volume technique, based on an approximate Riemann solver, for the inter-cell advective fluxes and bathymerty source terms, with the finite difference method, used to discretize the dispersive terms. Time integration is performed using a fourth order Adams-Basforth-Moulton predictor scheme while a fourth-order MUSCL-type reconstruction technique is implemented to compute the values at cell interfaces for use in the local Riemann problems. The bathymerty source term is discretised as to provide a well-balanced scheme, also in the presence of wet/dry fronts which are properly handled in the numerical model.

Two different option in order to handle wave breaking are presented and tested. The first one relays on the shock-capturing features of the finite volume method that allows an intrinsic representation of wave breaking, while the second option handles breaking through momentum conservation with energy dissipation based on an eddy viscosity concept. To assess the performance and expose the merits and differences of the two Boussinesq formulations and wave breaking options, the numerical model has been applied to a number of standard test cases, for solitary wave propagation and interaction, as well to reproduce laboratory data for wave propagation, wave breaking and runup on plane beaches, and wave transformation over fringing reefs.

NON-POLYNOMIAL SEXTIC SPLINE APPROACH FOR SOLVING VARIABLE COEFFIECIENT FOURTH-ORDER PARABOLIC EQUATIONS

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Abstract: In this paper fourth-order variable coefficient parabolic partial differential equation, that governs the behaviour of a vibrating beam, is solved by using a three level implicit method based on non-polynomial sextic spline in space and finite difference discretization in time. We also obtain a new high accuracy schemes of $O(k^4 + h^8)$.
The linear stability of the presented methods is investigated. We solve test problems numerically to validate the derived methods. Numerical comparison with other existing methods shows the superiority of the presented scheme. We Consider the undamped transverse vibrations of a flexible straight beam whose supports do not contribute to the strain energy of the system and is represented by,

$$\mu(x)\frac{\partial^2 u}{\partial t^2} + \eta(x)\frac{\partial^4 u}{\partial x^4} = f(x,t),\ L_0 \le x \le L_1, t > 0, \tag{1}$$

subject to the initial conditions $u(x,0) = g_0(x)$ and $u_t(x,0) = g_1(x)$, for $L_0 \le x \le L_1$, and with boundary conditions

$$u(L_0,t) = f_0(t),\ u(L_1,t) = f_1(t) \ \text{ and } \ u_{xx}(L_0,t) = p_0(t), u_{xx}(L_1,t) = p_1(t),\ t \ge 0$$

where u is the transverse displacement of the beam,$\mu(x) > 0$ and $\eta(x) > 0$ are mass per unit length and beam bending stiffness, t and x are time and distance variables respectively, $f(x,t)$ is dynamic driving force per unit mass.

Professor David M. Young, Jr.: His Research, Career, and Life

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Keywords: Successive Overrelaxation (SOR), large sparse linear systems, iterative methods/algorithms

The late David M. Young, Jr. (1923–2008) was an internationally known pioneer in the field of numerical analysis. His 1950 Harvard University dissertation is a classical piece of mathematical research. It established the mathematical framework for the Successive Overrelaxation (SOR) method, among other significant things. Also, Dr. Young's 1970 book on *Iterative Solution of Large Linear Systems* is a landmark in the scientific computing literature. Young's career evolved in parallel to the first fifty years of the modern scientific computing era—from the early days of computers to the modern parallel supercomputers. Professor Young was instrumental in the development of iterative algorithms and software for solving large sparse linear systems of algebraic equations. Such systems typically arise in the numerical solution of elliptical partial differential equations. We present an overview of DMY's extremely active career and life as a teacher, researcher, and an administrator, as well as a family man and avid tennis player, while always being a gentleman.

From his legacy of research papers and books, Professor Young was, and still is, an invaluable source of knowledge and inspiration to us all!

A progression of the backtrack optimization technique for forecasting potential financial crisis periods

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Key words: Financial crisis alert, Backtracking, Time series.

Financial crisis is a curse that follows any economic and financial system regardless its profitability and the level it functions. The appearance of crises across financial markets, especially during the 1990s that the internationalized markets adopted a rather approachable character, imposed severe costs in financial and social systems. Such situation enhance major withdrawn of funds from economies and finally affect the society itself. The recent global financial abnormal situation has motivated further interest empowered from the socio-economical consequences its results would enclose, which certify the importance of an immediate response to a crisis first symptoms towards minimizing its impact. Plethora of research and methodologies have developed towards resolving the issue of predicting a potential period of crisis. Their common characteristic is that most of them focus on the existence of indicator/s able to allocate the threshold rendering a crisis burst.

Recently we proposed an algorithm which, although it extracts indicator-based alerts, differentiates from the signal approaches on the indicator's nature. Moreover, the observation that a time series behavies similarly to a trace of a function with m variables, expanded the implementation of function properties on time series. Based on such observations, on this algorithm was exploited the Lipschitz constant as an indicator of a time series' acceleration to drastic changes. Its usage provided efficient evidence regarding its accuracy to an ex-ante chronical allocation of a future abnormal financial situation.

This idea is combined with that of using two different optimization methods, with different convergence characteristics, in order to envelop the future optima in a time range. Different convergence characteristics of the methods result to the interval that is eligible to envelop the local optima, plus on this study the local optima to foresee regards changes of the crisis indicator used; that is deductions of the Lipschitz constant.

This paper imposes the generation of a forward chronical interval that is vulnerable for a crisis to burst. *Some* approximations of the Lipschitz constant as a crisis indicator consist the time series in question. Further the application of two different optimization techniques over the Lipschitz-made time series results to a future period of time that is a chronical interval vulnerable for a crisis to burst. The preliminary obtained results provide strong evidence that the method may be used as an Early Warning System (EWS) in financial crisis.

Numerical Solution of Discontinuous Differential Systems: Approaching the Discontinuity Surface from One Side

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Key words: Discontinuous ODEs, Filippov theory, Runge-Kutta methods.

We present a numerical approach to treat discontinuous differential systems of ODEs of the type: $x' = f_1(x)$ when $h(x) < 0$ and $x' = f_2(x)$ when $h(x) > 0$, where $\Sigma := \{x : \ h(x) = 0\}$ is a smooth co-dimension one discontinuity surface, and with $f_1 \neq f_2$ for $x \in \Sigma$. Often, f_1 and f_2 are defined on the whole space, but there are applications where f_1 is not defined above Σ and f_2 is not defined below Σ. For this reason, we consider numerical schemes –based on a class of explicit Runge-Kutta methods– which do not evaluate f_1 above Σ (respectively, f_2 below Σ).

Generalized Iterative Methods for augmented linear systems*

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Key words: Iterative methods, augmented linear systems, SOR method

In this paper we study the solution of large sparse augmented linear systems. The generalized modified extrapolated SOR (GMESOR) method is considered. We find sufficient conditions for GMESOR to converge and determine its optimal iteration parameters and the corresponding minimum value of its convergence factor. Under the assumption that the eigenvalues of a key matrix are real it is shown that optimum GMESOR becomes equivalent to optimum GSOR [1], [2] whose convergence factor equals to the one of the Conjugate Gradient (CG) method. For comparison, we develop a similar analysis for the Generalized Modified Preconditioned Simultaneous Displacement (GMPSD) method.

References

[1] Z.-Z. Bai, B. N. Parlett and Z.-Q. Wang, On generalized succesive overrelaxation methods for augmented linear systems, Numer. Math. 102, (2005), 1-38.

[2] G. H. Golub, X. Wu and J. -Y. Yuan, SOR-like methods for augmented systems, BIT 41, (2001), 71-85.

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Nonmonotone Sign-based Algorithms for Neural Networks Learning

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Key words: Learning algorithms, nonlinear optimisation, nonlinear Jacobi, Rprop algorithm, neural network architectures.

Nonmonotone learning is in line with theories for cognitive development and is supported by recent advances in optimisation methods, which showed that nonmonotone optimisation algorithms possess useful properties, such as global and superlinear convergence, require fewer numbers of line-searches and function evaluations, and are effective for large-scale unconstrained problems.

In this work, we propose nonmonotone first-order learning methods that apply one-step subminimisation by employing an Resilient Propagation (Rprop)-based heuristic scheme to locate an approximation of the subminimiser along each weight direction operating in a nonmonotone way. This can be considered as a generalisation of the approach proposed by Anastasiadis et al. (2005) and Anastasiadis et al. (2006), which enforced monotone reduction of the learning error. The theoretical foundations of our approach are discussed and experiments are conducted on a variety of datasets using static and dynamic neural networks to empirically evaluate it. The results provide numerical evidence that supports our claims about the benefits of this approach.

