

THE FIRST ANNUAL MEETING OF APPLIED MATHEMATICS: FRONTIER ASPECTS OF APPLIED MATHEMATICS

WORKSHOPS



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A Scalable Parallel Eigensolver for Large-scale Simulations on Next-generation Computing Environments

Prof. Tetsuya Sakurai

Large-scale eigenvalue problems arise in wide variety of scientific and engineering applications such as nano-scale materials simulation, vibration analysis of automobiles, analysis of big data, etc. In such situations, high performance parallel eigensolvers are required to exploit distributed parallel computational environments. In this talk, we present the parallel eigensolver z-Pares, based on the so-called “Sakurai-Sugiura projection method” for large-scale interior eigenvalue problems. We evaluate its performance on some scientific and engineering applications executed on state-of-art supercomputers such as the K-computer at RIKEN. The hierarchical structure of this software enables effective utilization of vast computational resources. A stochastic estimation method for eigenvalue density is also presented. Some numerical experiments illustrate the efficiency of the proposed methods.

For material related to this talk, [click here](#).

A Newton-Type Method with Non-equivalence Deflation for Nonlinear Eigenvalue Problems Arising in Photonic Crystal Modeling

Prof. Tsung-Ming Huang

The numerical simulation of the band structure of three-dimensional dispersive metallic photonic crystals with face-centered cubic lattices leads to large-scale nonlinear eigenvalue problems, which are very challenging due to a high dimensional subspace associated with the eigenvalue zero and the fact that the desired eigenvalues (with smallest real part) cluster and close to the zero eigenvalues. For the solution of the nonlinear eigenvalue problem, a Newton-type iterative method is proposed and the nullspace-free method is applied to exclude the zero eigenvalues from the associated generalized eigenvalue problem. To find the successive eigenvalue/eigenvector pairs, we propose a new non-equivalence deflation method to transform converged eigenvalues to infinity, while all other eigenvalues remain unchanged. The deflated problem is then solved by the same Newton-type method, which is used as a hybrid method that combines with the Jacobi-Davidson and the nonlinear Arnoldi methods to compute the clustering eigenvalues. Numerical results illustrate that the proposed method is robust even for the case of computing many clustering eigenvalues in very large problems.

For material related to this talk, [click here](#).

Partial differential equations and graph theory from a perspective of a chemist

Prof. Henryk Witek

Many research areas in contemporary theoretical physics and theoretical chemistry are closely related to various research directions in numerical and applied mathematics. In many cases there is not enough interactions between theoretical chemists and applied mathematicians that would stimulate research collaborations between these two communities, collaborations that can prove useful and valuable for presumably both sides. Another difficulty impeding the research collaborations is the lack of satisfactory formal mathematical training for most theoretical chemists and physicists working on applied mathematical problems, which results in somewhat clumsy way of defining the questions and problems we would like to ask to the mathematicians. The current talk is supposed to cover two mathematical problems studied in my group over the period of last 5 years. The exposition will follow the "vague and clumsy" way of speaking of non-mathematicians but it is hoped that it will be clear enough to enable understanding and possible future collaborations on the outskirts of the presented divagations.

The first of the presented topics will concern a particular and very narrow problem in the theory of elliptic PDEs. I will talk about the possibility of solving in an exact and analytical manner the time-independent Schrodinger equation for the helium atom. Very accurate, numerical solutions to this problem are well-known and from the point of view of applied mathematics, the problem can be considered solved. However, the associated numerical techniques are limited only to a few-electron problems and it would be very valuable to have compact functional expressions approximating the exact wave function of the two-electron problem (i.e., helium) to utilize them in the description of many-electron wave functions. My talk will discuss perspectives of obtaining such estimates. Various open problems [1] associated with this process will be also discussed.

B.-H. He and H. A. Witek: Toward Exact Analytical Wave Function of Helium Atom: Two Techniques for Constructing Homogeneous Functions of Kinetic Energy Operator, J. Chin. Chem. Soc. in press (2015) DOI: [10.1002/jccs.201500086](https://doi.org/10.1002/jccs.201500086)

The second of the presented topics will focus on the possibility of describing stability of a specific class of chemical molecules (benzenoids) on the base of various topological invariants that can be defined from the corresponding molecular graphs.

