The workshop on Numerical Methods for Evolutionary Problems is jointly organized by the *Dipartimento di Energetica, Dipartimento di Matematica - Università di Firenze*, and the *Dipartimento Interuniversitario di Matematica - Università di Bari*. The members of the organizing committe are

- Donato Trigiante (Firenze)
- Luigi Brugnano (Firenze)
- Francesca Mazzia (Bari)
- Felice Iavernaro (Bari)

The organizing committe would like to thank

- Lidia Aceto
- Pierluigi Amodio
- Ivonne Sgura

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- Regione Puglia

Contents

1 Introduction

The main purpose of this workshop is to focus the state of art of the numerical methods for evolutionary problems. This is a wide and active field of research and therefore it is related to many other activities in numerical analysis.
In 1999 we have obtained a support from italian M.U.R.S.T. and, for related projects, in the last five years we have also got supports from GNIM (now G.N.C.S.).
In presenting the results of our activity, we have invited a few national and international leading experts in order to set such results in the mainstream of the international activities in the same fields.
Several innovative results have been obtained in the following areas:

- Numerical methods for ODEs (both IVPs and BVPs);
- Numerical methods for Delay ODEs;
- Preconditioning of matrices;
- Numerical methods for Volterra equations;
- Numerical codes;
- Numerical methods for Stocastic Volterra integral equations and ODEs;
- Numerical Linear Algebra;
- ABS and Quasi-Newton methods;
- Numerical methods for nonlinear programming.

We are glad to thank all the collaborators who have contributed to this project and, particularly, the experts B. Aulbach, A. Bellen, J. Cash, F. Chatelin, R. Chan, J. Gondzio, D. Marini, G. Mastroianni, E. Spedicato, P. van der Houwen, S. Vandewalle who, we are sure, will make successful this meeting.

2 Scientific Program

Monday, 17 September

9.15	–	9.50	**Opening Address by Donato Trigiante**

Plenary Lectures

9.50	–	10.40	**Peter Van der Houwen** Parallel aspects in RK and EBDF methods
10.40	–	11.00	– **Break** –
11.00	–	11.50	**Donatella Marini** A unified analysis of DG methods for elliptic problems

Contributed Talks

11.50	–	12.15	**Felice Iavernaro** On the solutions of symmetric BVMs for linear Hamiltonian Boundary Value Problems
12.15	–	12.40	**Nicoletta Del Buono** Numerical methods for isodynamical matrix flows with application to balanced realization in control theory
12.40	–	13.05	**Giovanni Gheri** On some numerical methods for spectral computations in regular and non regular Sturm-Liouville problems
13.05	–	15.00	– **Lunch** –

Contributed Talks

15.00	–	15.25	**Tiziano Politi** An Algorithm for the Computation of the G-Singular Values of a Real Matrix
15.25	–	15.50	**Lidia Aceto** On the properties of matrices defining BVMs
15.50	–	16.15	**Raffaella Pavani** Numerical treatment of second order neutral delay differential equations using deficient spline functions
16.15	–	16.40	– **Break** –
16.40	–	17.05	**Giulia Spaletta** Rounding error reduction in extrapolation methods
17.05	–	17.30	**Anna Napoli** Galerkin-type methods with Chebyshev nodes for initial value problems
17.30	–	18.30	**Special Lecture**

Tuesday, 18 September

Plenary Lectures

9.00 – 9.50 **Bernd Aulbach**
Discretization of invariant manifolds
a new approach using measure chains

9.50 – 10.40 **Alfredo Bellen**
Old and new aspects of the numerical integration of
Delay Differential Equations

10.40 – 11.00 – **Break** –

Contributed Talks

11.00 – 11.25 **Nicola Guglielmi**
Radau IIA methods for the numerical integration of
stiff delay differential equations

11.25 – 11.50 **Stefano Maset**
An asymptotically stable approach in the numerical solution
of Delay Differential Equations

11.50 – 12.15 **Lucio Torelli**
RK methods for Functional Differential Equations

12.15 – 12.40 **Margherita Carletti**
Instability regions in delay models with delay dependent parameters:
an application in the biosciences

12.40 – 13.05 **Beatrice Paternoster**
Adapting the parameters of the numerical method
to an oscillatory behaviour

13.05 – 15.00 – **Lunch** –

Plenary Lectures

15.00 – 15.50 **Raymond Chan**
A Preconditoner for Waveform Relaxation Iterations
of LMF-Based ODE Codes

Contributed Talks

15.50 – 16.15 **Pierluigi Amodio**
Parallel preconditioning techniques for the solution
of linear systems arising from fluid dynamics problems

16.15 – 16.40 – **Break** –

16.40 – 17.05 **Luca Bergamaschi**
Preconditioning of iterative eigensolvers

17.05 – 17.30 **Maria Teresa Vespucci**
On the Convergence of Krylov Linear Equation Solvers

17.30 – 18.30 **Special Lecture**

Wednesday, 19 September

Plenary Lectures

9.00	–	9.50	**Francoise Chaitin-Chatelin** Computing Thoughts
9.50	–	10.40	**Stefan Vanderwalle** Multi-level iterative methods for time-dependent partial differential equations
10.40	–	11.00	– **Break** –
11.00	–	11.50	**Jaff Cash** Continuation Methods for solving difficult two point BVPs.

Contributed Talks

11.50	–	12.15	**Francesca Mazzia** TOM: A Code for Boundary Value Problems
12.15	–	12.40	**Ivonne Sgura** BVMs for the numerical approximation of BVPs arising in modeling of Nonlinearly Elastic Materials
12.40	–	13.05	**Luigi Brugnano** Blended block implicit methods for the numerical integration of ODEs
13.05	–	13.30	**Cecilia Magherini** The BiM code for the numerical integration of ODEs
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20.30	–		– **Conference Dinner** –

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Numerical Techniques in Interior Point Methods for Optimization

9.50 – 10.40 **Emilio Spedicato**
ABS algorithms and ABSPACK

10.40 – 11.00 – **Break** –

Contributed Talks

11.00 – 11.25 **Ladislav Luksan**
A class of globally convergent ABS algorithms for nonlinear systems

11.25 – 11.50 **Zunquan Xia**
On the nonlinear ABS algorithm for problems
with singular Jacobian at solution

11.50 – 12.15 **Emanuele Galligani**
The Newton–Arithmetic Mean Method for
the Solution of Nonlinear Systems

12.15 – 12.40 **Luca Zanni**
Large Quadratic Programs in Training Support Vector Machines

12.40 – 13.05 **Carla Durazzi**
On a Parallel Interior–Point Method for
Quadratic Programs with Special Structure

13.05 – 15.00 – **Lunch** –

Plenary Lectures

15.00 – 15.50 **Giuseppe Mastroianni**
Polynomial Approximation and some Applications
to Integral Equations

Contributed Talks

15.50 – 16.15 **Elvira Russo**
High Performance Methods for Volterra Equations
with Weakly Singular Kernels

16.15 – 16.40 – **Break** –

16.40 – 17.05 **Giuliana Criscuolo**
Numerical approximation of some BEM singular integrals

17.05 – 17.30 **Maria Rosaria Capobianco**
Uniform and pointwise numerical approximation of the
weighted Hilbert transform on the real line

17.30 – 17.55 **Bruno Carpentieri**
Iterative solution and preconditioning of boundary integral
equations in electromagnetism

17.55 – 18.30 **Special Lecture**

Friday, 21 September

9.00	–	11.00	**Panel discussion**
11.00	–	11.20	**Concluding Address**

3 Abstract of Plenary Lectures

Discretization of invariant manifolds a new approach using measure chains
Bernd Aulbach
(Department of Mathematics, University of Augsburg, Germany)

Since invariant manifold theory comes in two versions (with continuous or discrete time) the question arises whether an invariant manifold of a given differential equation can be approximated by an invariant manifold of a corresponding difference equation. It is known that the answer to this question is affirmative for a large class of invariant manifolds (including stable, unstable, center, center-stable and center-unstable manifolds) for autonomous ordinary differential equations if the discretizations have constant step-size.