References

Anastasiadis, A., Magoulas, G.D., & Vrahatis, M.N. (2005). Sign-based Learning Schemes for Pattern Classification. *Pattern Recognition Letters*, 26, 1926-1936.

Anastasiadis, A., Magoulas, G.D., & Vrahatis, M.N. (2006). Improved sign-based learning algorithm derived by the composite nonlinear Jacobi process. *Journal of Computational and Applied Mathematics*, 191, 166-178.

The use of nonclassical pseudospectral method for solving nonlinear variational problems

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Key words: Variational problems, Nonclassical pseudospectral method, Orthogonal functions, Euler-Lagrange equation, Euler-Poisson equation.

In the large number of problems arising in analysis, mechanics, geometry, etc., it is necessary to determine the maximal or minimal of a certain functional. Problems in which it is required to investigate a function for a maximum or minimum are called variational problems.

In this paper we introduce an efficient computational method to solve variational problems for functional dependent on higher-order derivatives and functionals dependent on m functions in the following form:

(i)Extremize

$$J[x(t)] = \int_a^b F(t, x(t), x'(t), \ldots, x^{(n)}(t))dt,$$

with the given boundary conditions

$$x(a) = a_0, \;\; x'(a) = a_1, \;\; \ldots, \;\; x^{n-1}(a) = a_{n-1},$$

$$x(b) = b_0, \;\; x'(b) = b_1, \;\; \ldots, \;\; x^{n-1}(b) = b_{n-1}.$$

(ii)Extremize

$$J[x_1, x_2, \ldots, x_m] = \int_a^b F(t, x_1, x_2, \ldots, x_m, x_1', x_2', \ldots, x_m')dt,$$

with the given boundary conditions of the form

$$x_k(a) = x_k^0, \quad x_k(b) = x_k^1, \quad k = 1, 2, \ldots, m.$$

This method requires the definition of nonclassical orthogonal polynomials and collocation points (interpolation nodes) and it is applied to satisfy the Euler-Lagrange and Euler-Poisson equations (as ordinary differential equations) and it's boundary conditions at these collocation points. The application of the method to differential equations leads to an algebraic system. For the case of nonlinear differential equations, the resulting system is nonlinear system which can be solved using Newton's iterative method. Numerical examples are included to demonstrate the validity and applicability of the proposed method.

A new approach for solving systems of nonlinear equations via a forecasting hybrid technique

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Key words: nonlinear equations, ARMA models, time series forecasting.

Nonlinear problems are of interest to engineers, physicists and mathematicians because most physical systems are inherently nonlinear in nature. There is a class of methods for the numerical solution of a system of nonlinear equations which arise from iterative procedures. A feature of these repetitive processes is that they cannot use information from the path traced out from some/all previous points that finally leads to the solution of the system. Moreover, this sequence of points -generated by an iterative process- depends crucially on the nature of the involved nonlinear equations and the used iterative method.

Time series is a sequence of data points, measured typically at successive times spaced at uniform time intervals. Time series forecasting is the use of a model to forecast future events based on known past events; to predict data points before they are measured. Models for time series forecasting are the autoregressive (AR) models, the integrated (I) models, and the moving average (MA) models. These three classes depend linearly on previous data points. Combinations of these techniques produce autoregressive moving average (ARMA) and autoregressive integrated moving average (ARIMA) models.

Inspired by the idea of time series forecasting, in this paper, we treat the produced iterative points of any iterative process, at the last m steps, to be the known past events for the forecasting model. The proposed approach results to the next iteration of the iterative process, for every coordinate, through a hybrid way using a combination of the iterative process and the forecasting model of time series. Since the use of time series forecasting is an intermediate step in the iterative process it is necessary to take into account the complexity and the computational cost of this model. Thus, the simple ARMA models seem to be a good choice. Moreover, in order to avoid the recalculation of ARMA coefficients at each iteration, a recalculation of them is realized only when it is necessary.

Preliminary numerical examples on well-known test problems are promising.

High-order accurate numerical pressure correction based on Geometric MultiGrid schemes for the incompressible Navier-Stokes equations

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Key words: Geometric Multigrid techniques, Incompressible Navier-Stokes equations, Staggered grids, Compact Difference schemes, Schur Complement, preconditioned Bi-CGSTAB

Industrial and environmental applications of computational fluid mechanics, such as wind turbine blades, high-speed trains, naval transportation, aircraft wings, simulation of blood and atmospheric flow, require detail flowfield information. High order numerical methods offer higher resolution, over low accuracy schemes, for the numerical solution of the incompressible Navier-Stokes equations, for example by marching the solution in time with Runge-Kutta methods and discretizing in space by fourth-order compact difference schemes. The same order of accuracy should be maintained for the pressure correction applied to ensure incompressibility, a procedure which amounts in solving a Poisson-type equation. This is a highly demanding procedure, regarding computational cost, of the overall numerical method. The linear system to be solved is general, large and sparse, suggesting the use of iterative solvers to save computational cost. Estimation of the eigenvalues of the coefficient matrix showed that preconditioned iterative methods (specifically BiConjugate Gradient type methods with Jacobi preconditioning) converge faster than other classical solvers. Nonetheless, execution time for the solution of the linear system remains a forbidding factor for realistic applications. An improved performance is obtained using Schur Complement type iterations, but a significant convergence acceleration is achieved with the incorporation of geometric multigrid techniques into the iterative solver. The performance of several multigrid algorithms is investigated. The accuracy of the fourth-order compact difference scheme is not deteriorated by the incorporation of the multigrid technique, though realistic boundary conditions are effectively handled. The increase of scalability of the computation and the direct realization of the parallelism is ensured therefore, for the costly incompressibility problem. Multigrid schemes can accelerate the iterative solution process significantly (hundreds of times) even for fine discretizations.

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Parallel Schur Complement type iterations for Collocation linear systems

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Key words: Collocation Finite Element method, Red-Black Coloring Scheme, Bi-CGSTAB, Schur Complement, Grid Computers.

We consider the computationally intense problem of solving the large, sparse and non-symmetric system of equations arising from the discretization of Boundary Value Problems (BVPs) by the Collocation finite element method using Hermite bi-cubic elements. As the size of the problem directly suggests the usage of parallel iterative methods, we consider the implementation on distributed memory parallel architectures of a Schur Complement type technique with the Bi-Conjugate Gradient Stabilized (Bi-CGSTAB) iterative method. To induce scalability to our computation, we structure the Collocation matrix to a particular line Red-Black ordered form, leading to the development of well-structured parallel algorithm for the solution method. The realization of the algorithm took place on two different type of grid computers. First on a SUN X2200M2 with 16-nodes and 64 AMD Opteron type cores grid computer connected via an ethernet gigabit network and then on a HP c7000 with 32-nodes and 128 AMD Opteron type cores cluster computer. Speed-up measurements are used to reveal the efficiency of the parallel implementation.

Direct numerical simulations of plunging airfoils wakes using spectral/hp element method.

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Key words: Direct Numerical Simulation, Plunging/Flapping airfoils, Spectral/hp element method, Airfoil wakes.

Plunging airfoils are investigated for applications such as Micro-Air Vehicles (MAVs) and bird and fish like propulsion. Plunging or flapping wings can provide more propulsive efficiency than that of fixed wings, especially at small to moderate Reynolds numbers, where the MAVs (due to their small size) operate. Furthermore, it has been observed that birds and insects rely on detaching and separating vortices resulting from the flapping motion to create higher lift and thrust. Thus, understanding the flow over plunging airfoils and its dependence to varying the governing parametrs is of great interest. The Reynolds number, the frequency and amplitude of the plunge motion are the most important parameters to characterize the aerodynamics of plunging airfoils and their wakes. In this contribution the unsteady flow over a plunging 2D airfoil is simulated using a high-order numerical method associated with a moving frame of reference technique. Most numerical methods used in the scientific community are second-order accurate in time and space, we use here a high-order method to obtain more accurate and high resolution data that are used to characterize the boundary-layer over the airfoil and the wake patterns. The results are presented in terms of vorticity countours (particularly at the boundary-layer and the wake region), time averaged horizontal velocity and time series of the force coefficients. As predicted by theory and experiments, three wake patterns are identified, namely : drag producing wake (Karman Street), thrust producing wake (reversed Karman Street) and neutral wake. The mean incidence investigated is $\overline{\alpha} = 0^\circ$ and Reynolds number $4500 \leq Re \leq 10^4$. Furthermore, a non-zero mean incidence is considered $\overline{\alpha} = 12^\circ$ and the contribution of the leading-edge shedding to the lift and thrust production is discussed. The transition from a drag producing wake, to a neutral, and a thrust producing wake is observed when increasing the plunge frequency (at constant amplitude) and the amplitude (at constant frequency). These results are in accordance with previsous published experimental and computational investigations at $\overline{\alpha} = 0$. Moreover, we investigate the case where $\overline{\alpha} = 12$, varying the plunge amplitude frequency, and characterizing the wake patterns.

