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Invited talks

Extended Optimal Transportation Theory

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Optimal transportation theory goes back to Monge who solved a Civil Engineering problem where parcels of materials have to be displaced from one site to another one with minimal transportation cost. This problem was revisited by Kantorovich in 1942 and rephrased as an infinite dimensional linear program, the so-called Monge-Kantorovich problem, which established a bridge between Combinatorial Optimization, Probability theory and Statistics, as reported, for instance, in the recent book by Rachev and Rüschendorf.

In the late 80', a connection was made between Optimal Transportation Theory and non-linear Partial Differential Equations. In particular, a variant of the original Monge transportation problem was related to two of the most challenging (both analytically and numerically) non-linear PDEs, namely the (real) Monge-Ampère equations and the Euler equation of incompressible fluid mechanics. Nowadays, many other important PDEs, in particular the heat equation and several dissipative equations (porous medium equations, lubrication equations, limited flux diffusion equations, granular flow equations,...) have been neatly related to optimal transportation theory.

The aim of the talk is to describe an extension of the Monge-Kantorovich theory dealing with optimal deformations of fluid motions and related to classical Electrodynamics.

PDE and Wavelet Techniques for Image Compression

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In this talk, I will present an overview of our recent work on combining PDE and wavelet techniques for image compression. The first part will be on an adaptive ENO wavelet transform designed by using ideas from Essentially Non-Oscillatory (ENO) schemes for numerical shock capturing.

The second part of the talk is on using a variational framework, in particular the minimization of total variation (TV), to select and modify the retained standard wavelet coefficients so that the reconstructed images have fewer oscillations near edges.

Joint work with Dr. Haomiin Zhou at Caltech.

Heterogeneous Multiscale Methods

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The heterogeneous multiscale method is a framework for numerical approximations of problems with very different active scales. The original problem is discretized on the macro-scale and the missing data from the micro-scale is supplied by micro-scale simulations on sub-domains. The use of sub-domains is critical in order to reduce the overall computational complexity. Examples will be given from homogenization of partial differential equations, Brownian motion and molecular dynamics. The emerging theory will also be discussed.

A Level Set Approach for Solutions with Shocks of Order Preserving Evolution Equations

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There are several classes of evolution equations whose solution may develop jump discontinuities called shocks in finite time. A typical example is a conservation law. There are also second order examples including the curvature flow equation with a certain class of driving forces for graphs.

We are interested in what way we extend the solution after it develops shocks. For a conservation law an entropy solution is a suitable weak notion of a solution so that the problem is uniquely and globally solvable. For a certain class of first order equations the author introduced a notion of a proper viscosity solution which applies nonconservative equations as well as a conservation law. We extend this approach to a second order problem (having order preserving structure). We establish several comparison principle but it is sometimes too weak to guarantee the uniqueness of a solution.

A level set approach for graphs is very natural. However, without a suitable definition of a solution this approach also includes an overturned solution. We introduce a suitable definition of solutions for level set equations so that it is globally and uniquely solvable. The nonuniqueness question corresponds the fattening phenomena. So for a generic initial data our original problem is uniquely solvable.

Some part of this work is a joint work with Moto-Hiko Sato of the Muroran Institute of Technology at Muroran, Hokkaido.

Numerical Methods for the Solution of a System of Eikonal Equations with Dirichlet Boundary Conditions

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In this presentation, we discuss the numerical solution of a system of Eikonal equations with Dirichlet boundary conditions. Since the problem under consideration has infinitely many solutions, we look for those solutions which are nonnegative and of maximal (or nearly maximal) L^1 -norm. The computational methodology combines penalty, biharmonic regularization, operator splitting, and finite element approximations. Its practical implementation requires essentially the solution of cubic equations in one variable and of discrete linear elliptic problems of the Poisson and Helmholtz type. As expected, when the spatial domain is a square whose sides are parallel to the coordinate axes, and when the Dirichlet data vanishes at the boundary, the computed solutions show a fractal behavior near the boundary, and particularly, close to the corners.