In this talk we show that those results can be extended to non-autonomous differential equations (in Banach spaces) and numerical schemes with variable step-size. Our approach is based on the so-called "calculus on measure chains", a rapidly growing new theory which allows to treat continuous- and discrete-time equations simulaneously.

Old and new aspects of the numerical integration of Delay Differential Equations
Alfredo Bellen
(Dipartimento di Scienze Matematiche, Università di Trieste, Italy)

In the convergence, stability and asymptotic stability analysis of the numerical solution of the Cauchy problem

$$\begin{cases} y'(t) = f\big(t, y(t), y(t-\tau)\big), & t_0 \le t \le t_f \\ y(t) = \phi(t), & t \le t_0, \end{cases} \tag{1}$$

the theoretical and implementative difficulties essentially depend on the form of the delay function τ which may be constant ($\tau = const$), time-dependent ($\tau = \tau(t)$) or state-dependent ($\tau = \tau(t, y(t))$). The behaviour of τ determines, in particular, the propagation of discontinuities, if any, in the solution of (1) and hence in the attainable accuracy of the approximation. Although for constant delays the problem of accuracy has been deeply investigated and completely solved, much has still to be done for the other cases of time-dependent and state-dependent delay. In particular, for the latter, the discontinuities can not be located "a priori" and a reliable proof on the order of convergence still lacks for methods of order $p > 2$. Numerical experiments support the conjecture that the order of the method is preserved by including the computed discontinuiuties as mesh points. On the other hand, even for constant delays, the stability analysis is still unsatisfactory. In fact, it has been proved that, for linear systems, no Runge-Kutta method exists which preserves the unconditional stability on the

whole class of asymptotically stable equations. A completely different approach, based on the formulation of (1) as an abstract Cauchy problem, provides a numerical approximation that preserves the stability property. In the class of equations with time-dependent delays most depends on the behaviour of the delay. An emblematic example is given by the well-known pantograph equation

$$\begin{cases} y'(t) = ay(t) + by(qt), \quad 0 \le t \le t_f \\ y(0) = y_0, \end{cases} \tag{2}$$

where the deviating argument qt, $0 < q < 1$, leads to the delay function $\tau(t) = (1-q)t$ which is simultaneously vanishing and unbounded in $(0, \infty)$. These peculiarities entail some problems in the implementation of the first step as well as in the storage of the solution in the long run integration. The use of a quasi-geometric mesh allows integrating (2) by a method wich preserves the superconvergence of the method and the stability of the solution as well.

Continuation Methods for solving difficult two point BVPs.
Jeff Cash
(Imperial College, London, U.K.)

A very powerful approach for solving stiff two-point boundary values is to use continuation. This is in theory a rather simple idea but is surprisingly difficult to implement efficiently in paractice. Some of the difficulties associated with the derivation of continuation methods are described and a particular algorithm is developed. Some numerical results show the expected effectiveness of the continuation approach on some highly stiff problems.

A Preconditoner for Waveform Relaxation Iterations of LMF-Based ODE Codes
Raymond Chan & X. Jin & V. Sin & L. Song
(The Chinese University of Hong Kong, Shatin, Hong Kong)

We consider the solution of ordinary differential equations by the waveform relaxation iteration in conjunction with the boundary value methods. The waveform relaxation iteration differs from the classical iterative methods in that it is a continuous-in-time analogue of the stationary methods and it iterates with functions. In this talk, we will discuss the use of block-circulant-circulant-block preconditioners for solving the linear systems arising from the application of boundary value methods in each iteration of the waveform relaxation method. These techniques are very effective in speeding up the convergence rate of the resulting iterative process. Numerical experiments are presented to illustrate the effectiveness of our methods.

Computing Thoughts
Francoise Chaitin-Chatelin
(University of Toulouse I and CERFACS, Toulouse, France)

We present a mathematical reflexion about the act of computing. We revisit the notion of numbers which are the building blocks of computation. We contrast exact computation (used in Pure Mathematics) with inexact computation (used in Applied Mathematics). Special attention is given to finite precision computation.

Numerical Techniques in Interior Point Methods for Optimization
Jacek Gondzio
(Department of Mathematics & Statistics, Edinburgh, U.K.)

In the first part of the talk, we shall introduce the interior point methods (IPMs) for linear, quadratic and nonlinear optimization. IPMs form a major feature of the optimization landscape for 16 years. Their theory [5] and implementation [1] are very well understood. Following [4], to derive the primal-dual interior point algorithm one should:

- replace nonnegativity constraints on the variables with logarithmic barrier penalty terms;
- move equality constraints to the objective with the Lagrange transformation to obtain an unconstrained optimization problem and write first order optimality conditions for it; and
- apply Newton's method to solve these first order optimality conditions (i.e. to solve a system of nonlinear equations).

We shall do this exercise.

In the second part of the talk, we shall focus our attention on the numerical methods of linear algebra applied in IPMs. We examine several topics:

- the exploitable special structures of linear systems arising in IPMs for linear, quadratic, and nonlinear programming (we also address the consequences of non-convexity in nonlinear program);
- the use of direct methods for positive definite and indefinite symmetric systems arising in IPMs [1];
- the long perceived and unavoidable (but benign in practice) ill-conditioning of linear systems [2,3];
- the alternative approaches to solving linear algebraic subproblems including iterative methods.

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A unified analysis of DG methods for elliptic problems

Donatella Marini
(Dipartimento di Matematica and I.A.N.–C.N.R., Pavia, Italy)

We provide a framework for the analysis of a large class of discontinuous methods for second-order elliptic problems. It allows for the understanding and comparison of most of the discontinuous Galerkin methods that have been proposed for the numerical treatment of elliptic problems by diverse communities over three decades. We shall show that virtually all the DG methods introduced so far can be rewritten in a suitable variational form that allows to study easily properties such as consistency, stability, and error estimates.

In particular, we shall include the original method by Bassi-Rebay [4], its stabilized version [5], [7], and variants [8]; the LDG method by Cockburn and Shu [9], the interior penalty method by Douglas and Dupont [10], two penalty methods by Babuška-Zlamal [3], and Brezzi et al. [8], respectively, and the method by Baumann and Oden [6], with its stabilized version by Rivière, Wheeler and Girault [11].

For an exhaustive discussion we refer to [1], [2].

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Polynomial Approximation and some Applications to Integral Equations

G. Mastroianni
(Dipartimento di Matematica, Università della Basilicata, Italy)

The polynomial approximation in related functional spaces is an important tool in Numerical Analysis. In this talk I present a short survey on the subject and some applications to the numerical treatment of integral equations.

ABS algorithms and ABSPACK

Emilio Spedicato
(Università di Bergamo, Italy)

We review the main theoretical results on ABS algorithms for linear systems and optimization, including Diophantine equations. We discuss their numerical performance in the framework of the project ABSPACK, with comparison with other well known packages.

Parallel aspects in RK and EBDF methods

Peter van der Houwen & Jason Frank & Jacques de Swart
(CWI, Amsterdam, The Netherlands)

If the nonlinear systems arising in s-stage RK methods are solved by Newton iteration, then we are faced with linear systems of dimension sd, d denoting the IVP dimension. For large d the direct solution of these linear systems is costly. On parallel computers, these costs can be reduced by using a parallel inner iteration process. This technique is quite flexible and can be extended to the whole class of implcit General Linear Methods. The first part of the talk describes this parallel, iterative linear solver. Performance results can be found in the Bari Test Set for IVP solvers which has already or will soon be released. The second part of the talk is concerned with parallel aspects of extended backward differentiation formulas (EBDFs) and their modified forms (MEBDFs). These methods were proposed by Cash in the 1980s for solving IVPs for stiff ODE systems. In a recent performance evaluation of various IVP codes, it turned out that the variable-step-variable-order MEBDF code often performs more efficiently than codes like RADAU5, DASSL and VODE. This motivated us to look at possible parallel implementations of EBDF-type methods. In particular, we considered the original 3-stage EBDF method and the higher stage versions introduced by Cash and Psihoyios in 1998. These methods can be generalized such that the system matrix in the modified Newton method, used for solving the nonlinear relations, can be block-diagonalized. This enables an efficient parallel implementation. L-stable methods up to order 6 with the same computational complexity per processor as the conventional BDF methods can be constructed. Numerical experiments with the order 6 method show that on four processors a speedup factor in the range [2, 4] can be expected.