The numerical solution of Volterra integral equation by the forward-jumping method

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Key words: Volterra-Uryson equation, convergence, reduced computational cost.

As it is known, the integral equations play an important role in pure and computational mathematics. They are useful also for the numerical calculations in many problems of mechanical fluctuations in theoretical physics. Remark that investigation researches of the integral equations with variable boundaries began with Abel's works. The new beginning in the theory of integral equations is due mainly to Volterra. For the numerical solution of such equations we often use quadrature methods. In this work we use the forward-jumping method with constant coefficients and give sufficient conditions for its convergence.

Let's consider the following nonlinear Volterra type integral equation:

$$y(x) = f(x) + \int_{x_0}^{x} K(x, s, y(s))ds, \quad x \in [x_0, X]. \tag{1}$$

Sometimes this equation is referred to as Volterra-Uryson equation.

Suppose that $K(x, s, y)$ a continuous function in some closed domain G and the equation (1) has unique solution on the segment $[x_0, X]$.

Applying a quadrature method to equation (1) we have:

$$y_n = f_n + \sum_{i=1}^{n} \alpha_i K(x_n, x_i, y_i). \tag{2}$$

As it is apparent from (2), the amount of computing work for the kernel function $K(x, s, y)$ at the point x_n equals to n, and at the point x_{n+1} equals to $n + 1$. In this regard, the amount of computing work increases during the transaction from one point to another. For the numerical solution of equation (1) we suggest the forward-jumping method, which is free from the noted disadvantage:

$$\sum_{i=0}^{k-m} \alpha_i (y_{n+i} - f_{n+i}) = h \sum_{j=0}^{k} \sum_{i=0}^{k} \beta_{i,j} K(x_{n+j}, x_{n+i}, y_{n+i}).$$

We also find sufficient conditions for the convergence of the suggested method.

Remark that the investigation of the forward-jumping methods began from Kowell's work, published in 1910, which is fundamental to applied numerical solution of ordinary differential equations.

Properties of the Sylvester Hadamard matrices and their applications

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Key words: Sylvester Hadamard matrices, Sign property, D-optimal designs, Pivot patterns.

In 1867 Sylvester had noted that if one took a ± 1 matrix, S, of order t whose rows are mutually orthogonal then $\begin{bmatrix} S & S \\ S & -S \end{bmatrix}$ was an orthogonal ± 1 matrix of order $2t$. Matrices of this form are called Sylvester Hadamard matrices and are defined for powers of 2.

The first few Sylvester-Hadamard matrices of orders $2^p,\ p = 1, 2, 3$ are given below. For information, we give in an additional last column the number of times the sign changes as we proceed from the first to the last element across the row:

$$S_2 = \left[\begin{array}{cc|c} 1 & 1 & 0 \\ 1 & - & 1 \end{array}\right],\ S_4 = \left[\begin{array}{cccc|c} 1 & 1 & 1 & 1 & 0 \\ 1 & - & 1 & - & 3 \\ 1 & 1 & - & - & 1 \\ 1 & - & - & 1 & 2 \end{array}\right],\ S_8 = \left[\begin{array}{cccccccc|c} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \\ 1 & - & 1 & - & 1 & - & 1 & - & 7 \\ 1 & 1 & - & - & 1 & 1 & - & - & 3 \\ 1 & - & - & 1 & 1 & - & - & 1 & 4 \\ 1 & 1 & 1 & 1 & - & - & - & - & 1 \\ 1 & - & 1 & - & - & 1 & - & 1 & 6 \\ 1 & 1 & - & - & - & - & 1 & 1 & 2 \\ 1 & - & - & 1 & - & 1 & 1 & - & 5 \end{array}\right]$$

In this paper we study properties of Sylvester Hadamard matrices that lead to interesting applications. More specifically,

1. The sign property

If a ± 1 matrix of order n, S_n, has all the sign changes 0, 1, ..., $n-1$ then its equivalent with a Sylvester Hadamard matrix.

This property is well known to users of the Walsh functions but has not been emphasized in the mathematical literature. This has prompted us to mention it explicitly here.

2. D-optimal designs embedded in Sylvester Hadamard matrices

We will study which D-optimal designs (± 1 matrices with maximal determinant) of dimension m can be embedded in a Sylvester Hadamard matrix of dimension n.

3. Pivot patterns of Sylvester Hadamard matrices

We will study the pivot patterns of S_{16}, S_{32}, S_{64} and we will try to answer open questions concerning the appearing pivot values such as:

Question For a Hadamard matrix of order 16, the determinant of its lower right 4×4 principal submatrix can take the value 8 only if the matrix is in the Sylvester Hadamard equivalence class ?

On some finite volume schemes applied to nonlinear dispersive wave equations

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Key words: finite volume method, dispersive PDEs, solitary waves, run-up, water wave, inundation.

The complete water wave problem remains a difficult task despite recent progresses in this field. Its intrinsic complexity and stiffness prevent from efficient simulations in complex and large domains. Consequently, a number of approximative models have been proposed. In the present work we consider weakly nonlinear/weakly dispersive wave regime which is modelled by the family of Boussinesq type equations [1]. In the present study we apply some finite volume schemes to these models.

Our numerical schemes are tested on various practical problems [2]. First, we consider some classical questions of soliton dynamics: solitary wave propagation, conservation of invariants, interactions, dispersive shock formation. A comparison with experiments on solitons head-on collision is also performed.

Finally, special attention is given to the run-up of long waves on a plane beach. We modify Peregrine's [1] system to derive a new nonlinear and dispersive system appropriate for the study of long wave runup. Validation by experimental data is presented for the run-up of non-breaking and breaking solitary waves on a plane beach. Some applications to tsunami wave modelling are also discussed.

References

[1] PEREGRINE, D. H. 1967. Long waves on a beach, *J. Fluid Mech.*, **27**, 815–827.

[2] DUTYKH, D., KATSAOUNIS, TH. & MITSOTAKIS, D. 2010. On some finite volume schemes applied to nonlinear dispersive wave equations for the study of solitary waves and the runup of long waves in 1D, *to appear*.

An Extended Origin-Based Method for Solving Capacitated Traffic Assignment Problem

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Key words: Capacitated traffic assignment problem, Origin-Based Algorithm, Penalty strategy, Topological order.

In this paper, we have proposed a new algorithm for solving Capacitated Traffic Assignment Problem (CTAP). The proposed method first approximates original problem with a sequence of standard Traffic Assignment Problem (TAP) by an inner penalty strategy and then this subproblems have been solved by recently proposed Origin-Based (OB) algorithm with some modifications. This algorithm will be more useful for large scale problems since all computation in OB algorithm is done under a topological order.

The time-dependent spectral method for solving equations of dynamic nonlinear elasticity

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Key words: nonlinear dynamic equation, von Kármán elastic plate, time-dependent spectral method, Fourier transform, Runge-Kutta scheme.

AMS subject classification: 35Q74, 35L57, 74K20, 74S25, 65T40, 65L06.