On the Engquist Majda Absorbing Boundary Conditions for Hyperbolic Systems

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In their classical paper [1], the authors presented a methodology for the derivation of far field boundary conditions for the absorption of waves that are almost perpendicular to the boundary. In this paper we derive a general order absorbing boundary conditions of the type suggested by Engquist and Majda. The derivation utilizes a different methodology which is more general and simpler. This methodology is applied to the two and three dimensional wave equation, to the three dimensional Maxwell's equations and to the equations of advective acoustics in two dimensions.

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Floating Particles

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We consider the problem of self-assembly due to capillarity of small heavier- and lighter-than fluid particles floating on a free surface. Problems of self-assembly, symmetry breaking dynamics and anti-diffusion of uniform dispersions in thin films rimming a rotating cylinder are discussed. Some results of direct numerical simulation of the motions of floating particles (Singh and Joseph 2002) based on the method of Lagrange multipliers (DLM) for the solids and level set methods for the free surface, all on fixed grids, are presented.

Multi-Energy Levels and Time Scales for Coupled Schrodinger Dynamics

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We consider coupled nonlinear Schrodinger equations model the Bose-Einstein condensates with multiple hyperfine spin states. Even in the simplest cases, both vortices and domain walls may arise. They could be energetically and dynamically stable. Due multi-levels of Hamiltonian energy involved, there are different time scales in these nonlinear schrodinger flows. They provide challenging issues for analysis and, they may be also interesting from numerical and computational point of views.

A Mathematician's Perspective on Molecular Biology

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Coming from the field of applied mathematics, I have spent the past two years working on molecular biology, with the ultimate goal of merging mathematical and molecular techniques to create new tools for investigating biological processes at the "genomic" scale. In this talk, I will briefly summarize the present state of genomics (in language a mathematician can understand), and then attempt to answer the frequently asked question "where's the math?". Towards this end, I will present my "insiders" perspective on the role of mathematics in molecular biology, and illustrate it with examples drawn from the history of molecular biology and from my own current research projects.

Image Inpainting and Camouflage: Do Not Believe What You See

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Inpainting is the art of modifying an image in a form that is not detectable to an ordinary observer. The applications of this are numerous, from special effects in movies to wireless image transmission. In this talk we will describe novel algorithms for image inpainting that we have been developing in the last few years. The algorithms are based on partial differential equations such as those used to model fluids. We will also show the connections of our algorithms with biological processes.

Some Low Order Quadrilateral Reissner-Mindlin Plate Elements

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In this talk, we give an overview for recent development of some low order quadrilateral Reissner-Mindlin plate elements. General design guidelines for such elements are supplied. Error estimates for all these methods are reviewed. The main technical ingredients for performing error analysis are clarified and underpinned. In particular, the interplay of the accuracy and the mesh distortion are carefully studied.

hp-Adaptive Finite Element Approximation of Partial Differential Equations with Nonnegative Characteristic Form

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We present an overview of recent developments concerning the a posteriori error analysis of hp-version finite element approximations to hyperbolic problems and second-order partial differential equations with degenerate second-order terms. After highlighting some of the conceptual difficulties in error control for hyperbolic problems, such as the lack of correlation between the local error and the local finite element residual, we concentrate on a specific discretisation: the hp-version of the discontinuous Galerkin finite element method. The method is capable of exploiting both local polynomial-degree-variation (p-refinement) and local mesh subdivision (h-refinement), thereby offering greater flexibility and efficiency than numerical techniques which only incorporate h-refinement or p-refinement in isolation. The decision as to whether to h-refine or p-refine is based on a new algorithm for Sobolev-index estimation via truncated Legendre series expansions.

We shall be particularly concerned with the derivation of a posteriori bounds on the error in output functionals of the solution for partial differential equations with nonnegative characteristic form; relevant examples include the lift and drag coefficients for a body immersed into an inviscid fluid, the local mean value of the field, or its flux through the sections of the boundary of the computational domain.

The theoretical results will be illustrated by numerical experiments.

