Contributed Session 07: Scientific Computation and Numerical Algorithms

Time-splitting scale-selective numerical scheme for atmospheric modeling

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The atmosphere is a complex system supporting processes of different space and time scales. Accordingly, the complete 3D mathematical models of the atmospherecontain 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. Stability analysis of the scheme shows that the time step is restrictedonly by the maximum velocity of advection. The performed numerical experiments show computational efficiency of the designed scheme and accuracy of the predicted atmospheric fields.

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A method to solve fractional differential equations

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Fractional order differential equations (FDE) are generalizations of integer order differential equations and became an important tool in mathematical modeling, in recent years. Several solution techniques for FDE's were studied in earlier works. We give a new method to solve first order FDE's using a transformation. This new method has many advantages like its speed, simplicity and applicability. Some examples are also given to show that this technique works properly. Finally, an application of the method is given to solve an epidemic model.

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Complexity analysis of a winding number algorithm by iterated function methods

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The winding number of plane curves is a geometric quantity often used in the context of complex analysis to locate the zeros and poles of a rational function. It is usually applied to study the stability of linear systems or as two-dimensional bisection procedure for approximating function zeros. We present an analysis of computational complexity of an algorithm for calculating the winding number, using dynamical systems techniques .

The algorithm is based on an adaptive insertion process of interpolation points in the given curve Δ (Ying-Katz process). This process may be viewed as the iteration, in the space of polygonal curves (not finite-dimensional) $\mathbb{C}^* = \bigcup_{i=1}^{\infty} \mathbb{C}^i$, of the application $f_\Delta : \mathbb{C}^* \to \mathbb{C}^*$ carrying $P = (\Delta(s_0), \Delta(s_1), ..., \Delta(s_n))$ to $f_\Delta(P) = (..., \Delta(s_i), \Delta(\frac{s_i+s_{i+1}}{2}), \Delta(s_{i+1}), ...)$ if the points $\Delta(s_i)$ and $\Delta(s_{i+1})$ are in not consecutive quadrants in the plane, and $f_\Delta(P) = P$ otherwise. The fixed points of f_Δ are the sampling polygons of Δ with vertices in consecutive quadrants.

We show that the iteration of f_Δ reaches a fixed point in a finite number of iterations because there is a termination function, related to the distance from the origin of the curve. We also demonstrate the correctness of the algorithm from certain property that is invariant along the orbits of f_Δ.

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Constructing extensions of nonstandard finite difference schemes

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We consider both the nonstandard finite difference schemes of Mickens and the higher order methods of Erdogan and Ozis. The latter's method formulates a method to calculate some of the denominator functions and nonlocal approximations that characterize Micken's schemes. We extend this analysis by presenting a construction for nonlinear functions of the form

$$\frac{d^2y}{dt^2} = f(t, y, y')$$

and systems of differential equations. We present analysis and numerical results to demonstrate both the effectiveness of the technique and when this method is best used.

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On functions having the fixed point property

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In this paper, necessary and sufficient conditions are given for a family of functions with the fixed point property to be equivalent to the Axiom of Choice.

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Uncertainty quantification with probabilistic cellular automata

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Development of real-time tools for uncertainty propagation is of increasing interest in industrial applications such as monitoring of infrastructure grids. However, it faces major challenges due to the complexity of the underlying models. To meet these challenges we suggest to source out large parts of the computations into a preprocessing procedure. Our ideas are demonstrated by the propagation of initial value uncertainties under deterministic PDE dynamics. In particular we introduce a discretization of PDEs which is based on a variant of the set oriented method. As preprocessing it translates PDEs to completely discrete (in time, space and state) dynamical systems: probabilistic cellular automata. These automata are much simpler than the usual models and become accessible to very efficient simulation techniques. The goal is to use an automaton to approximate the evolution of a system's probability density in real-time. It is observed that the solution of the approximating system converges to the exact solution for refinement of the discretization's resolution. To test our results we consider the reactive transportation of chemical pollutants in drinking water. We compare our method to Wiener's polynomial chaos approach as implemented in conventional solvers.