The nonlinear dynamic equations of bending of thin elastic von Kármán plate are solved by means of the time-dependent spectral method. The plate is simply supported and subjected to the external constant force (compressive or stretching) λ applied at the edges of the plate. The following system of coupled two nonlinear dynamic partial differential equations is considered

$$\begin{aligned} h\rho\, w_{tt} - \rho\frac{h^3}{12}\Delta w_{tt} + hc\, w_t + D\Delta^2 w + L_\lambda w &= h[w,\psi], \ \text{in } \Omega, \\ \Delta^2\psi &= -\tfrac{E}{2}[w,w], \end{aligned} \tag{1}$$

where $[w,\psi] = \partial_{11}w\partial_{22}\psi + \partial_{11}\psi\partial_{22}w - 2\partial_{12}w\partial_{12}\psi$, $w(t,x,y)$ is a deflection, $\psi(t,x,y)$ is the Airy stress potential, $w,\ \psi \in C(0,T;W^{2,2}(G))$, $\Omega = (0,T]\times G$, $G = (0,l_1)\times(0,l_2)$ is the shape of the plate. Furthermore, h, ρ, c, D and E are physical parameters of the plate and L_λ is a differential operator characterizing the external forces (compression and tension) on the edges of the plate.

The initial and boundary conditions for (1) read

$$\begin{aligned} &w(0,x,y) = u(x,y),\ w_t(0,x,y) = v(x,y) \ \text{ in } \ G, \\ &w = \Delta w = 0,\ \psi = \Delta\psi = 0 \ \text{ in } \ (0,T]\times\partial G, \end{aligned} \tag{2}$$

where $u, v \in W^{2,2}(G)$. According to the classical results of dynamic nonlinear elasticity theory the initial-boundary value problem (1), (2) has a unique solution. The solution we expand in partial sums of double Fourier's series. The global basis functions are the eigenfunctions of the Laplacian under the Dirichlet conditions. Using Galerkin's projections for (1), (2) we have

$$\mathbf{H}\mathbf{w}_N''(t) + \hat{c}\mathbf{w}_N'(t) + \mathbf{K}_1\mathbf{w}_N(t) - \mathbf{B}_\lambda\mathbf{w}_N(t) = \mathbf{A}_{1,N}(\mathbf{w}_N(t), \mathbf{K}_2^{-1}\mathbf{A}_{2,N}(\mathbf{w}_N(t),\mathbf{w}_N(t))). \tag{3}$$

Here $\mathbf{w}_N(t)$ is a vector with components which are the time-dependent Fourier coefficients, $\hat{c} = hc$, the matrices $\mathbf{H}$, $\mathbf{K}_1$, $\mathbf{K}_2$ and $\mathbf{B}_\lambda$ arise from approximations of the differential operators, and $\mathbf{A}_{1,N}$, $\mathbf{A}_{2,N}$ denote approximations of the nonlinear geometric terms in (1). The equation (3) is reduced to two first order ordinary differential equations. For solving the obtained system with the found initial conditions $\mathbf{w}_N(0)$, $\mathbf{w}_N'(0)$ the fourth order Runge-Kutta scheme is applied.

AN IMPLICIT FINITE DIFFERENCE SCHEME FOR FOCUSING SOLUTIONS OF THE GENERALIZED DAVEY-STEWARTSON SYSTEM

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Key words: The Generalized Davey-Stewartson system, global existence, blow-up.

The generalized Davey-Stewartson (GDS) system is given by

$$
\begin{aligned}
& i\, u_t + \sigma u_{xx} + u_{yy} = \kappa \mid u \mid^2 u + \gamma(\varphi_{1,x} + \varphi_{2,y})u \\
& \varphi_{1,xx} + m_2\varphi_{1,yy} + n\varphi_{2,xy} = (\mid u \mid^2)_x \\
& \lambda\varphi_{2,xx} + m_1\varphi_{2,yy} + n\varphi_{1,xy} = (\mid u \mid^2)_y
\end{aligned}
$$

where u and φ_1, φ_2 are, respectively, the complex- and the real-valued functions of spatial coordinates x, y and the time t. The parameters $\sigma, \kappa, \gamma, m_1, m_2, \lambda, n$ are real constants and σ is normalized as $\mid \sigma \mid = 1$. The GDS system has been derived to model $2+1$ dimensional wave propagation in a bulk medium composed of an elastic material with couple stresses [1]. The parametric relation $(\lambda - 1)(m_2 - m_1) = n^2$ follows from the structure of the physical constants and plays a key role in the analysis of these equations. The GDS system is classified according to the signs of parameters $(\sigma, m_1, m_2, \lambda)$. In this study, we consider (+,+,+,+) elliptic-elliptic-elliptic (EEE) and (–,+,+,+) hyperbolic-elliptic-elliptic (HEE) cases.

In this study, the generalized Davey-Stewartson (GDS) system is solved by a numerical method which is based on an extension of the relaxation method introduced in [2]. In the hyperbolic-elliptic-elliptic case, we numerically test the relaxation method by using the analytical blow-up profile. In the elliptic-elliptic-elliptic case, we compare the numerical results with the analytical global existence and blow-up results [3] for certain ranges of parameters. Numerical tests show that the relaxation method does not miss the blow-up phenomena and provides accurate results for the GDS system.

REFERENCES

[1] Babaoglu, C., Erbay, S., 2004. Two dimensional wave packets in an elastic solid with couple stresses, Int. J. Nonlinear Mech. 39, 941-949.

[2] Besse, C., Bruneau, C. H., 1998. Numerical study of elliptic-hyperbolic Davey-Stewartson system: Dromions simulation and blow-up, Math. Model Meth. Appl. Sci. 8, 1363-1386.

[3] Eden, A., Erbay, H. A., Muslu, G. M., 2008. Closing the gap in the purely elliptic generalized Davey-Stewartson system, Non. Anal. TMA 69, 2575-2581.

Auxiliary variational inequality principle and projection methods for MHD propulsion system

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Key words: JSM theory, variational inequalities, marginal turbulence.

In this paper we show how one could extend Jones-Soward-Mussa (JSM) theory (2000): analytic and computational solution for $E \to 0$ and $Pr/E \to \infty$ and another MHD related problems e.g., Zhang (2001) ansatz for: $E << 1$ arbitrary but fixed and $0 \leq Pr < \infty$ the so-called enhanced Nearly Geostrophic Inertial Wave (NGIW) approach. Such extension represents a construction of a new MHD plasma convection and magnetoconvection force theory. Different theoretical and computational aspects are presented. We proposed the auxiliary variational inequality as well as the projection method as a replacement of asymptotic analysis for the solution of some complicated MHD as well as MHD turbulence and thruster problems. We also suggest some variational formulation extension for a similar class of mathematical and engineering problems.

Rescaling Systems of Ordinary Differential Equations: Control of Stiffness and Parallel-in-Time Integration

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Key words: Initial Value Problems, Stiff Systems, Rescaling, Sliced-time Computations, Parallel in time Integration.

Consider the first order initial value problem in which one seeks $Y : [0, T] \to \mathbb{R}^k$, such that:

$$(S) \qquad \begin{cases} \frac{dY}{dt} = F(Y), & 0 < t \leq T \leq \infty, \\ Y(0) = Y_0, \end{cases}$$

The rescaling methodology we are presenting starts with a time-slicing procedure, governed by a uniform stopping criterion that makes solving the IVP (S), that could be stiff, equivalent to solving a sequence of initial value shooting problems (S_n).
Then, a change of variables (of both the time-variable and the solution) is made:

$$\begin{cases} t = T_{n-1} + \beta_n s, \quad \beta_n > 0 \\ Y(t) = Y_{n-1} + D_n Z(s), \end{cases}$$

and yields an equivalent sequence of rescaled initial value shooting problems (S'_n) in which the time and the solution are set to zero at the onset of every slice allowing each of them to be solved through a local approach:

$$(S'_n) \qquad \begin{cases} \frac{dZ_n}{ds} = G_n(Z_n)(s)), & 0 < s \leq s_n \\ Z_n(0) = 0, \\ H[Z_n(s_n)] = 0. \end{cases}$$

The change of the time-variable uses a time-rescaling factor β_n that intends to control the growth of G_n and of its jacobian, i.e. control the stiffness of the original problem. When combined with a relevant End-Of-Slice condition, $H[Z_n(s_n)] = 0$, this technique provides the rescaled systems (S'_n) with a property of **uniform similarity** which infers for certain forms of $F(.)$, the uniform boundedness of the rescaled solutions $\{Z_n(s)\}$ on all slices. While originally intended to kill the

stiffness of the problem (S), the rescaling methodology can be also at the basis of parallel time integration.
The paper aims at presenting cases of applications of such technique and in particular its efficiency in devising parallel algorithms for time-dependent evolution problems.

References

[1] M.BERGER, R.KOHN. *Rescaling algorithm for the numerical calculation of blowing-up solutions.* Commun. Pure Appl. Math. 41 (1988) 841-963.