The talk is based on joint work with Paul Houston, University of Leicester, UK.

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Technical reports are available from:

<http://web.comlab.ox.ac.uk/oucl/work/andre.suli/biblio.html>

Stochastic Differential Equations for Driven Lattice Systems

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Exact Langevin equations for the fluctuations in the occupation numbers of driven lattice models are derived from their master equations. The asymptotic equivalence of the Langevin description and the lattice models is demonstrated by direct comparison with kinetic Monte Carlo simulations. The passage to the continuum limit is then considered for models with analytic and with non-analytic transition rules. As an example of the first case, we show how the stochastic equation of motion for the asymmetric exclusion process yields Burgers' equation in the continuum limit. For the second case, we consider a model of deposition with local relaxation based on height minimization and obtain the Edwards-Wilkinson stochastic differential equation in the continuum limit. We conclude with a discussion about the extension of our approach to other types of lattice models.

Shock Wave for Supersonic Flow Past a Perturbed Cone

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In this talk I will present some results on the global existence of shock wave solutions to the 3-D supersonic flow past a curved cone. This is a fundamental problem in gas dynamics and serves as a basic model in the theory of shock waves in multi-dimensional space. We first treat the case that the flow is stationary and past an infinite curved and symmetric cone. In this case, the flow is governed by the potential equations as well as the boundary conditions on the shock and the surface of the body. It is shown that the solutions to this problem exists globally in the whole space with a pointed shock attached at the top of the cone and tends to a self-similar solution under suitable conditions. For a general perturbed cone, a local existence theory for both steady and unsteady is also established. I will discuss a new method based on a global weighted energy estimate proposed in this work.

Universal Solver CIP for All Phases of Matter

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We present a review of the CIP method that is known as a general numerical solver for solid, liquid, gas and plasmas. This method is a kind of semi-Lagrangian scheme and has been extended to treat incompressible flow in the framework of compressible fluid. Since it uses primitive Euler representation, it is suitable for multi-phase analysis. The recent version of this method guarantees the exact mass conservation even in the framework of semi-Lagrangian scheme. Comprehensive review is given for the strategy of the CIP method that has a compact support and subcell resolution including front capturing algorithm with functional transformation, pressure-based algorithm.

Contributed talks

Zooming into an Image with ENO Interpolation

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Image interpolation is frequently performed by simple techniques, such as data-independent bilinear and cubic interpolation, or zero padding in the frequency domain. While there are inherent advantages in using linear methods, they are easy to analyze and lead to fast and efficient algorithms, in many occasions the quality of the zoomed images obtained with linear (i.e. data independent) techniques can be quite unsatisfactory.

Applying a data-independent interpolatory technique is, in a certain way, equivalent to assuming that the data available is low pass and that the high pass data is zero. However, real life images cannot be considered low pass, in fact, the 'edges' in an image, i.e. the places where there is an abrupt change in luminosity in the image, can only be enhanced if some kind of 'high pass' information is taken into account.

To zoom into an image while avoiding at the same time the blurring effects observed in linear techniques, one can use data-dependent, hence nonlinear, algorithms.

In recent years, adaptive interpolation algorithms have been developed to incorporate properties of the human visual system. The goal of these methods is to extract certain local characteristics from the pixel neighborhood and interpolate missing pixels in a fashion that seems better suited for human perception than simple linear filtering.

In this paper we propose to enlarge an image using a particular type of nonlinear techniques. The basic filters will be obtained via an interpolatory procedure, however the type of interpolation used will be data-dependent: In smooth regions we use filters that come from linear average interpolants, while close to an edge we shall construct the filter by interpolating using only data that on one side of the edge, that is, crossing 'jumps' on the image data is avoided.

Adaptive Mesh Redistribution Method in Hyperbolic Problems of Gas Dynamics

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It is well known that if the solution of flow equations has regions of high spatial activity, a standard fixed mesh technique is ineffective, since it should contain a very large number of mesh points. In case of hyperbolic problems of gas dynamics it is domains containing shock waves, contact discontinuities, detonation waves. A moving mesh adaptation algorithm can be applied to reduce computational costs in practical modeling. In such an approach the grid nodes are relocated so that to increase mesh concentration in the domains of steep moving wave fronts.