Multi-level iterative methods for time-dependent partial differential equations

Stefan Vandewalle
(Katholieke Universiteit Leuven, Belgium)

The spatial discretisation of time-dependent partial differential equations by means of finite differences, finite elements or finite volumes leads to systems of ordinary differential equations of very large dimension. Such ODE-systems can no longer be solved efficiently by classical ODE-software. Their solution requires specialised solvers that take the structure of the semi-discrete PDE-problems into account.

We will first consider linear multistep and implicit Runge-Kutta time-stepping schemes. Their implementation necessitates the solution of linear or nonlinear algebraic systems with a size that is a constant multiple of the number of ODEs (or spatial discretisation points). It will be shown that these systems can be solved very efficiently, i.e., with a complexity that is linear in the number of unknowns, when multilevel PDE-algorithms are used.

Next we consider time-stepping schemes where the solution is advanced time-window by time-window. The discrete solution is then computed block-wise, i.e., on several time-levels simultaneously. Such methods have been studied in the boundary-value-method and waveform relaxation literature. The size of the linear algebra problems to be solved is equal to those arising in standard time-stepping schemes multiplied by the number of time-levels in the time-window. It will be shown that a suitable modification of the multi-level method can tackle these problems very efficiently. The limiting case of infinite length time-windows leads to an algorithm which can be easily analysed theoretically by means of a Fourier-Laplace analysis. The analysis leads to sharp convergence rate estimates, which will be verified by numerical experiments.

Finally, we will deal with a number of special cases such as time-periodic problems, strongly anisotropic problems and delay partial differential equations.

4 Abstract of Contributed Talks

4.1 Numerical Methods for ODEs

On the properties of matrices defining BVMs
Lidia Aceto & Donato Trigiante
(Dipartimento di Energetica, Università di Firenze,Italy)

When we approximate the solution of the initial value problem

$$\begin{cases} y'(t) = f(t, y(t)), & t \in [t_0, T] \\ y(t_0) = y_0 \end{cases}$$

by using at consecutive grid points of a uniform mesh with stepsize h the same Boundary Value Method (BVM) [1], with $(\nu, k-\nu)$-boundary conditions, we obtain the discrete problem which may be written in matrix form as follows:

$$A\,\mathbf{y} - hB\,\mathbf{f} = \mathbf{v},$$

where the vectors $\mathbf{y}$ and $\mathbf{f}$ contain the unknowns, $\mathbf{v}$ is the known vector and the coefficient matrices A and B are Toeplitz band matrices.
In this talk we shall present the conditions needed for a Toeplitz band matrix to be positive definite. Such result will provide a useful tool to study the stability problem for BVMs in an alternative way. Classically such problem has been carried out by using the theory of difference equations. Here we shall prove that the necessary condition to obtain in each class of BVMs an $A_{\nu,k-\nu}$-stable method is that the matrices A and B arising from its application are positive definite. In particular, our attention will be focused on the following class of methods: Generalized BDF (GBDF) and Top Order Methods (TOMs).

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Numerical methods for isodynamical matrix flows with application to balanced realization in control theory
Nicoletta Del Buono & Luciano Lopez & Carmen Mastroserio
(Dipartimento Interuniversitario di Matematica, Università di Bari, Italy)

Recently several numerical methods have been proposed for solving isospectral problems which are matrix differential systems whose solutions preserve the spectrum during the evolution. In this talk we consider matrix differential systems called *isodynamical flows* in which only a component of the matrix solution

preserves the eigenvalues during the evolution and we propose procedures for their numerical solution.

Applications of such numerical procedures may be found in systems theory, in particular in balancing realization problems.

On some numerical methods for spectral computations in regular and non regular Sturm-Liouville problems

G.Gheri & Paolo Ghelardoni & Marco Marletta
(Dipartimento di Matematica Applicata, Università di Pisa, Italy)

In the regular Sturm-Liouville problems (SLPs) the main difficulty in the spectral computations arises from the approximation of the eigenvalues of higher index. Thus some particular procedure right for the purpose to correct the approximations obtained seems to be necessary. In this frame the class of the boundary value methods (BVMs) equipped with symmetric properties represents a mighty tool. Actually the symmetric schemes preserve the analyticity of the computed solutions on some discretization parameter allowing to set up an effective spectral correction procedure.
With regard to non regular SLPs, the presence of internal singularities is responsible of a decay of the accuracy of some classical methods. In particular, in the case of an eigenvalue embedded in the continous spectrum, the Magnus series method and JWKB method exhibit a somewhat poor approximation endowments and the standard BVMs experience a degeneration of their order of convergence. Nevertheless some BVMs employed in a non standard form act as in the regular case. Furthermore the symmetric schemes enable that enhanced estimates may still be obtained despite the fact that the problem is $\lambda-$nonlinear.

On the solutions of symmetric BVMs for linear Hamiltonian Boundary Value Problems

Felice Iavernaro & Pierluigi Amodio & Donato Trigiante
(Dipartimento di Matematica, Università di Bari, Italy)

We consider the application of a symmetric Boundary Value Method to solve the linear Hamiltonian Boundary Value Problem

$$\left\{ \begin{array}{l} \mathbf{y}' = JS\mathbf{y}, \quad t \in [t_0, t_f], \\ B_0\mathbf{y}(t_0) + B_f\mathbf{y}(t_f) = \mathbf{b}, \end{array} \right. \qquad J = \left(\begin{array}{cc} 0 & I \\ -I & 0 \end{array} \right), \tag{3}$$

on a uniform mesh with stepsize h (S is symmetric and positive definite). Denoting by $\mathbf{y}(t_n)$ and $\mathbf{y}_n$ the solutions of (3) and of the BVM respectively, for a p order method it is easy to check that the Hamiltonian function $\sigma = (\mathbf{y}(t_n))^T S\mathbf{y}(t_n)$ and its approximation $\sigma_n = \mathbf{y}_n^T S\mathbf{y}_n$, satisfy the relation $\sigma_n = \sigma + O(h^p)$, that is the convergence properties of the Hamiltonian function evaluated on the numerical solution are the same as those of the underlying method.

We firstly prove that symmetric schemes of even order (ETRs, ETR_2s, TOMs) posses a superconvergence property, namely they produce a solution

satisfying $\sigma_n = \sigma + O(h^{p+2})$. After that, the continuous and the discrete problems are shown to be deeply interconnected each other according to the following symmetric properties:

(i) the solution of (3), projected on the given mesh, may be regarded as a solution generated by a symmetric BVM of even order applied to a Hamiltonian problem obtained perturbing (3) by an Hamiltonian term $O(h^p)$;

(ii) apart the initial and final additional conditions, the solution of a symmetric BVM of even order applied to (3) may be regarded as the projection on the mesh of the solution of a Hamiltonian problem obtained perturbing (3) by an Hamiltonian term $O(h^p)$.

From this correspondence a number of interesting properties satisfied by the true solution may be directly transferred to the numerical one. The additional methods work as a perturbation over this favourable situation, but their effect disappear very quickly as long as we move towards the middle of the time integration interval.

Galerkin-type methods with Chebyshev nodes for initial value problems

A. Napoli & F. Costabile
(Università della Calabria, Italy)

For the numerical solution of systems of nonlinear first-order ordinary differential equations we employ polynomial Galerkin-type method to devise global methods.