[2] B.LE MESURIER, G.PAPANICOLAOU, C.SULEM, P.L.SULEM. *The focusing singularity of the nonlinear Shrodinger equation.* In Directions in Partial Differential Equations, Editors Crandall M. et Al., Academic Press (1987) 159-201.

[3] N.R. NASSIF, D. FAYAD AND M.CORTAS, *Sliced-Time Computations with Re-scaling for Blowing-Up Solutions to Initial Value Differential Equations*, ICCS 2005 Proceedings, V.S. Sunderam. et al. (Eds), Springer-Verlag, LNCS 3514 (2006), pp. 58–65.

[4] N.R. NASSIF, N. MAKHOUL-KARAM AND Y. SOUKIASSIAN, *A New Approach for Solving Evolution Problems in Time-Parallel Way*, ICCS 2006 Proceedings Part I, Springer-Verlag Berlin Heidelberg, 3991 (2006), pp. 148–155.

[5] N.NASSIF, N.MAKHOUL-KARAM, Y.SOUKIASSIAN.*Computation of blowing-up solutions for second-order differential equations using re-scaling techniques*. JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, VOLUME 227, ISSUE 1, MAY 2009, PP. 185-195.

A Hybrid Branch & Bound Algorithm for Bound Constrained Optimization

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Key words: Bound constrained optimization, Newton's method, Hull Interval Newton method

In this work a hybrid branch & bound algorithm is proposed for finding the global minimum of a nonlinear function with constant bound constraints. The proposed hybridization consists in finding efficient initial guesses for the classic Newton's method for unconstrained optimization, utilizing an interval branch & bound method for solving interval equations, the Hull Interval Newton method. In particular, the Hull Interval Newton method is employed for finding regions where the objective function is locally quadratic, or are near to areas where the objective function is locally quadratic. The classic Newton's method is initialized by a point from these regions, aiming to converge rapidly to a local minimum. Utilizing properly the found local minima, new regions are arisen, and, finally, the proposed procedure converges to a global minimum of the objective function. The overall approach intends to produce "good" initial points for the classic Newton's method, as well as, to provide a certainty in finding a global minimum utilizing an interval methodology. In addition, the used interval methodology is enhanced by the speed and the low-cost behavior of the real Newton's method. The above assertions are verified by the stated numerical results.

Maximum-norm error estimate of the finite volume approximation for a convection-diffusion equation

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Key words: finite volume method, error estimate, convection-diffusion.

We consider the finite volume (FV) approximation in the sense of [1] for a convection-diffusion equation for $u = u(x,t)$ of $\overline{\Omega} \times [0,T]$,

$$\begin{cases} u_t - \nabla \cdot (\nabla u - bu) = f \quad \text{in} \quad \Omega \times (0,T), \\ u = g \quad \text{on} \quad \partial\Omega \times (0,T), \quad u|_{t=0} = u_0 \quad \text{on} \quad \Omega, \end{cases}$$

where $\Omega \subset \mathbb{R}^2$ denotes a polygonal domain in $\mathbb{R}^2$; T a positive constant; $b : \Omega \times (0,T) \to \mathbb{R}^2$, $f : \Omega \times (0,T) \to \mathbb{R}$, $g : \partial\Omega \times (0,T) \to \mathbb{R}$ and $u_0 : \Omega \to \mathbb{R}$ are given smooth functions.

The purpose of this paper is to prove an error estimate in L^∞ norm, under some appropriate assumptions,

$$\|u - u_h^n\|_{L^\infty(0,T;\Omega)} = O(h + \Delta t) \quad (h \downarrow 0),$$

where u_h^n denotes the FV approximation under consideration with the space and time discretization parameters h and Δt. To prove this uniform convergence result, we basically follow the method of Tabata [2]. In fact, one of the crucial points of Tabata's method is that FV schemes are treated as finite difference schemes defined on irregular meshes, and it can be directly applied to analysis of FV schemes defined on admissible meshes.

References

[1] R. Eymard, T. Gallouët and R. Herbin: *Finite Volume Methods*, Handbook Numer. Anal. **VII** (2000) 713–1020, Elsevier.

[2] M. Tabata: *Uniform convergence of the upwind finite element approximation for semilinear parabolic problems*, J. Math. Kyoto Univ. **18** (1978) 327–351.

Stability Analysis of A Model Using Non Standard Finite Difference Schemes

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Key words: Stability analysis, nonstandard finite difference equation, numerical solution, HIV viruses

In this paper, we developed a non standard numerical scheme for a model used by Perelson, Kirschner and Boer. This model is the interaction of HIV with $CD4^+T$. The model is given by the following system of differantial equations

$$\begin{array}{l} \frac{dT}{dt} = p - \alpha T + rT(1 - \frac{T+I}{T_{\max}}) - kVT, \\ \frac{dI}{dt} = kVT - \beta I, \\ \frac{dV}{dt} = N\beta I - \gamma V, \end{array} \tag{1}$$

with the initial conditions: $T(0) = r_1, I(0) = r_2, V(0) = r_3$. The concentration of $CD4^+T$ cells, the concentration of infected $CD4^+T$ cells by the HIV viruses and free HIV virus particles are denoted respectively by $T(t), I(t), V(t)$.

Nonstandard Finite Difference Schemes are a generalization of the usual discreate models of diferantial equations. They gives us more stable results than classical discretization by using denominator function. We will analyse stability of the model. If the differential equations have a constant solution with a particular stability property, the discrete model should also have this constant solution with exactly the same stability property. We will consider this rule and establish some criterions by choosing suitable denominator functions. By applying the Schur-Cohn criterion, we conclude if the model asymptotically stable or not.

Collocation with discontinuous Hermite elements for a tumor invasion model with heterogeneous diffusion in $1+1$ dimensions

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Key words: Collocation, Hermite cubics, Backward Euler, Gliomas modeling.

Over the past few years, mathematical modeling for studying highly diffusive brain tumors has been well developed. Gliomas are common malignant brain tumors characterized by their aggressive diffuse invasion of brain normal tissue. The basic mathematical model used to study highly diffuse tumors, and at the same time incorporates the brain tissue heterogeneity (white and grey matter), considers a reaction-diffusion equation with a discontinuous diffusion coefficient; namely

$$\frac{\partial \bar{c}}{\partial \bar{t}} = \nabla \cdot \left(\bar{D}(\bar{\mathbf{x}}) \nabla \bar{c} \right) + \rho \bar{c} \tag{1}$$

with

$$\bar{D}(\bar{\mathbf{x}}) = \begin{cases} D_g & , \quad \bar{\mathbf{x}} \text{ in Grey Matter} \\ D_w & , \quad \bar{\mathbf{x}} \text{ in White Matter} \end{cases} . \tag{2}$$

Working towards the development of high order numerical approximation schemes, here, concentrating on the one space dimension case, we develop and study the implementation of a Hermite Collocation method with Discontinuous Hermite elements to treat first derivative discontinuities at internal interface points, as the spatial discretization method, combined with Backward (implicit) Euler (BE) time discretization schemes. Numerical experiments are included to demonstrate the performance of the method.

The Computation of Conformal Modules by Domain Decomposition

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Key words: Numerical conformal mapping; Conformal module; Domain decomposition

Let $Q := \{\Omega;\ z_1, z_2, z_3, z_4\}$ be a (generalized) quadrilateral, consisting of a Jordan domain Ω and four specified points z_1, z_2, z_3, z_4 in counterclockwise order on its boundary, and let R_H denote a rectangle of base 1 and height H of the form $R_H := \{(\xi, \eta),\ 0 < \xi < 1,\ 0 < \eta < H\}$. Then, the conformal module $m(Q)$ of Q is the unique value of H for which Q is conformally equivalent to the rectangular quadrilateral $\{R_H;\ 0, 1, 1 + iH, iH\}$. By this it is meant that for $H = m(Q)$, and for this value only, there exists a unique conformal mapping of Ω onto R_H that takes the four specified points z_1, z_2, z_3, z_4 of Q, respectively, onto the four vertices $0, 1, 1 + iH, iH$ of R_H.

Apart from being an important domain functional from the function theoretic point of view, the conformal module of a quadrilateral is also intimately related to certain physical constants that occur in engineering applications. In particular $m(Q)$ plays a very central role in applications involving the measurement of resistance values of integrated circuit networks. For these reasons, the problem of determining $m(Q)$ is of interest both from the theoretical and the practical points of view.