Coupled algorithm of using the Godunov's type solver and adaptive moving mesh has been offered in [1, 2, 3]. In this approach after every mesh iteration the finite-volume flow solver updates the flow parameters at the new time level directly on the curvilinear moving grid without interpolation from one mesh to another [3, 4]. Thus, we eliminate the errors caused by interpolation procedure which smears the discontinuities. This scheme on one hand utilizes the idea of the Godunov's scheme on the deforming meshes [5] and on the other hand is of the second-order accuracy in time and space.

Method of adaptive grid generation has been suggested in [6] and it is based on the theory of harmonic maps. Method is variational, i.e. we consider the problem of minimizing a finite-difference function approximating the Dirichlet's functional written for surfaces. The discrete functional has an infinite barrier at the boundary of the set of grids with all convex quadrilateral cells and this guarantees unfolded grid generation during computations both in any simply connected, including nonconvex, and multiply connected 2D domains. This folding-resistant property is very important since if any of the cells becomes folded we have to stop calculation of the flow problem and use special procedures to continue modeling. The barrier property is also of particularly importance in the vicinity of shock waves where the cells are very narrow and maximal aspect ratio achieves 50 and larger [7].

When modeling 2D hyperbolic problems with discontinuous solution on the moving adaptive mesh it is possible to reduce the errors, caused by shocks smearing over the cells, by many factors of ten and, therefore, to decrease significantly, by several times [7], the overall error.

We present examples of modeling 2D gas flows in ideal approach having complicated wave structures and flow with combustion process when the detonation wave arises.

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High-Order Semi-Discrete Central-Upwind Schemes for Multi-Dimensional Hamilton-Jacobi Equations

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We present high-order semi-discrete central-upwind numerical schemes for approximating solutions of multi-dimensional Hamilton-Jacobi (HJ) equations of the form

$$\frac{\partial}{\partial t}\phi(x, t) + H\left(\frac{\partial}{\partial x}\phi(x, t), x\right) = 0, \quad x \in R^N.$$

This scheme is based the use of fifth-order central interpolants, like those developed in [1]. in fluxes presented in [3]. These interpolants use the weighted essentially non-oscillatory (WENO) approach to avoid spurious oscillations near singularities, and become "central-upwind" in the semi-discrete limit. This scheme provides numerical approximations whose error is as much as an order of magnitude smaller than those in previous WENO-based fifth-order methods [2, 1]. These results are discussed via examples in one, two and three dimensions. We also present explicit N -dimensional formulas for the fluxes, provide a proof that these fluxes are monotone and discuss the connection between this method and that in [2].

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How Accurate can we Compute the Length of Level Curves?

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The computation of the length of a curve *via* a parametrization is a classical geometrical problem, (Lagrangian). From an Eulerian point of view, however, we have a fixed grid and it is desirable to evaluate both the curve and its important geometrical quantities (area inclosed, normal vectors, curvature, ...) by using that same fixed grid. Thus, level set methods work in this context, and an alternate formulation for the evaluation of these variables is needed. This alternate formulation, sometimes, is not only advantageous, but

necessary. Lagrangian parametrization is very restrictive and it assumes the curves do not have essential morphological changes.

The formula for the length of a level curve in terms of a level set function, (implicit function), lacks of accurate numerical methods for its evaluation, as opposed to the parametrized version (Lagrangian), though it keeps the usual advantages of the level set methods (see [3]).

In this presentation, we introduce different discretizations of the Eulerian length formulas in order to analyze how accurate we can evaluate the length of level curves, in the presence of kinks and multiple connected components.

These algorithms will be tested in different well known curves, and we shall use them to measure the evolution of the interfaces of different physical states by translations, rotations or other, more complex, transformations.