The basic idea is to approximate y' by a linear combination y'_n of some system of orthogonal polynomials ϕ_k of degree k and determine the coefficients of y'_n by requiring that it provides Galerkin-type approximation on the hole given interval, using an appropriate discrete inner product.

Some methods which uses Chebyshev polynomials of first and second kind are studied which result to be collocation methods. The stability of the equivalent implicit Runge-Kutta methods is studied by classical proceedings. Extension to the solution of second order differential equations is outlined.

Adapting the parameters of the numerical method to an oscillatory behaviour

Beatrice Paternoster
(Dipartimento di Matematica e Informatica, Università di Salerno, Italy)

We have been considering the possibility of adapting the parameters of a numerical methods for ODEs to the special form of the solution. In particular, in the case of second order ODEs with oscillatory solutions, if the location of the frequencies are known in advance, we can tune the parameters to the frequencies to provide better approximations to the oscillations. We use and compare three

differents approaches, First, assuming that the dominant frequencies ω_j are a priori given, we extend trigonometric and mixed collocation to two step Runge-Kutta methods. Then we derive a phase-fitted Runge-Kutta-Nyström (RKN) method which results exact in phase for linear problems with periodic solutions. Finally, only assuming that the frequencies are located in a given nonnegative small interval $[\omega_1, \omega_2]$, we adapt the parameters of the RKN method through least squares minimization.

Numerical treatment of second order neutral delay differential equations using deficient spline functions

Raffaella Pavani & Franca Calio' & Elena Marchetti
(Politecnico di Milano, Italy)

As well known, it is standard practice first to reduce a $qth-$order ordinary differential equation (ODE) to a first-order system. However, as pointed out in [5] "the only exception is when the equation is second order, for which special numerical methods have been devised". As we showed in two previous papers about second order neutral delay differential equations (NDDE), such a special method can be easily implemented using deficient spline functions. Therefore for NDDE it can be advisable not to resort to reduction, provided that such a reduction can be seriously problematic for some NDDE problems

In particular we considered the following second order NDDE problem:

$$\begin{cases} y''(x) = f(x, y(x), y(g(x)), y'(g(x)), & x \in [a, b] \\ y(x) = \varphi(x), \quad y'(x) = \varphi'(x), \quad x \in [\alpha, a], \alpha \leq a, \alpha = \inf_{x \in [a,b]}(g(x)) \end{cases}$$

As well known, recently a lot of robust efficient delay differential equation solvers were implemented and used as public domain software. However just a small subset of them deals even with neutral cases; anyway reduction is always used. Therefore our aim is to make it as easy as possible to solve effectively the previous NDDE problem, without reduction.

To this end we merge two classical techniques: the approximation of the solution by means of deficient spline functions and the use of a collocation method in order to compute the approximating function.

In [2] we presented the numerical method in details; moreover we extended Theorems assuring convergence and consistency provided in [1] for the first order problem, to the second order problem.

In [3] *we improve the stability result*: whereas for the first order NDDE problem the method is stable only for spline order $m < 4$, for the second order NDDE problem, we prove the stability for spline order $m < 5$.

A major disadvantage of special methods implemented for second order ODE is that the accumulation of rounding errors is very fast and is proportional to $1/h^2$, where h is the used stepsize [4]. However we show that our method for second order NDDE can use variable steps; therefore it converges efficiently even when relatively large values of stepsize are mostly used.

Our algorithm implemented in MATLAB reveals simple and flexible; moreover for problems whose solution exhibits low regularity, it provides an excellent numerical solution and can require less flops than other public domain software

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An Algorithm for the Computation of the G-Singular Values of a Real Matrix

Tiziano Politi & Giovanni Di Lena & Giuseppe Piazza
(Dipartimento Interuniversitario di Matematica, Politecnico di Bari, Italy)

The well-known Singular Values Decomposition (SVD) states that every matrix A can be written in the form

$$A = U\Sigma V,$$

where U and V are orthogonal and Σ is diagonal with nonnegative entries. In this work we consider the problem to compute a special SVD decomposition of the matrix A called $G-SVD$. In this case given a real diagonal matrix G with main elements equal to ± 1, the $G-SVD$ of a matrix is a decomposition of the same kind of the usual SVD but matrices U and V are orthogonal with respect to the metric defined by G and not to the usual Euclidean metric. The elements of matrix Σ are called $G-$singular values.
In this work we study some theoretical aspects about the conditions for the existence of the $G-SVD$ and propose a qd-type algorithm to compute the $G-$singular values.
The first step of the algorithm is the bidiagonalization of the matrix using the $G-$orthogonal matrices called Hyperbolic Houselder Transforms.
The second step is the numerical computation of the $G-$singular values of a bidiagonal matrix. We have considered also a modified algorithm which includes the computation of a shift at each step (as the algorithms for the computation of the singular values). Some numerical tests are given.

Rounding error reduction in extrapolation methods

Giulia Spaletta & Mark Sofroniou
(Dipartimento di Matematica, Università di Bologna, Italy)

Extrapolation methods are very efficient when high accuracy is desired in a numerical solution of an ordinary differential equation.

An example of Hairer is used to demonstrate how high order methods can suffer from cumulative rounding error propagation.

A new formulation for reducing the effect of cumulative rounding errors will be outlined and numerical examples will be given to illustrate the benefits over the standard formalism.

Finally, several features of a developmental implementation of extrapolation methods in Mathematica will be illustrated.

4.2 Delay Differential Equations

Instability regions in delay models with delay dependent parameters: an application in the biosciences
Margherita Carletti
(Istituto di Biomatematica, Università di Urbino,Italy)

In this work we describe a method to determine the instability regions of the positive equilibria in delay models involving delay dependent parameters. The method relies on a geometric stability switch criterion introduced by Beretta and Kuang in [2] and it is here applied to a $2D$ model of phage-bacteria interaction in an open marine environment [1]. As for similar delay models, the numerical experiments show that, as time delay increases, stability changes from stable to unstable to stable, implying that large delays can be stabilizing, thus contradicting the common scenario provided by delay models with delay independent parameters [3].

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Radau IIA methods for the numerical integration of stiff delay differential equations

Nicola Guglielmi
(Università dell'Aquila, Italy)

We consider initial value problems for delay differential equations

$$\begin{aligned} M\,y'(t) &= f\Big(t, y(t), y\big(\alpha_1(t,y(t))\big), \dots, y\big(\alpha_m(t,y(t))\big)\Big), \\ y(t_0) &= y_0, \qquad y(t) = g(t) \quad \text{for} \quad t < t_0, \end{aligned} \tag{1}$$

where M is a constant $d \times d$ matrix and $\alpha_i(t, y(t)) \le t$ for all $t \ge t_0$ and for all i. The value $g(t_0)$ may be different from y_0, allowing for a discontinuity at t_0.

Allowing the matrix M to be singular, the above formulation includes all kinds of differential-algebraic delay equations as well as problems of neutral type.

We discuss how collocation methods based on Radau nodes can be applied to solve problems of type (1). We consider both theoretical properties of such methods and practical implementation aspects [1,2].

In particular we focus attention on the following issues:

(i) choice of the continuous extension;

(ii) stability and accuracy of the numerical process;

(iii) error control and stepsize selection strategies;

(iv) efficient solution of the algebraic equations.

Finally we show the practical behaviour of such methods on real-life examples [3,4].

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An asymptotically stable approach in the numerical solution of Delay Differential Equations

Stefano Maset
(Department of mathematical sciences, University of Trieste, Italy)

It is known (see [1]) that there do not exist Runge-Kutta (RK) methods unconditionally preserving the asymptotic stability when they are applied to linear systems of Delay Differential Equations (DDEs)

$$y'(t) = Ly(t) + My(t-\tau). \tag{1}$$

In other words for any RK method there exist problems (complex system of dimension 2 or real system of dimension 4) where the method has stability restriction on the stepsize. In view of such a very negative result we now present an approach for solving DDE which unconditionally preserves the asymptotic stability on all systems of DDE with L, M matrices of arbitrary dimension. We restate the DDE as an abstract Cauchy problem (equivalently as an hyperbolic PDE) and then we use a classic RK method on the abstract problem. At every step of the method we have to solve a Boundary Value Problem which can be solved exactly.