In this talk we consider some of the computational and application aspects of the problem of determining $m(Q)$, and give an outline of a highly efficient domain decomposition method for computing the conformal modules of elongated quadrilaterals of the type that occur frequently in applications. (This is a report of joint work with N.S. Stylianopoulos.)

MatLab Workshop: Parallel and Distributed Computing

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MATLAB is a high level structured language and an interactive development environment for technical computing and algorithm development. It has enabled scientists and engineers to efficiently process and analyze data, develop and deploy algorithms and applications. Furthermore, Parallel and Distributed Computing capabilities available recently in MATLAB, allow users to solve computationally and data intensive problems by taking advantage of the latest multiprocessing systems: multicore desktops, computer clusters, grid and cloud computing services. It is now possible to interactively prototype and develop distributed and parallel applications, briefly touch upon the parallel data structures, such as distributed arrays, and programming constructs such as parallel for loops, parallel numeric algorithms and message passing functions. Using typical numerical computing problems as examples, this workshop describes how to use MATLAB parallel tools to take full advantage of the performance enhancements offered by multicore / multiprocessor computing environments. Presenter will demonstrate hands - on examples in multithreading computation of basic linear algebra functions and element wise operations on matrices, optimization of an expensive objective and constrain function, Monte Carlo simulation of a stochastic differential equation and FFT computation on distributed arrays.

Phase-field method for computationally efficient modeling of the solidification of binary alloy with magnetic field effect

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Key words: Numerical procedure and applications, phase-field model, magnetic field, binary alloy, solidification, dendrites

We present a new 2D phase-field model with anisotropy, applied to the dynamics and structure of free dendrite growth during solidification process of binary alloys under the action of magnetic field. The physics of solidification problem of Ni-Cu alloy such as conditions for crystal growth rate are discussed and show good qualitative agreement with numerical simulations.

In order to improve the quality and properties of mixtures, the major industrial challenges lie in the possibility to control the metal structure and defects, that occur during the solidification process. It has been observed experimentally that hydrodynamic motions in liquid phase have a considerable influence on structure and dynamic behavior of developing dendrites. Moreover, it has been shown that the velocity of the melt and direction of flow can be controlled by applying magnetic field and electric current. To study the effect of magnetic field on the evolution of microstructure of dendrites, we have constructed a phase field model to simulate directional solidification and dendritic crystal growth under the action of magnetic field. The mathematical formulation for the model is composed of magnetohydrodynamic, concentration and phase-field systems which are time-dependent, non-linear and coupled systems.

The modeling, the numerical procedure and details of assigning the numerical parameters are provided. The nature of the problem constrains us to use very fine meshes in some physical regions. The results demonstrate that the physics of solidification process can be simulated and captured by using our approach.

Extended procedures for convergence acceleration

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Key words: Extrapolation, Convergence acceleration, Sequence transformation, Annihilation operator.

Let (S_n) be a sequence of real or complex numbers converging to a limit S_∞. If the convergence is slow, it will be transformed into a new sequence (T_n) converging to the same limit by a *sequence transformation*. The idea behind a sequence transformation is *extrapolation to the limit*. Well–known examples of this idea are Richardson's extrapolation and Aitken's Δ^2 processes. It is important to study many different sequence transformations since it was proved that a transformation able to accelerate the convergence of all sequences cannot exist.

In this talk, new procedures for the extrapolation to the limit of slowly convergent sequences and functions are proposed. They are based on the notions of error estimates and annihilation operators. We obtain generalizations of the discrete and confluent E-transformation, which are the most general sequence and function transformations known so far. Many transformations yet studied are included into the new formalism.

Particular cases, such as Drummond's transform and extensions are given. A new expression for the E–transformation, using generalized divided differences, is also obtained, and generalized.

These transformations are related to Padé and Padé-type approximants.

This is a joint work with C. Brezinski (Laboratoire Paul Painlevé, Université des Sciences et Technologies de Lille, France).

NA*lab*: A Matlab graphical environment for studying the behavior of numerical methods in undergraduate courses

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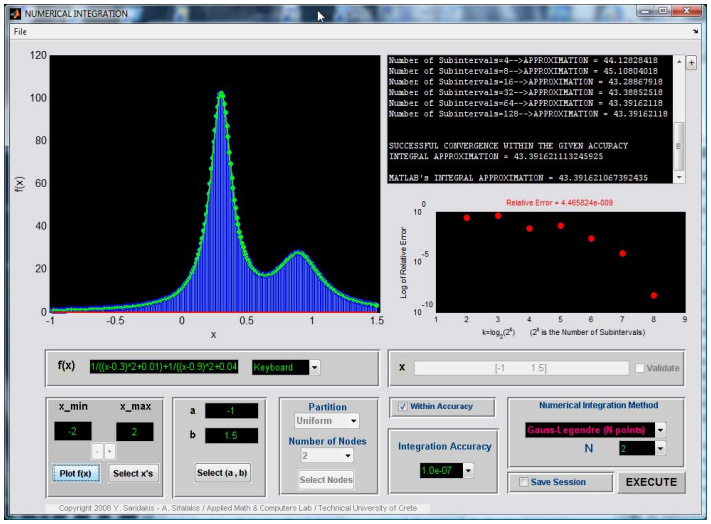
Key words: Matlab, Education, Numerical Analysis, Software.

Traditionally, the study of numerical methods belongs to the core educational courses in science and engineering curricula. Understanding their underlying mechanisms, their behavior and performance were always central educational issues. Working towards this direction we developed NA*lab*, a graphical Matlab environment, to accompany the lectures of a traditional numerical analysis introductory course as the main laboratory tool. At this stage of development, NA*lab* consists of three modules pertaining to the areas of: (a) Root Finding (Bisection, Regula-Falsi, Hybrid methods, Newton-Raphson, Secant, Steffensen, Muller), (b) Interpolation - Function Approximation (Lagrange, Hermite, Linear/Hermite/Natural Splines), and (c) Numerical Integration (Riemman, Trapezoidal, Simpson, Romberg, Gauss-Legendre). The graphical user interfaces (GUI) used in NA*lab* are designed to include both input and output data at all times, while results are presented using both geometrical and numerical approaches. The successful deployment of NA*lab* in the lab sections of the Numerical Analysis courses in all engineering departments of Technical University of Crete encourages its future development.



A parallel algorithm specifying determinants of ± 1 matrices

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Key words: ± 1 matrices, Determinants, Parallel algorithm.

An interesting problem appearing in several applications is the specification of all possible values of determinants for matrices with elements ± 1. Let B be an $n \times n$ matrix with elements ± 1. It holds that (i) $det\ B$ is an integer and 2^{n-1} divides $det\ B$;

(ii) when $n \leq 6$, the only possible values for $det\ B$ are the following, and they do all occur:

n	1	2	3	4	5	6
det B	1	0,2	0,4	0,8,16	0,16,32,48	0,32,64,96,128,160

Table 1. Possible determinant values for $n \times n$ ± 1 matrices.

In this work we study the extention of the above results for matrices of higher order. For this purpose, we developed a parallel algorithm specifying first the determinants of a 7×7 matrix with elements ± 1. The basic steps of this algorithm are:

STEP1: Create all possible $128 = 2^7$ vectors with elements {-1,1}
Distribute in the available multiple processors the following tasks:
STEP2: Create all 7×7 matrices corresponding to the 7^{128} possible combinations of vectors.
STEP3: Evaluate the determinant for each matrix by applying Gaussian elimination with complete pivoting.

By executing this algorithm, we specified that the possible values for the determinant of a 7×7 matrix with elements ± 1 are

$$0,\ 64,\ 128,\ 192,\ 256,\ 320,\ 384,\ 448,\ 512,\ 576$$

and they do all occur.
The time required for the calculation of these determinants (to find each one of them at least once) was 30 minutes.
The extention of this algorithm for the computation of all possible values of the determinants of ± 1 matrices of dimension 8 that can occur, which is an open problem, is under construction.

Numerical and Algorithmic Aspects of Orthogonal Sequences in Combinatorial Design Theory

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Key words: Orthogonal designs, sequences, algorithm, complexity analysis, software.

Combinatorial Design Theory studies questions about arrangements of elements of a finite set into subsets so that certain properties are satisfied. Combinatorial Design Theory has applications in cryptography, coding theory, numerical analysis, telecommunications and other areas.