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On the Simplified Keller-Segel System Modelling Chemotaxis²

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In this paper we study the global in-time and blow-up solutions for the simplified Keller-Segel system modelling chemotaxis, which actually is the initial-boundary problem of the following parabolic-elliptic system:

$$(P) \quad \begin{cases} \frac{\partial u}{\partial t} = \nabla \cdot (\nabla u - \chi u \nabla v), & x \in \Omega, t > 0, \\ 0 = \Delta v - \gamma v - \beta |v|^{p-1} v + \alpha u, & x \in \Omega, t > 0, \\ \frac{\partial u}{\partial n} = \frac{\partial v}{\partial n} = 0, & x \in \partial\Omega, t > 0, \\ u(x, 0) = u_0(x), & x \in \Omega. \end{cases}$$

where χ, α, β and γ are positive constants, $p > 1$, Ω is a bounded smooth domain in \mathbf{R}^N , n denotes the unit outward normal vector of $\partial\Omega$. For the initial function u_0 we suppose that

(i) $u_0 \geq 0$ and u_0 is not identical to 0 in Ω ,

(ii) u_0 is smooth on $\overline{\Omega}$.

²Research supported by the NSFC and the 973 Key Project of the MOSTC.

We prove that there is a critical number which determines the occurrence of the solution to be blow-up in two dimensional case for $1 < p < 2$. In three or higher dimensional cases, we show that the radial symmetrical solution may blow up if $1 < p \leq \frac{N}{N-2}$ ($N \geq 3$) for the problem with nonnegative initial value.

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Acceleration Methods for Total Variation-based Image Restoration

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In this paper, we apply a fixed point method to solve the total variation-based image restoration problem. An algebraic multigrid method is used to solve the corresponding linear equations. Krylov subspace acceleration is adopted to improve convergence in the fixed point iteration. A good initial guess for this outer iteration at finest grid is obtained by combining fixed point iteration and geometric multigrid interpolation successively from the coarsest grid to the finest grid. Numerical experiments demonstrate that this method is efficient and robust.

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Spectral Convergence of Mapped Chebyshev Methods

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Classical Chebyshev collocation methods are often used in the solutions of PDE of diverse fields such as but not limited to the Euler equations of the gas dynamics. The methods yield very high rate of convergence for sufficiently smooth solutions and is well known as spectral accuracy. For large number of grid points $N \gg 32$, the differentiation operator of the methods D has large roundoff error that grows in the order of N^2 . Furthermore, for the explicit time stepping scheme, the CFL is often very restrictive and Δt is bounded by $O(N^{-2})$.

The source of such restrictive time steps are credited to the agglomeration of the Chebyshev points near the boundaries, yielding a minimal grid spacing of order $\Delta x_{\min} = O(N^{-2})$. It is reasonable to argue that smaller grid spacing allows higher wavenumbers and, therefore, faster dynamics, requiring shorter time steps.

Kosloff and Tal-Ezer have addressed this issue and proposed to map the Chebyshev points to a new set of collocation points with a greater minimal grid spacing in order to alleviate the time step restriction. The mapping is given in the form of $x = \arcsin(\alpha\xi)/\arcsin(\alpha)$, where $\alpha \in (0, 1)$ is a parameter determining the strength of the endpoints separation.

On their seminal work, they claimed the mapping reduces the spectral radius of the derivative operator D from $O(N^2)$ to $O(N)$, therefore, increasing the allowed time step from $O(N^{-2})$ to $O(N^{-1})$ for hyperbolic problems and from $O(N^{-4})$ to $O(N^{-2})$ for parabolic ones. The mapping stretches the grid spacing on the boundary pushing the points to the center of the domain, generating a quasi-uniform grid. While many good properties arise from this new distribution of points, as a smaller roundoff error and a better resolution for higher modes, the map has singularities at $y = \pm \frac{1}{\alpha}$, which incurs in some approximation error. A way of choosing the parameter α in order to avoid the influence of the map singularity in the numerical scheme was proposed and confirmed numerically.