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RK methods for Functional Differential Equations

Lucio Torelli & Stefano Maset & Rossana Vermiglio
(Department of mathematical sciences - University of Trieste,Italy)

The class of functional differential equations comprises discrete delay and distributed delay equations. The approach for numerically solving them is different in these two cases.
In this talk we show how RK-like schemes can be applied to general functional differential equations

$$y'(t) = f(t, y_t) \tag{1}$$

This approach requires only the computation of the functional f and gives new methods which works for both discrete and distributed delays. At every step of the RK method a functional algebraic equation arises which is solved by using interpolatory projection on finite dimensional spaces.

4.3 Solutions of large linear systems arising from ODEs and PDEs

Parallel preconditioning techniques for the solution of linear systems arising from fluid dynamics problems
Pierluigi Amodio & Aldo Bonfiglioli
(Dipartimento di Matematica, Università di Bari, Italy)

We analyze the solution of sparse linear systems arising from the discretization of CFD (Computational Fluid Dynamics) problems simulating both compressible and incompressible flows. The coefficient matrix of the linear system has a symmetric sparsity structure, and each element is a square block of fixed size (from 1 to 4) which contains information as velocity, pressure, etc.

The number of nonzero blocks per rows depends on the position of the discretized element in the domain, but it is less or equal to 7. Moreover, after a suitable reordering, the coefficient matrix has a band structure with a small bandwidth.

For the solution of the above system it is necessary to consider an iterative method (for example GMRES) with a proper preconditionings. We analyze parallel preconditionings known as Additive Schwarz methods which are among the most used for CFD problems.

In such methods the original domain is divided in subdomains which are elaborated by different processors, but the boundaries of each subdomain are overlapped among the processors in order to speed the convergence.

After an overview about the properties of such algorithms, we analyze a new preconditioning which increases the convergence rate of the iterative method and reduces the number of communications among the processors.

Title Preconditioning of iterative eigensolvers
Luca Bergamaschi & G. Gambolati& G. Pini & M. Putti & F. Sartoretto
(Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate, Università di Padova, Italy)

The Jacobi-Davidson method (JD) has been recently proposed [5] to find a number of eigenpairs close to a prescribed value.

In this communication we present a comparison [3] of this method with ARPACK [4] and the DACG method [1] in the solution of large sparse spd eigenproblems arising from discretization of the diffusion equation. In particular, we analyze the role of preconditioning in the solution of the indefinite system of the form (A - *I)x = b which is required at every step of the Jacobi-Davidson iteration [2]. Numerical tests show the high sensitivity of JD to preconditioning.

We parallelized the preconditioned JD obtaining an appreciable degree of parallelism when using both the Jacobi and AINV preconditioners, the latter revealing, on the average, more robust and efficient.

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On the Convergence of Krylov Linear Equation Solvers

M.T. Vespucci & C.G. Broyden
(University of Bergamo, Italy)

In this paper we show that the reduction in residual norm at each iteration of CG and GMRES is related to the first column of the inverse of an upper Hessenberg matrix that is obtained from the original coefficient matrix by way of an orthogonal transformation. The orthogonal transformation itself is uniquely defined by the coefficient matrix of the equations and the initial vector of residuals. We then apply this analysis to MINRES and show that, under certain circumstances, this algorithm can exhibit an unusual (and very slow) type of convergence that we refer to as QTRoscillatory convergence.

4.4 Reliable scientific codes

Blended block implicit methods for the numerical integration of ODEs

Luigi Brugnano & Cecilia Magherini
(Dipartimento di Matematica "U.Dini", Università di Firenze, Italy)

We recall the basic facts concerning a new approach for naturally defining efficient nonlinear splittings for the numerical implementation of block implicit methods for ODEs. The approach, first derived in [1] and then further analyzed

in [2], relies on the basic idea of defining a numerical method as the combination (*blending*) of two suitable component methods. By carefully choosing the methods, it is shown that very efficient implementations of block implicit methods can be obtained [3]. Moreover, some of them, characterized by a diagonal splitting, are well suited for parallel computers. A corresponding computational code [4] will be presented in a companion talk.

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The BiM code for the numerical integration of ODEs

Cecilia Magherini & Luigi Brugnano

(Dipartimento di Matematica "U.Dini", Università di Firenze, Italy)

In this talk, numerical results obtained with a recently developed sequential code for ODEs [1,2], based on a blended implementation of Block Implicit Methods (BiM), are presented. The BiM code uses a variable order-variable stepsize strategy, with methods of order 4-6-8-10-12-14. Numerical tests from the CWI testset [3], comparing the new code with the most efficient existing ones, prove its effectiveness. The possibility of getting an improvement of the performance through a parallel implementation of the code, is also sketched.

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TOM: A Code for Boundary Value Problems

Francesca Mazzia & Donato Trigiante
(Dipartimento Interuniversitario di Matematica, Bari, Italy)

Many choices need to be made in order to construct an efficient code for Boundary Value ODE Problems (BVP). The most crucial certainly are:

1. the discrete method;
2. the stepsize variation strategy;
3. the method for solving the nonlinear problems.

The existing codes, for example COLNEW, TWPBVP and MIRKDC [1,2, 6, 10], are based on different classes of methods such as collocation at gaussian points and mono-implicit Runge Kutta. The present code [7,8,9] is based on symmetric multistep formulas of highest order (TOMs) defined in [5].

Concerning the second choice, i.e. the mesh selection strategy, it is important especially when dealing with continuous problems whose solutions are of multiscale nature. Most of the existing codes base the mesh selection on an estimate of the local error. Such choice makes the code sensitive to the step size variation and, moreover, it does not provide any information about the conditioning of both continuous and discrete problem. We assume the principle that both the discrete and continuous problems should share the order of magnitude of the conditioning parameter.

In [3, 4] two quantities were defined which are related to the conditioning of the continuous problems and the corresponding discrete ones. Such parameters were also used to find a monitor function for the step size variation strategy.

Such step size variation has been refined and used in the present code [9]. It drastically reduces the computation cost, and moreover it also provide the correct mesh when we information about the behavior of the continuous solution is available.

Finally, for what concerns the the third major problem, i.e. the solution of the nonlinear problems, we use a quasilinearization strategy [8].

The effectiveness of choices made is shown by some numerical experiments on stiff problems. We also provide the corresponding results from COLNEW, TWPBVP and MIRKDC in order to show that the performance of the code is reasonable.

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BVMs for the numerical approximation of BVPs arising in modeling of Nonlinearly Elastic Materials

Ivonne Sgura & C. O. Horgan & G. Saccomandi
(Dipartimento di Matematica, Università di Lecce, Italy)

The purpose of this research is to investigate the mechanical problem of the *shearing* of the annular region between two concentric rigid cylinders occupied by an incompressible isotropic nonlinearly elastic material. The deformation is driven by an axial pressure gradient [4]. This kind of geometry, despite of its simplicity, occurs in many engineering applications (for example the rubber bush mountings in cab suspensions, etc...).

The problem is formulated as a two-point BVP for a second-order nonlinear ODE. Two classes of neo-Hookean materials are considered [3,5]. The first class models limiting chain extensibility at the molecular level and the second class is of power-law type, that includes modeling of biological materials.

Our purpose is to investigate the behavior of the solutions for different values of the pressure gradient in order to predict the possible breaking points in the material. The numerical experiments are performed with the experimental code *TOM* [6]. The code uses a class of BVM [2], with the quasi-linearization technique [7] and a mesh selection strategy based on the conditioning of the problem [1,8]. We provide numerical results regarding *softening* power-law materials and we show that a *boundary layer* behavior is exhibited near the bonded surfaces. We perform further numerical experiments for *hardening* materials showing that an interior *localization* is exhibited, that is a cusp occurs in the axial displacement profile when large pressure gradients are considered. The numerical results highlight the contrasting behavior between softening and hardening rubber-like or biological materials.