Orthogonal designs constitute a special class of combinatorial designs that preserves orthogonality in the sense of mutual Euclidean product, and problems related to their existence and construction are directly amenable to algebraic formulations that enable the application of powerful combinatorial tools and computational methods. Orthogonal designs boil down to their numerical counterparts, Hadamard and weighing matrices, upon suitable substitution of their variables with integer values or integer matrices. Prolific methods for constructing the later designs often involve the use of orthogonal sequences in suitable arrays.

For a sequence $A = [a_1, a_2, \ldots, a_n]$ of length n the periodic autocorrelation function, PAF, $P_A(s)$ and the non-periodic autocorrelation function, NPAF, $N_A(s)$ are defined as

$$P_A(s) = \sum_{i=1}^{n} a_i a_{i+s} \ , s = 0, 1, \ldots, n-1 \quad N_A(s) = \sum_{i=1}^{n-s} a_i a_{i+s} \ , s = 0, 1, \ldots, n-1.$$

where in PAF we consider (i+s) modulo n. Sequences of previous kind are referred to as orthogonal, in the sense that the sum of their autocorrelations is zero. Periodic and non-periodic (sometimes are also called aperiodic) ternary complementary pairs are used to construct sequences with desirable properties for radar applications and cryptographic systems. Moreover, these sequences intervene in coded aperture imaging and higher-dimensional signal processing applications. The structure and the number of steps encountered for an interpretation of these methods in terms of a computer implementation, has shown in the past that it is an ideal case for meta-meta programming.

Recently, we established new formalisms on PAF and NPAF of orthogonal sequences suitable for efficient computation of their autocorrelation, by using signed difference sets. A complexity analysis of the proposed combinatorial algorithms for the check of the autocorrelation has revealed that for sequences of small weight our formalism is optimal, and we cannot expect asymptotically better algorithms. These formalisms, allows further consideration of meta-programming techniques and the development of numerical software aided by high-performance computing, for the deployment of several combinatorial design databases.

Iterative Refinement Techniques for Solving Block Linear Systems of Equations

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Key words: Iterative refinement, k-fold iterative refinement, linear systems, least squares problem, block matrices, condition number, numerical stability, symmetric matrices.

In many practical applications we need to solve a linear system of equations $Ax = b$, where $A \in \mathbf{R}^{N,N}$ is nonsingular and has special block structure. We assume that the matrix A is partitioned into $s \times s$ blocks, i.e. $A = (A_{ij})$, where $A_{i,j} \in \mathbf{R}^{n_i,n_j}$ is refereed to as the (i, j) block of A, $\{n_1, \ldots, n_s\}$ is a given set of positive integers, $n_1 + \ldots + n_s = N$.

Very often, the block matrices A_{ij} are sparse and many of them are zero. Numerical algorithms should exploit the structure of the matrix A. We would like to use algorithms that produce solutions y accurate to full machine precision. If $A + E$ has the same block structure as A: $A_{ij} = 0$ implies that $E_{ij} = 0$. If $A = (A_{ij})$ is symmetric then it is reasonable to have a numerical solution y being a solution of slightly perturbed symmetric system $(A + F)y = b$. We partly resolve this problem using blockwise approach. We prove that if $A = (A_{ij}) \in \mathbf{R}^{N,N}$ is a block symmetric matrix and y is a solution of a nearby linear system $(A + E)y = b$, then there exists $F = F^T$ such that y solves a nearby symmetric system $(A + F)y = b$, if A is symmetric positive definite or the matrix $\mu(A) = (\|A_{ij}\|_2)$ is diagonally dominant. Our blockwise analysis extend existing normwise and componentwise results on preserving symmetric perturbations.

We consider some ways in which iterative refinement may be used to improve the computed results. We present various kinds of iterative refinement techniques, eg. k-fold iterative refinement, for the solution of a nonsingular system $Ax = b$ with A partitioned into blocks using only single precision arithmetic. Fixed precision iterative refinement may give solutions to full single precision even when the initial solution have no correct significant figures. Very often, one or two steps are sufficient to terminate successfully the process. Extensive numerical testing was done in MATLAB to compare the performance of some direct methods for solving linear system of equations of special block matrices.

Some applications of the results for the least squares problem (LS) will be also considered.

High dimensional Interpolating Cubature rules on transformed Lattice grid

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Key words: Cubature rules, Chebyshev polynomials, Transformed Lattice grid

In this talk we present a new way to construct s-dimensional interpolatory cubature rules of given algebraic polynomial degree, d, By design the new rules have the desired polynomial degree. Our focus is therefore to construct rules with positive weights and low Legesgue number. We will provide some numerical evidence of the quality of the new rules.

The idea is to apply a cosine transform to an integration lattice and assign the appropriate weights to make the cubature rule having the desired degree. This is similar to constructing the 1d Clenshaw-Curtis rules by a cosine transform of the trapezoidal rule.

Integration lattices form the abscissa set for Lattice rules [1] , which are, like the trapezoidal rule, known to be of high trigonometric degree and thus excellent for periodic function. While Clenshaw-Curtis rules, although of polynomial degree only N, has recently been shown to as good as the celebrated Gauss-Legendre rules with equal number of abscissas [2].

References

[1] Sloan, I.H., Joe, S.: Lattice methods for multiple integration. Oxford University Press (1994)

[2] Trefethen, L. Nick.: Is Gauss quadrature better than Clenshaw-Curtis? Siam Review **50(1)**, 67–87 (2008)

Global and linear rate of convergence of higher order methods on Powell's Singular Function

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Key words: System of nonlinear equations, Halley's method.

To remove singularities at the root of a nonlinear equation $f(x) = 0$ Schröder in 1870 suggested to consider the nonlinear equation

$$g(x) \equiv f(x)/f'(x) = 0$$

provided that $f'(x) \neq 0$ in a neighborhood of the solution x^* except at x^*. We can extend this to a system of nonlinear equations $F(x) = 0$ where $F : \mathbb{R}^n \to \mathbb{R}^n$ is at least two times continuously differentiable. We now follow Schröder and apply Newton's method on $G(x) = 0$ where

$$G(x) \equiv F'(x)^{-1}F(x) = 0$$

provided the Jacobian matrix $F'(x)$ is nonsingular in a neighborhood of the solution x^* except possibly at x^*. The method will have second order rate of convergence under suitable assumptions. We show that Schröders method is closely related to the super-Halley method on $F(x) = 0$. Super Halley is a member in the Halley Class of methods. All methods in the Halley Class have third order rate of convergence under suitable assumptions. Other well known methods in the Halley class are the Chebyshev method and the (original) Halley method. We will explore relationship between these method and the underlying quadratic Taylor model these methods rely on. It will be shown that the methods inherit the rate of convergence from the approximation they generate of the quadratic model.

We will illustrate the methods using classical problems where the Hessian/Jacobian is singular at the solution and thus violates the assumption needed for higher rate of convergence. In particular we will consider the function introduced by M.J.D. Powell in 1962. The Powell singular function is an unconstrained optimization problem. However, the function is also used as nonlinear least squares problem and system of nonlinear equations. The function is a classic test function included in collections like MINPACK, Hoch and Schittkowski and CUTE as well as an example problem in text books. The function is convex and the Hessian or Jacobian matrix is singular at the solution. The function is stated as a difficult test case. In addition to the above methods we consider Newton's method and show that the methods have global convergence. However, they all have a linear rate of convergence. We will illustrate these properties with numerical experiments.

NUMERICAL SOLUTION OF NONLINEAR FREDHOLM INTEGRO-DIFFERENTIAL EQUATIONS BY CHEBYSHEV WAVELETS

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Key words: Chebyshev wavelets, Integro-differential equation, Galerkin method.

In this paper, the continues Chebyshev wavelets constructed on the interval [0, 1] are used to solve the high-order nonlinear Fredholm integro-differential equation. The nonlinear part of the integral equation is approximated by Chebyshev wavelets, and the nonlinear integral equation is reduced to a system of nonlinear equations. Numerical examples illustrates the pertinent features of the method.