To this purpose we will present a specific extension of the usual definition of a perfect matching of a graph and we will define a combinatorial object called Zhang-Zhang (ZZ) polynomial that can be used to enumerate all possible perfect matchings. A recursive algorithm [7] for computing the ZZ polynomials will be presented together with a number of its applications. [8,6] The main part of the talk will be concerned with various open problems related to the asymptotic behavior [1-5] of the ZZ polynomials for various classes of benzenoids.

1. C. P. Chou, J.-S. Kang, H. A. Witek: Closed-form formulas for the Zhang–Zhang polynomials of benzenoid structures: Prolate rectangles and their generalizations, *Discr. Appl. Math.* in press (2015) DOI: 10.1016/j.dam.2015.06.020
2. C. P. Chou, H. A. Witek: Two Examples for the Application of the ZZDecomposer: Zigzag-Edge Coronoids and Fenestrenes, *MATCH Comm. Math. Comput. Chem.* 73, pp. 421-426 (2015)
3. H. A. Witek, G. Mos, C. P. Chou: Zhang-Zhang Polynomials of Regular 3- and 4-tier Benzenoid Strips, *MATCH Comm. Math. Comput. Chem.* 73, pp. 427-442 (2015)
4. C. P. Chou, H. A. Witek: Determination of Zhang-Zhang Polynomials for Various Classes of Benzenoid Systems: Non-Heuristic Approach, *MATCH Comm. Math. Comput. Chem.* 72, pp. 75-104 (2015)

5.C. P. Chou, H. A. Witek: Closed-Form Formulas for the Zhang-Zhang Polynomials of Benzenoid Structures: Chevrons and Generalized Chevrons, MATCH Comm. Math. Comput. Chem. 72, pp. 105-124 (2015)

6.C. P. Chou, H. A. Witek: ZZDecomposer: A Graphical Toolkit for Analyzing the Zhang-Zhang Polynomials of Benzenoid Structures, MATCH Comm. Math. Comput. Chem. 71, pp. 741-764 (2014)

7.C. P. Chou, H. A. Witek: An Algorithm and FORTRAN Program for Automatic Computation of the Zhang-Zhang Polynomial of Benzenoids, MATCH Comm. Math. Comput. Chem. 68, pp. 3-30 (2012)

8.C. P. Chou, Y. Li, H. A. Witek: Zhang-Zhang Polynomials of Various Classes of Benzenoid Systems, MATCH Comm. Math. Comput. Chem. 68, pp. 31-64 (2012)

I hope that the presented topics will stimulate interactions between the communities of applied mathematicians and theoretical chemists, leading to many fruitful collaborations.

For material related to this talk, [click here](#).

Accurate Implementation of Doubling Algorithms for M -matrix Algebraic Riccati Equations

Prof. Jungong Xue

Structure-preserving doubling algorithms (SDAs) are very efficient iterative methods for computing the unique minimal nonnegative solution to an M -matrix algebraic Riccati equation (MARE). They are globally and quadratically convergent. However, the initialization phase and the doubling iteration kernel in any SDA involve inverting nonsingular M -matrices. A nonsingular M -matrix can be inverted by the GTH-like algorithm to almost full entrywise relative accuracy, provided a triplet representation of the matrix is known. Recently, Nguyen and Poloni (*Numer. Math.*, 130(4):763--792, 2015) discovered a way to construct triplet representations in a cancellation-free manner for all involved M -matrices in the alternating directional doubling algorithm (ADDA), the best among all known SDAs, for a special class of MAREs arising from Markov-modulated fluid queues. In this paper, we extend Nguyen's and Poloni's work to all MAREs by also devising a way to construct the triplet representations cancellation-free. Our construction,

however, is not a straightforward extension of theirs. It is made possible by an introduction of novel recursively computable auxiliary nonnegative vectors. As the second contribution, we propose an entrywise relative residual for an approximation solution. The residual has an appealing feature of being able to revealing the entrywise relative accuracy in the approximation. This is in marked contrast to the usual legacy normalized residual which reflects relative accuracies of large entries well but not so much those of very tiny entries. Numerical examples are presented to demonstrate and confirm our claims.

For material related to this talk, [click here](#).

Performance Engineering for Extreme-Scale PDE-Constrained Optimizations on Petascale Architectures

Prof. Olaf Schenk

One of the outstanding challenges of computational sciences and engineering is large-scale nonlinear parameter estimation governed by partial differential equations. These inverse problems are known as PDE-constrained optimization problems and are significantly more difficult to solve than PDE forward problems. Several algorithmic and performance engineering advances are discussed to solve these problems under uncertainty in operationally-compatible time. The new developments include novel incomplete augmented sparse factorizations, stencil-code optimizations, and multicore- and GPU-based dense matrix implementations. In addition, achieving scalability for the optimization process implemented on large-scale computing platforms comprised of tens of thousands of multicore processors is a task that offers many challenges. We will address these issues and will present numerical parallel results both in two and three space dimensions from seismic applications that illustrate the usefulness of the approach.