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4.5 Optimization problems

On a Parallel Interior–Point Method for Quadratic Programs with Special Structure

C. Durazzi & V. Ruggiero
(Department of Mathematics, University of Ferrara, Italy)

A crucial issue for an efficient implementation of Interior-Point (IP) methods is the solution of the linear system arising at each iteration for finding the search direction. The present state–of–the–art codes on IP methods for linear and quadratic programming (LP, QP) problems use direct inner solvers. However, iterative methods can be used with success on special classes of large–scale problems, having a particular structure in the matrix of the linear constraints.
In particular, for the solution of LP and separable QP problems, we proposed in [Durazzi, Ruggiero, Zanghirati, JOTA, 2001] a parallel IP method, named IPPCG method, that uses the preconditioned conjugate gradient algorithm for solving the normal equations, obtained by the reduction of the linear inner system. For non separable QP problems, an extension of the IPPCG method is considered in [Durazzi, Ruggiero, 2001], where, at each step of the method, instead of the normal equations, the reduced KKT system is solved by an iterative method. Also in this case, following the suggestions in [Luksan, Vlcek,

Numer. Linear Algebra Appl., 1998], a PCG method with convenient indefinite preconditioner can be used.
Furthermore, a sufficient condition for an approximate solution of the inner linear system is devised so that the global and the local superlinear convergence of the IPPCG method is assured. This condition can be used as an adaptive stopping rule for the iterative inner solver.
Numerical experiments on parallel computers confirm the effectiveness of the IPPCG method for programs with special structure, such as discrete quadratic optimal control problems or stochastic programming and robust optimization problems.

The Newton–Arithmetic Mean Method for the Solution of Nonlinear Systems
Emanuele Galligani
(Dipartimento di Matematica Università di Modena e Reggio Emilia, Italy)

This paper is concerned with the development of the Newton–Arithmetic Mean method for large systems of nonlinear equations with block–partitioned jacobian matrix.
This method is well suited for implementation on a parallel computer; its degree of decomposition is very high.
The convergence of the method is analysed for the class of systems whose jacobian matrix satisfies an affine invariant Lipschitz condition. An estimation of the radius of the attraction ball is given.
Special attention is reserved to the case of weakly nonlinear systems; theorems about the monotone convergence of the method are proved under the hypothesis of positive boundedness on the nonlinear mapping.
An application of the method for solving real paractical problems related to the study of reaction–diffusion processes and of interacting populations is described.

A class of globally convergent ABS algorithms for nonlinear systems
Ladislav Luksan
(Czech Science Academy)

We present a globally convergent modification of the nonlinear ABS algorithm based upon the globalization technique developed by Luksan. Numerical results within the ABSPACK project show that the modified algorithm is very robust, providing actually the best performance of all tested codes in terms of number of solved problems.

On the nonlinear ABS algorithm for problems with singular Jacobian at solution
Zunquan Xia
(Dalian Un. Technology)

We discuss the performance of the ABS nonlinear algorithms in the case where the Jacobian is rank deficient at a local solution. We show the existence of ABS methods that keep a q-quadratic rate of convergence in this case.

Large Quadratic Programs in Training Support Vector Machines
Luca Zanni & Gaetano Zanghirati
(Department of Mathematics, University of Modena and Reggio-Emilia, Italy)

We consider the numerical solution of the quadratic programming (QP) problem arising in training the learning machines named Support Vector Machines (SVMs). Given a training set $D = \{(\mathbf{p}_i, y_i),\ i = 1, \ldots, n,\ \mathbf{p}_i \in R^m,\ y_i \in \{-1, 1\}\}$ of labeled examples, the SVM learning technique performs pattern recognition by finding a decision surface obtained by solving a convex quadratic program of the form:

$$\begin{array}{rl} \text{minimize} & \frac{1}{2}\mathbf{x}^T G\mathbf{x} - \sum_{i=1}^n x_i \\ \text{subject to} & \sum_{i=1}^n y_i x_i = 0, \qquad 0 \le x_j \le C, \qquad j = 1, \ldots, n. \end{array} \tag{1}$$

The size of the quadratic program is equal to the number of training examples and, consequently, in many interesting applications we must solve a large QP problem ($n \gg 10000$). Since the matrix G is dense, the main approaches for solving this large quadratic program are based on special decomposition techniques, that avoid explicit storage of G by splitting the original problem into a sequence of smaller QP subproblems. The aim of this work is to introduce an efficient iterative solver for these QP subproblems when problem (1) arises in training SVMs with Gaussian kernels, that is, when the entries G_{ij} of G are defined by $G_{ij} = y_i y_j \exp\left(-\|\mathbf{p}_i - \mathbf{p}_j\|^2/(2\sigma^2)\right)$. The solver is a projection-type method that requires a matrix-vector multiplication and the solution of a singly constrained separable QP problem at each iteration. An appropriate updating rule for the projection parameter of the method is proposed in order to produce a good convergence rate. The effectiveness of the approach is evaluated by solving several benchmark problems and by comparison with well known QP packages. Furthermore, a parallel implementation of the decomposition technique is tested on a multiprocessor system.

4.6 Integral Equations

Uniform and pointwise numerical approximation of the weighted Hilbert transform on the real line
M. R. Capobianco & G. Criscuolo
(Istituto per Applicazioni della Matematica CNR, Napoli, Italy)

The importance of the Hilbert transform coming from its many applications, justifies some interest in its numerical evaluation. Besides appearing in several physical and engineering problems, the Hilbert transform is the main part of

singular integral equations on $\mathbf{R}$.
We propose an algorithm to compute the weighted Hilbert transform $H(wf)$ assuming that the density function f has good integration properties at the limits of the integration interval; these assumptions are the same ones to assure the boundedness of $H(wf)$. The proposed procedure is of interpolatory type and it uses as quadrature nodes the zeros of the orthogonal polynomials $p_m(w), m = 1, 2, \ldots$ with respect to the weight function w on $\mathbf{R}$; namely we approximate $H(wf)$ by $H_m(wf) = H(w\mathcal{L}_m(w; f))$, where $\mathcal{L}_m(w)$ denotes the Lagrange interpolating operator corresponding to the matrix having as elements the zeros of $p_m(w), m = 1, 2, \ldots$.
The results obtained in [1] are stronger than those ones proved in [4] where, in order to prove the main result for the quadrature rule, the boundedness of the operator H and Lm(w) are examined in unrelated way. Indeed, the authors of [4] do not prove the uniform converge and the stability of the quadrature rule $H(w\mathcal{L}_m(w; f))$ as we show, and they appealed to more complicated interpolatory procedure. Further, in [4] only the case of the Hermite weight is examined. The main observation is that if one wants to use only the zeroes of the orthogonal polynomials for interpolation, one can use instead good bounds on the functions of the second kind. The same formula of [4], based on polynomial interpolation at the zeros of orthogonal polynomials associated with the weight function under consideration, augmented by two carefully chosen extra points, has been proved in [3] for a much class of weights that have varing rates of decay. Furthermore, under the same assumptions on the functions f and w, we propose a Gauss type quadrature to evaluate H(wf). We give results about the convergence and the stability of the proposed procedure with respect to the distance of the singularity from the quadrature nodes. Taking into account these results, we describe the principal computational aspects of a new algorithm to evaluate $H(wf)$ (see also [2]).