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A discontinuous Galerkin least-squares finite element method for solving Fisher's equation

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Fisher's equation is a semilinear parabolic reaction-diffusion equation, which was introduced to investigate the dispersion of a mutant gene through a population in a one-dimensional habitat. Fisher's equation admits traveling wave solution, for which it is challenging to obtain reliable numerical approximation. In particular, for equations under strong reactions, the solutions evolve into shock-like waves, which is a classical difficult problem in numerical computation. In this paper, we introduce a discontinuous Galerkin least-squares finite element method for solving Fisher's equation, which produces accurate and stable solutions in uniform meshes. Numerical results are provided to confirm the efficiency of the method. A comparison study of several numerical methods is also included.

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Conformal conservation laws and geometric integration for damped Hamiltonian PDEs

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Conformal conservation laws are defined and derived for a class of multi-symplectic equations with added dissipation. In particular, the conservation laws of energy and momentum are considered, along with those that arise from linear symmetries. Numerical methods that preserve these conformal conservation laws are presented in detail, providing a new framework for proving a numerical method exactly preserves the dissipative properties considered. The conformal methods are compared analytically and numerically to standard conservative methods, which includes a thorough inspection of numerical solution behavior for linear equations. The semi-linear wave equation and nonlinear Schrodinger equation with added dissipation, as well as an elliptic boundary value problem, are used as examples to demonstrate the results.

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Determining important parameters in the dynamics of a three-compartment model of abiotic nutrient pool, autotroph and detritus

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We conduct a systematic parameter ranking for an existing three-compartment model of abiotic nutrient pool, autotroph and detritus. We commence by describing this important model and highlighting a few characterizations of the complexities in the model. Using existing set of parameter values and assuming initial conditions, we were able to conduct this rigorous parameter ranking. Our present method permits us to deduce interesting conclusions about the relative importance of individual parameters within the model. This method also permits us to gain some insights into the ability of the model to show what happens within the African ecological system. Considering alternative parameter values, we test the behavior of this model which has allowed us to identify a deficiency in one part of the model. For this complex model (a nonlinear system of ordinary differential equations with a large number of parameters), we observe in this group of six parameters that the experimental time is ranked as an important parameter than the harvesting rate of autotroph biomass that is removed from the system.

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Sensitivity analysis of a partially coupled system of differential equations without delay

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For a class of non-linear partially coupled differential equations of first order, we propose a numerical sensitivity analysis based on the behavior of the solution trajectories due to a variation of a model parameter when other parameters are fixed. The numerical algorithms were written and corresponding cumulative percentage changes are calculated. Numerical results are presented and discussed. We observe in this rigorous sensitivity analysis over a time interval that the experimental time, T and the ratio of nutrient mass to total biomass in autotroph and detritus, Υ are the most sensitive and the least sensitive parameters respectively. We will expect this contribution to provide insights in understanding the role of parameter estimation in this important scientific problem.

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Fully fuzzy systems of linear equations

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The systems of linear equations arise in various fields of Engineering and Sciences like Electrical, Civil, Economics, and Dietary etc. Many times in real applications it is difficult to obtain the precise values of the parameters involved in the systems rather an interval in which their values fall can only be estimated by expert knowledge. In such situation it may be convenient to represent such parameters can be represented by fuzzy numbers (refer [1]). Our work extends the results for the solution of linear algebraic equations with fuzzy numbers (refer [2]) to the system of linear equations with fuzzy parameter using matrices. The fuzzy system is first converted into crisp using α-cuts. From the solution of converted crisp system, the solution of fuzzy system can be obtained if they satisfy the conditions given in our main result.

References:
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Modeling the thermal conductance of phononic crystal plates

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We present a method to model the phonon thermal conductance in porous phononic crystal plates. The goal is to optimize the figure of merit for materials, which is the primary criterion for the efficiency of a thermoelectric device. Values of about three or higher allow for the construction of thermoelectric generators based on the Seebeck effect, which are more efficient than conventional electrical generators. The quantity to be optimized for the phononic crystals slabs is the Landauer-Büttiker thermal conductance, which can be achieved by varying the geometrical structure concerning width and thickness of the sample as well as pore size, shape and density.To obtain the Landauer-Büttiker thermal conductance we have to determine the phonon mode distribution by solving the elastic equations of motion for the considered systems. Making use of the periodicity of the system, the equations of elastic wave propagation can be Fourier transformed. This yields a generalized eigenvalue problem for every vector $\mathbf{k}$ in the Brillouin zone. Making use of parallelization we can efficiently compute the dispersion relation and the corresponding phonon mode distribution in a straightforward way.

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