For material related to this talk, [click here](#).

Modeling of the dissipation tensor transport equation

Dr. Celine Lo

This work aims at developing a model for the dissipation tensor to close the Reynolds-stress tensor transport equations. In the context of second-moment closures, the modelling of anisotropies of the dissipation phenomenon generally involves an algebraic expression dependant on the Reynolds stress tensor. However, due to the evidence of considerably different near-wall behavior of the Reynolds-stress components from that of the dissipation tensor, instead of using an algebraic model, a transport equation for each of the components of the tensor is solved. To ensure the numerical stability of the solution, a transport equation for a modified dissipation tensor, for which the boundary conditions are zero at the wall, is solved. Due to the lack of direct numerical simulation data for the exact transport equation of the dissipation tensor, the conventional “a priori” approach as well as the “a differential a priori” method are used to develop the model. This latter methodology, introduced by Parneix and Durbin (1996), consists in freezing some variables by using Direct Numerical Simulation data and solving differential equations for the remaining quantities. The model is tested against the fully developed turbulent channel flow to validate the performance of the model predictions.

The interplay between theory and computation in the study of 3D Euler equations.

Prof. Yizhao Thomas Hou

Whether the 3D incompressible Euler equations can develop a singularity in finite time from smooth initial data is one of the most challenging problems in mathematical fluid dynamics. This question is closely related to the Clay Millennium Problem on 3D Navier-Stokes Equations. We first review some recent theoretical and computational studies of the 3D Euler equations. Our study suggests that the convection term could have a nonlinear stabilizing effect for certain flow geometry. We then present strong numerical evidence that the 3D Euler equations develop finite time singularities. To resolve the nearly singular solution, we develop specially designed adaptive (moving) meshes with a maximum effective resolution of order 10^{12} in each direction. A careful local analysis also suggests that the blowing-up solution is highly anisotropic and is not of Leray type. A 1D model is proposed to study the mechanism of the finite time singularity. Very recently we prove rigorously that the 1D model develops finite time singularity. Using a very delicate method of analysis which involves computer aided proof, we prove the existence of a discrete family of self-similar profiles for a variant of this model. Moreover, we show that the self-similar profile enjoys some stability property..

For material related to this talk, [click here](#).

Bound-preserving high order schemes in computational fluid dynamics

Prof. Chi-Wang Shu

We give a survey of our recent work with collaborators on the construction of uniformly high order accurate discontinuous Galerkin (DG) and weighted essentially non-oscillatory (WENO) finite volume (FV) and finite difference (FD) schemes which satisfy strict maximum principle for nonlinear scalar conservation laws, passive convection in incompressible flows, and nonlinear scalar convection-diffusion equations, and preserve positivity for density and pressure for compressible Euler systems. A general framework (for arbitrary order of accuracy) is established to construct a simple scaling limiter for the DG or FV method involving only evaluations of the polynomial solution at certain quadrature points. The bound preserving property is guaranteed for the first order Euler forward time discretization or strong stability preserving (SSP) high order time discretizations under suitable CFL condition. One remarkable property of this approach is that it is straightforward to extend the method to two and higher dimensions on arbitrary triangulations. We will emphasize recent developments including arbitrary equations of state, source terms, integral terms, shallow water equations, Lagrangian schemes, equations with delta function solutions, relativistic hydrodynamics, and positivity-preserving high order finite volume scheme and piecewise linear DG scheme for convection-diffusion equations. Numerical tests demonstrating the good performance of the scheme will be reported.

For material related to this talk, [click here](#).

Quantum Hydrodynamics and Turbulence in Atomic Bose-Einstein Condensates

Prof. Makoto Tsubota

For the abstract of this talk, please [click here](#).

For material related to this talk, [click here](#).