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Iterative solution and preconditioning of boundary integral equations in electromagnetism

B. Carpentieri[1] & I.S. Duff, L. Giraud and G. Sylvand
(CERFACS, Toulouse, France)

In recent years, there has been a significant amount of work on the simulation of electromagnetic wave propagation phenomena, addressing various topics ranging from radar cross section to electromagnetic compatibility, to absorbing materials, and antenna design. The *Boundary Element Method* (BEM) has been successfully employed in the numerical solution of this class of problems, proving to be an effective alternative to common discretization schemes like Finite Element Methods (FEM's) and Finite Difference Methods (FDM's). The idea of BEM is to shift the focus from solving a PDE defined on a closed or unbounded domain to solving a boundary integral equation over the finite part of the boundary. The discretization by the boundary element method results in linear systems with dense complex matrices which are very challenging to solve. With the advent of parallel processing, this approach has become viable for large problems and the typical problem size in the electromagnetics industry is continually increasing. Direct dense methods based on Gaussian elimination are often the method of choice because they are reliable and predictable both in terms of accuracy and cost. However, for large-scale problems, they become impractical even on large parallel platforms because they require storage of n^2 double precision complex entries of the coefficient matrix and $\mathcal{O}(n^3)$ floating-point operations to compute the factorization, where n denotes the size of the linear system. Iterative Krylov subspace based solvers are a promising alternative provided we have fast matrix-vector multiplications and robust preconditioners.

In this talk we present results concerning the use of iterative Krylov solvers for the numerical solution of boundary integral equations in electromagnetism with special emphasis on the design of robust preconditioners, a crucial component of Krylov methods in this context. We consider in particular a sparse approximate inverse preconditioner based on Frobenius-norm minimization that use a static nonzero pattern selection. We report on results on the numerical scalability of the preconditioner on large problems in collaboration with AEDS, implemented in its FMM code. Finally we consider two possible multilevel extensions for the sparse approximate inverse. The first is based on the introduction of low-rank corrections which intend to improve the quality of the sparse approximate inverse computed on difficult problems. The second is based on inner-outer solution schemes in the FMM context which use different level of accuracy for the M-V products.

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Numerical approximation of some BEM singular integrals
G. Criscuolo
(Università degli Studi di Napoli "Federico II", Italy)

Very recently, Mastroianni and Monegato have derived error estimates for the numerical approach to evaluate the integral

$$\int_a^b \int_{-1}^1 \frac{f(x,y)}{x-y} w(x)dxdy, \tag{1}$$

where $(a,b) \equiv (-1,1)$, or $(a,b) \equiv (a,-1)$, or $(a,b) \equiv (1,b)$, $f(x,y)$ is a smooth function on both variables, and $w(x) = w^\alpha(x) = (1-x^2)^\alpha, \alpha > -1$. When $y \in (-1,1)$, the inner integral is defined in the Cauchy principal value sense. The results shown in [2] have wide interest in the applications. Indeed, in the applications of Galerkin boundary element methods, for the solution of onedimensional singular and hypersingular equations, one has to deal with integrals which after proper normalization are of the type (1). Further, twodimensional singular integrals of form (1) arise in some aeroelasticity problems (see the references in [2]). Using the same numerical approach to evaluate (1) proposed in [2], we improve the corresponding error estimates. Furthermore, we generalize the results in [2] for a wider class of weights and for different choice of the quadrature nodes. The more general results about the convergence of the numerical approach to evaluate (1) are of interest in the applications (see also [1]).

References

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High Performance Methods for Volterra Equations with Weakly Singular Kernels
E. Russo & G. Capobianco & M.R. Crisci
(Dipartimento di Matematica e Informatica, Università di Salerno, Italy)

Large systems of Volterra Integral Equations with weakly singular kernels arise in many branches of applications such as, for example, reaction-diffusion problems in small cells.

In order to get accurate solutions in a reasonable time frame, high performances numerical methods are required. Methods of this kind are the iterative Waveform Relaxation that split the system into uncoupled subsystem and so realize a massive parallelism across the system. However, fully parallel WR methods are usually slowly convergent.

In order to construct fast convergent fully parallel WR methods, the authors introduce non-stationary continuous and discrete time WR methods. The convergence analysis is performed.

Non-stationary Richardson WR method is constructed in such a way to optimize the speed of convergence. A significant error bound is obtained, which allow to predict the number of iterations required to get a given tolerance and to determine the class of problems for which the method is more suitable.

A parallel code based on this method is under construction.

5 List of Partecipants

Lidia Aceto: Università di Firenze, Dipartimento di Energetica, via C. Lombroso 6/17 - 50134 Firenze – aceto@ingfi1.ing.unifi.it – Phone: +39 055 4796745.

Pierluigi Amodio: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – amodio@dm.uniba.it – Phone: +39 080 5442703.

Bernd Aulbach: Institut fr Mathematik, Lehrstuhl fr nichtlineare Analysis, Universitt Augsburg - D-86135 Augsburg, Germany – bernd.aulbach@math.uni-augsburg.de – Phone: : +49 (0821) 598 - 2156

Alfredo Bellen: Università di Trieste, Dipartimento di Scienze Matematiche, via Valerio 12/1 - 34100 Trieste – bellen@univ.trieste.it – Phone: +39 040 6762608.

Luca Bergamaschi: Università di Padova, via Belzoni 7 - 35131 Padova – berga@dmsa.unipd.it – Phone: +39 049 8275927.

Luigi Brugnano: Università di Firenze, Dipartimento di Matematica, viale Morgagni 67/a - 50134 Firenze – brugnano@math.unifi.it – Phone: +39 055 4237116.

Marco Caliari: Università di Padova, Dip. di Matematica Pura ed Applicata, via Di Vittorio 22 - 37064 Povegliano Veronese (VR) – mcaliari@math.unipd.it – Phone: +39 0457970980.

Giovanni Capobianco: Università di Salerno, via S. Allende - Baronissi (SA) – gcapobianco@unisa.it – Phone: +39 089965269.

Maria Rosaria Capobianco: Istituto per Applicazioni della Matematica - I.A.M. - C.N.R., via P. Castellino 111 - 80131 Napoli – capobian@iam.na.cnr.it – Phone: +39 0815608101/5608288.

Angela Cardone: Università di Salerno, via S. Allende - Baronissi (SA) – angelacard@katamail.com – Phone: +39 089965269.

Margherita Carletti: Università di Urbino, Istituto di Biomatematica, Località Crocicchia - 61029 Urbino (Pu) – m.carletti@mat.uniurb.it – Phone: +39 0722304275.

Bruno Carpentieri: CERFACS, 42, av. Gaspard Coriolis - 31057 Toulouse CEDEX (Francia) – carpenti@cerfacs.fr – Phone: +33 (0) 5 61 19 30 14.

Jeff Cash : Imperial College of Science, Technology and Medicine, Department of Mathematics, Huxley Building, Imperial College, 180 Queen's Gate - London, SW7 2BZ – j.cash@ic.ac.uk – Phone: No. : +44 171 594 8538.

Francoise Chaitin-Chatelin: University of Toulouse I and CERFACS, 42, av. G. Coriolis - 31057 Toulouse Cedex
– chatelin@cerfacs.fr

Raymond Chan: Department of Mathematics, Chinese University of Hong Kong, Shatin, Hong Kong – rchan@math.cuhk.edu.hk - na.rchan@na-net.ornl.gov – Phone: (852) 2609-7970.

Francesco Costabile: Università della Calabria - 87036 Arcavacata di Rende (CS) – costabil@unical.it – Phone: +39 0984 493827.

Maria Rosaria Crisci: Università di Salerno, via S. Allende - Baronissi (SA) – rcrisci@unisa.it – Phone: +39 89965269.

Giuliana Criscuolo: Università di Napoli, Dipartimento di Matematica ed Applicazioni, via Cintia - 80126 Napoli – criscuo@matna2.dma.unina.it – Phone: +39 081 675696.

Nicoletta Del Buono: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – delbuono@pascal.dm.uniba.it – Phone: +39 080 5442204.

Giovanni Di Lena: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – dilena@dm.uniba.it – Phone: +39 080 5442707.

Carla Durazzi: Università di Ferrara, Dipartimento di Matematica, via Machiavelli 35 – dzc@dns.unife.it – Phone: +39 0532 291025.