A Local Discontinuous Galerkin Scheme for the Nonlinear Parabolic -p-Laplace Type Equation

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Key words: parabolic p-Laplacian, Local discontinuous Galerkin, stability analysis,

In this work a local discontinuous Galerkin (LDG) scheme is presented for the approximation of the solution u of the following p-Laplacian problem:
let Ω be a bounded domain in $\mathbb{R}^d,\ d = 1, 2, 3$ and let $(0, T]$ be the time interval, find u such that

$$u_t - \nabla \cdot (|\nabla u|^{p-2}\nabla u) = f \ in\ \Omega \times (0, T] \quad (1)$$

$$u_0(x) = u(x, 0), \quad (2)$$

$$(|\nabla u|^{p-2}\nabla u) \cdot \mathbf{n} = u_N \ on\ \Gamma_N \times (0, T] \quad (3)$$

$$u = u_D \ on\ \Gamma_D \times (0, T], \quad (4)$$

where $|.| : \mathbb{R}^d \to \mathbb{R}$ is the Euclidean norm, $\partial\Omega = \Gamma_N + \Gamma_D$, $\mathbf{n}$ is the outward normal vector to $\partial\Omega$, $p \geq 2$ and the functions $f : \Omega \times (0, T] \to \mathbb{R}$, $u_0 : \Omega \to \mathbb{R}$, $u_N : \Gamma_N \times (0, T] \to \mathbb{R}$, $u_D : \Gamma_D \times (0, T] \to \mathbb{R}$ are given.

Classical finite element methods for the problem (1) have been proposed by many authors, see e.g. [1]. The last decade many DG methods have extensively presented for the numerical solution of hyperbolic type problems, but effective DG methods for the numerical simulation of general (more realistic) problems as (1) have not presented. The purpose of this work is in this direction. LDG methods was introduced by Cockburn and Shu [2]. The basic idea of LDG method is to rewrite the parabolic equation as a first order system of equations and to solve for u and $\nabla u = \mathbf{q}$ as independent unknowns. A particular feature of LDG methods is that u and $\mathbf{q}$ are approximated in the same degree polynomial space. For the semi-discrete approximate solution we are going to present a-priori bounds (stability bounds) in case of general boundary conditions as well as numerical solutions for classical benchmark problems.

References

[1] Barrett W. J. and Liu W. B. Finite element approximation of the parabolic p-laplacian. *SIAM J. Numer. Anal*, 31(2):413–428, 1994.

[2] Cockburn B. and Shu C.W. The local discontinuous Galerkin method for time dependent convectiondiffusion systems,. *SIAM J. Numer. Anal*, 6(35):24402463, 1998.

Spectral Equivalence between Toeplitz and Trigonometric Matrix Algebras Matrices.

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Key words: Spectral equivalence, trigonometric matrix algebras, Toeplitz matrices, preconditioning, multigrid method.

Spectrally equivalence between two sequences of matrices is a property that plays an important role in the numerical solution of linear systems since it can be used to construct efficient preconditioners for the preconditioned conjugate gradient method, and to form optimal multigrid schemes.

In this work, we prove the existence of matrices, $\tau_n(f)$, belonging to τ algebra that are spectrally equivalent with ill conditioned Toeplitz matrices $T_n(f)$. For that, we assume that the generating function f is real valued, nonnegative, continuous, with isolated roots of maximum order $\alpha \in \mathbb{R}^+$. Specifically, we prove that for $0 \leq \alpha \leq 2$ there exist a proper clustering of the eigenvalues of $\tau_n(f)^{-1}T_n(f)$ around unity. For $2 < \alpha < 4$, a weak clustering for the spectrum of the aforemention matrix is achieved, where the minimum eigenvalue is bounded from bellow, while a constant number, independent of n, of eigenvalues tend to infinity. The results are generalized to cover the more interesting, from theoretical and practical point of view, case of Block Toeplitz with Toeplitz Blocks (BTTB), matrices. Based on these theoretical statements we propose τ preconditioners that lead to superlinear convergence both in $1D$ and $2D$ case when the condition number of the Toeplitz matrix is $o(n^4)$. Finally, we show that the spectrally equivalence also holds between circulant matrices and ill-conditioned Toeplitz matrices. The main difference is that the continuous symbol which generates the Toeplitz matrix should have discrete roots of order less than 2. We perform many numerical experiments, whose results confirm the validity of theoretical analysis.

Discernibility-based Algorithms for Classification

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Key words: Classification, pattern recognition, discernibility, ensemble, feature resampling, k-nearest neighbor, distance metrics

There has been a great deal of research on classification systems, aiming at the development of general methods and specialised techniques to tackle particular classification problems. These techniques often employ the statistical properties of the data involved, or adaptive mechanisms to exploit every little piece of information that may reveal a useful property of the data, leading to a reliable classification. Yet, datasets not always follow the assumed statistical distribution and many classifiers tend to become "confused" when dealing with large datasets, as the excessive information that is there often compromises the classifiers' performance, sometimes due to the problem of overfitting. This can be attributed to the fact that they often consider all patterns being equally important, instead of taking into account their underlying structure which may yield more useful information for the classification process.

In this paper we propose an approach to enhance the pattern classification process by taking into account the geometry of class structure in datasets of interest. This is based on the recently proposed Discernibility concept, through one of its indexes, namely the Spherical Index of Discernibility. We demonstrate how this index can be applied to enhance distance-based classifiers, such as the k-nearest neighbor, as well as information fusion in diverse classifier ensembles. The ensemble used in our work comprised of a number of different classifiers in order to ensure a high level of diversity in the errors of the classification. A number of experiments, using multiple rounds of 10-fold cross validation, are conducted on a variety of datasets to empirically evaluate the proposed approach. The results appear to be quite promising improving the performance on the classification process.

NUMERICAL MODELLING OF INTERACTION BETWEEN CAROTID ARTERY WALLS AND BLOOD

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Key words:Carotid artery, Blood flow, Solid-fluid interaction, Stress-stretch relation

INTRODUCTION. We first present an experimental determination of carotid artery properties by using strips of human carotid artery. The strips were taken in the longitudinal and in the circumferential directions assuming that the carotid artery wall has the orthotropic characteristics. The material was subjected to uniaxial tension and the stress-stretch curves were obtained for various rates of deformation. It was found that the rates do not have significant effects on the passive response of the material. Next, we employ the measured non-linear stress-stretch dependence to determine the coefficients in the analytical form of this dependence by a standard fitting procedure. We give description of the numerical procedure, considering the carotid artery as a thin-walled shell structure subjected to blood pressure. We calculated behaviour complete human carotid artery by solving coupled problem interaction between artery walls and blood pressure on its. METHODS. A total number of 30 segments of carotid artery were used. Different initial strip lengths were taken in the longitudinal and in the circumferential directions and strained continuously using various strain rates. The developed force was measured by an isotonic transducer (Elunit, Yugoslavia) and recorded using PIC digital recording system (ECM, Yugoslavia). As the initial length we considered the measured strip length just before visible change in tension was recorded on PIC digital recording system. Pulsatile flow waveform in the carotid artery during systole and diastole phases is taken from literature (Perktold and etc., 1991; 1994) RESULTS. We employ the measured nonlinear stress-stretch curves in our material model within finite elements for geometrically and materially nonlinear analysis. We give description of the numerical procedure, considering carotid artery as a shell structure subjected to pressure loading. We calculated behavior of complete human carotid artery observing unsteady blood flow through artery, namely it was performed dynamic analysis interaction between artery walls solid and blood fluid. It was performed comparing obtained numerical results velocity fields in XY symmetry plane, von Mises stress distribution, wall shear stresses, etc. with results received for case when walls are considered as elastic and with results in literature. DISCUSSION. We have presented a new methodology which employ experimentally determined

real characteristics of carotid artery walls, represented through constitutive stress-stretch relation. Non-linear stress-stretch characteristics are employed as the basis for non-linear orthotropic material models in the finite element method. Large displacements and large strains are considered during interaction between artery walls and blood. The numerical simulations demonstrate the possibilities of modelling the complex mechanical behaviour of carotid artery, treated as a thin-walled structure. The proposed methodology provides a solid basis for deeper understanding of the carotid artery response during interaction between walls and blood.

Adaptive Monte Carlo Methods for SDEs

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Key words: Itô stochastic differential equations, weak approximation, Drift Implicit Euler method, adaptive method, Monte Carlo method.

We propose a general framework to construct adaptive methods for the weak approximation problem of Itô stochastic differential equations, which we apply on variances of the Drift Implicit Euler method.

Joint work with Ernesto Mordecki (Universidad de la República, Montevideo, Uruguay), Anders Szepessy (KTH, Stockholm, Sweden), Raul Tempone (KAUST, Thuwal, Saudi Arabia).