A charged nanopore model for nanofiltration (NF)

Prof. Tyzz-Leng Horng

Nanofiltration (NF) using membranes with numerous nanopores has gained its popularity in water treatment like desalination. Overlapped electric double layer (EDL) in charged nanopores makes the membrane to be ion selective and reach high rejection rate for salts when driving electrolyte through nanopores by pressure. It has its advantage over reverse osmosis (RO) with smaller pressure exerted and larger water throughput. Here a charged nanopore model is used to describe the physics and geometry of NF. Since the salt rejection process involves convection, diffusion and electro-migration of ions, joint of Poisson-Nernst-Planck (PNP) and Navier-Stokes (NS) equations is employed to study this problem. Steric effect would be significant inside nanopores, and a modified model of PNP with steric effect considered is actually used here. The computational results will be compared with traditional 1D model such as DSPM-DE (Donnan Steric Pore Model-Dielectric Exclusion), and the mechanism of salt rejection will be discussed. We hope we can gain as much physical insights as possible from such a model of simple geometry, and apply to much complicated charged nanopores like ion channel on cell membrane in the future.

Keywords: Desalination, nanofiltration, electric double layer, Poisson-Nernst-Planck equations, Navier-Stokes equations, steric effect.

For material related to this talk, [click here](#).

Analysis of Non-linear Implicit Solutions to the Euler Equations for Hypersonic and Shocked Flows

Prof. Matthew Smith

The Finite Volume Method (FVM) has become one of the cornerstone techniques for the numerical solution to the Euler and Navier-Stokes equations. Both of these equations are fundamentally non-linear in nature: fluxes across cell surfaces cannot be described by linear combinations of the conserved quantities without an approximation in the form of a linearization, which may be problematic for high speed (hypersonic) flows and flows with shock waves present. This does not present a challenge when we employ an explicit approach, since fluxes are evaluated in the previous time step's values. However, a truly implicit approach requires the simultaneous evaluations of fluxes – and evaluation of the time derivative – which is non-trivial due to the presence of non-linear terms. In this work, we analyze the use of a modified Quasi-Newton-Raphson method to the solution of both steady and transient multi-dimensional flow problems. The residual is computed directly using the Euler Equations such that $R(z) = dU(z)/dt + dF(z)/dx$ where z is our solution array holding our primitives (ρ, u, v, T). In order to facilitate a general investigation into the flux calculator employed, the Jacobian for the system is computed using Finite Differences.

The resulting Jacobian matrix ($4 \times N \times 4N$ in size for a 2D problem with N cells) is non-symmetrical but diagonally dominant. The modification to z at each iteration is computed using the Bi-Conjugate Gradient Stabilized (BiCGStab) method, where we employ a variety of preconditioners to accelerate this phase of the convergence. Results will be shown and discussed during the presentation, from which we can draw several important conclusions: (i) a higher order time discretization must be employed in transient implicit computations, which is demonstrated here using an Adams-Moulton formulation, (ii) both temporal and spatial accuracy play significant roles in the condition number of the Jacobian, which higher orders in space and lower orders in time leading to higher condition numbers, (iii) steady simulations require a special modification to the original N-R approach in order to maintain physical stability in the solution as required by the Finite Volume solver. Finally, if time permits, we shall discuss the application of this work to parallel computation using heterogeneous architectures.

For material related to this talk, [click here](#).

Mathematical modeling and simulation in acupuncture

Dr. Yannick Deleuze

Acupuncture requires a long-term training to handle acupoints. Four main techniques exist: (1) development of a local mechanical stress field by needle motions (lifting thrusting cycle or rotation) at acupoints; (2) development of a local temperature field by directly applying a heating moxa (mugwort herb) stick on the skin or indirectly by applying this stick on the acupuncture needle (moxibustion) at acupoints; (3) development of a local electrical field by applying a small electric current between a pair of acupuncture needles (electroacupuncture, or percutaneous electrical nerve stimulation) at acupoints; (4) stimulation of photosensitive GPCRs by laser light (laser acupuncture) at acupoints.

Acupuncture effects result from a set of signals sent from activated mastocytes at given acupoints to local nerve endings, capillaries, heart, and brain. Mastocytes are activated by a mechanical stress field (mechanotransduction), heating (thermotransduction), a electrical field (electrotransduction), or laser light (phototransduction). Whatever the operation mode, calcium entry in the mastocyte triggers degranulation and release of chemoattractants, neural stimulants, and endocrine substances. The process is sustained by recruitment of mastocytes (chemotaxis).

A mathematical analysis leads to a theorem for blow-up condition as well as an analytical solution useful for validation. Numerical simulations are also carried out using a finite element method with mesh adaptivity.

For material related to this talk, [click here](#).