Emanuele Galligani: Università di Modena e Reggio Emilia, Dipartimento di Matematica, via Campi 213/B - 41100 Modena – galligani@unimo.it – Phone: +39 059 2055206.

Giuseppe Gambolati: Università di Padova, via Belzoni 7 - 35131 Padova – gambo@dmsa.unipd.it – Phone: +39 049 8275916.

Paolo Ghelardoni: Università di Pisa, Dipartimento di Matematica Applicata, via Bonanno 25B - 56126 Pisa – ghelardoni@dma.unipi.it – Phone: +39 050 554096.

Giovanni Gheri: Università di Pisa, Dipartimento di Matematica Applicata, via Bonanno 25B - 56126 Pisa – gheri@dma.unipi.it – Phone: +39 050 554096.

Raffaella Giova: Dipartimento di Matematica e Applicazioni, via Cintia - 80126 Napoli – rgiova@unina.it – Phone: +39 081 675704.

Jacek Gondzio: Department of Mathematics & Statistics, University of Edinburgh - EH9 3JZ Edinburgh, U.K. – gondzio@maths.ed.ac.uk

Maria Italia Gualtieri: Università della Calabria - 87036 Arcavacata di Rende (CS) – gualtier@unical.it – Phone: +39 0984 493831.

Liana Guercia: Università di Lecce, Dipartimento di Matematica, via Provinciale Lecce-Arnesano P. O. Box 193 - 73100 Lecce – guercia@ingle01.unile.it – Phone: +39 335 411396.

Nicola Guglielmi: Università dell'Aquila, via Vetoio (Coppito) - 67010 L'Aquila – guglielm@univaq.it – Phone: +39 0862 433158.

Felice Iavernaro: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – felix@dm.uniba.it – Phone: +39 080 5442703.

Luciano Lopez: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – lopezl@pascal.dm.uniba.it – Phone: +39 080 5442678.

Ladislav Luksan: Czech Academy Sciences, Pod Vodarenskou Vezi - Praha – luksan@uivt.cas.cz – Phone: +420266053260.

Renzo Lupini: Università di Urbino, Istituto di Biomatematica, Località Crocicchia - 61029 Urbino (Pu) – lupini@mat.uniurb.it – Phone: +39 0722304223.

Cecilia Magherini: Università di Firenze, Dipartimento di Matematica, viale Morgagni 67/a - 50134 Firenze – c.magherini@math.unifi.it – Phone: +39 055 4237166.

Donatella Marini: Dipartimento di Matematica, Università di Pavia and I.A.N.–C.N.R. Via Ferrata 1, 27100 Pavia, Italy – marini@ian.pv.cnr.it – Phone: +39 0382 505638.

Angeles Martinez: Università di Padova, via Belzoni 7 - 35131 Padova – acalomar@dmsa.unipd.it – Phone: +39 049 8275900.

Stefano Maset: Università di Trieste, Dipartimento di Scienze Matematiche, via Valerio 12/1 - 34100 Trieste – maset@univ.trieste.it – Phone: +39 080 5442662.

Giuseppe Mastroianni: Università della Basilicata, Dipartimento di Matematica, C.da Macchia Romana - 85100 Potenza – mastroianni@unibas.it – Phone: +39 0971205836.

Carmen Mastroserio: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – carmen@pascal.dm.uniba.it – Phone: +39 080 5442662.

Francesca Mazzia: Università di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – mazzia@dm.uniba.it – Phone: +39 080 5442702.

Eleonora Messina: Università di Napoli, Dipartimento di MAtematica, via Cintia - 80126 Napoli – eleonora.messina@dma.unina.it – Phone: +39 081 675652.

Igor Moret: Università di Trieste, Dipartimento di Scienze Matematiche, via Valerio 12/1 - 34100 Trieste – torelli@univ.trieste.it – Phone: +39 040 6762602.

Anna Napoli: Università della Calabria - 87036 Arcavacata di Rende (CS) – napolia@unical.it – Phone: +39 0984 493829.

Paolo Novati: Università di Trieste, Dipartimento di Scienze Matematiche, via Valerio 12/1 - 34100 Trieste – novati@univ.trieste.it – Phone: +39 040 6762676.

Carmela Paracelli: Università di Lecce, Dipartimento di Matematica, via Provinciale Lecce-Arnesano P. O. Box 193 - 73100 Lecce – paracell@ingle01.unile.it – Phone: +39 0832 344356.

Lionello Pasquini: Università di Roma, Dipartimento di Matematica – lionello.pasquini@uniroma1.it – Phone: +39 06 49913201.

Beatrice Paternoster:Universita' di Salerno Dipartimento di Matematica e Informatica - 84081 Baronissi (SA) Italy beapat@dia.unisa.it Phone: : +39 (0)89 965328 Fax : +39 (0)89 965272.

Raffaella Pavani: Politecnico di Milano - 20133 Milano – rafpav@mate.polimi.it – Phone: +39 02 2399 4516.

Mario Pedrazzoli: Università di Pisa, Dipartimento Matematica Applicata, via Diotisalvi 2 - 56126 Pisa – m.pedrazzoli@ing.unipi.it – Phone: +39 050 554096.

Giorgio Pini: Università di Padova, Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate, via Belzoni 7 - 35131 Padova – pini@dmsa.unipd.it – Phone: +39 049 8275915.

Tiziano Politi: Politecnico di Bari, Dipartimento di Matematica, via Orabona 4 - 70125 Bari – pptt@pascal.dm.uniba.it – Phone: +39 080 5963684.

Valeria Ruggiero: Università di Ferrara, Dipartimento di Matematica, via Machiavelli 35 – Ferrara – rgv@dns.unife.it – Phone: +39 0532 291008.

Elvira Russo: Università di Napoli, via Cintia - 80126 Napoli – elvrusso@unina.it – Phone: +39 081675654.

Ivonne Sgura: Università di Lecce, Dipartimento di Matematica, via Provinciale Lecce-Arnesano P. O. Box 193 - 73100 Lecce – ivonne.sgura@unile.it – Phone: +39 0832 320591.

Mark Sofroniou: Wolfram Research Inc., Champaign, Illinois, USA – marks@wolfram.com – Phone: +39 051 398247.

Giulia Spaletta: Università di Bologna, Dipartimento di Matematica, Piazza Porta S. Donato 5 - 40127 Bologna – spaletta@cs.unibo.it – Phone: +39 051 2094482.

Emilio Spedicato: Università di Bergamo, piazza Rosate 2 - 24129 Bergamo – emilio@unibg.it – Phone: +39 035 277514.

Lucio Torelli: Università di Trieste, Dipartimento di Scienze Matematiche, via Valerio 12/1 - 34100 Trieste – torelli@univ.trieste.it – Phone: +39 040 6762677.

Donato Trigiante: Università di Firenze, Dipartimento di Energetica, via C. Lombroso 6/17 - 50134 Firenze – trigiant@cesit1.unifi.it – Phone: +39 055 4796726.

Peter van der Houwen: senna2@wolmail.nl

Stefan Vandewalle: Katholieke Universiteit Leuven, Department of Computerscience Celestijnenlaan 200A, B-3001 Leuven, Belgium – stefan.vandewalle@cs.kuleuven.ac.be

Maria Teresa Vespucci: Università di Bergamo, viale Marconi 5 - 24044 Dalmine (BG) – vespucci@spm.it – Phone: +39 035 223991.

Xia Zunquan: Dalian University Technology, c/o prof. Spedicato

Gaetano Zanghirati: Università di Ferrara, Dipartimento di Matematica, via Machiavelli 35 - Ferrara – g.zanghirati@unife.it – Phone: +39 0532 291025.

Luca Zanni: Università di Modena e Reggio Emilia, Dipartimento di Matematica, via Campi 213/B - 41100 Modena – zanniluca@unimo.it – Phone: +39 059 2055206.

Giovanni Zilli: Università di Padova, Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate, via Belzoni 7 - 35131 Padova – zilli@dmsa.unipd.it – Phone: +39 049 8275900.