This new distributions of points given above has distinct resolution properties than the classical Chebyshev points. A conjecture about the resolution power of the new set of points was stated in their paper with regards to the choice of the parameter α , in order to obtain better accuracy for higher wavenumbers. However, only heuristically results and arguments were obtained.

Another important issue related to the above mapping is maintenance of the spectral convergence of the Chebyshev method. Despite claimed the loss of spectral convergence by some works, spectral convergence of the mapped method has been analytically studied and interpolation error estimates have been obtained by Abril-Raimundo et al.

In this talk, we provide an analytical proof for the conjecture about the resolution power by means of the stationary phase method. We also will present a much simpler proof of the spectral convergence of the mapped Chebyshev methods, not involving error estimates, but enhancing the necessary geometrical aspects for keeping spectral convergence. In this way, the techniques can be naturally generalized to include other mappings of the Chebyshev points.

Shock-Vortex Interaction at High Mach Numbers

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We perform a computational study of the interaction of a planar shock wave with a cylindrical vortex. We use a particularly robust High Resolution Shock Capturing scheme, Marquina's scheme, to obtain high quality, high resolution numerical simulations of the interaction. In the case of a very-strong shock/vortex encounter, we observe a severe reorganization of the flow field in the downstream region, which seems to be due mainly to the strength of the shock. The numerical data is analyzed to study the driving mechanisms for the production of vorticity in the interaction.

Trigonometric Spectral Methods on Lattices

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Trigonometric spectral methods can be very accurate for solving periodic problems on rectangular domains. They obtain their answers by sampling the input function on a grid. This article shows how spectral methods can be extended to the situation where the input function is sampled on the nodeset of an integration lattice, a generalization of a grid. The error analysis is derived for a general approximation problem. Numerical examples illustrate how spectral methods on lattices can give higher accuracy than spectral methods on grids.

Motion of Liquid Drops on a Solid Surface

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Inside a proton-exchange-membrane fuel cell, condensation of water vapor may occur and subsequent removal of liquid drops is of primary interest. In this talk, we will discuss the motion of a liquid drop on a solid surface driven by gas flows. In particular, we will discuss the behaviour of the liquid-gas-solid three-phase contact point and related modeling issues. We first outline a front-tracking approach for computing the motion of a two-dimensional drop, based on Peskin's immersed boundary method. For thin liquid drops, we will re-formulate the problem using lubrication theory and some discussions will be given for including the effect of surface property and condensation. Numerical results will also be presented.

Atomistic-Continuum Method for the Simulation of Crystalline Materials

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Traditionally two apparently separate approaches have been used to model a continuous medium. The first is the continuum theory, in the form of partial differential equations describing the conservation laws and constitutive relations. This approach has been impressively successful in a number of areas such as solid and fluid mechanics. It is very efficient, simple and often involves very few material parameters. But it becomes inaccurate for problems in which the detailed atomistic processes affect the macroscopic behavior of the medium, or when the scale of the medium is small enough that the continuum approximation becomes questionable. Such situations are often found in studies of properties and defects of micro- or nano- systems and devices. The second approach is atomistic, aiming at finding the detailed behavior of each individual atom using molecular dynamics or quantum mechanics. This approach can in principle accurately model the underlying physical processes. But it is often times prohibitively expensive.

Recently an alternative approach has been explored that couples the atomistic and continuum approaches [1-7]. The main idea is to use atomistic modeling at places where the displacement field varies on an atomic scale, and the continuum approach elsewhere. The most successful and best-known implementation is the quasi-continuum method [1-2] which combines the adaptive finite element procedure with an atomistic evaluation of the potential energy of the system. This method has been applied to a number of examples [8-10], and interesting details were learned about the structure of crystal defects.

Extension of the quasi-continuum method to dynamic problems has not been straightforward [5-7]. The main difficulty lies in the proper matching between the atomistic and continuum regions. Since the details of the lattice vibrations, the phonons, which are an intrinsic part of the atomistic model, cannot be represented at the continuum level, conditions must be met that the phonons are not reflected at the atomistic-continuum interface. Since the atomistic region is expected to be a very small part of the computational domain, violation of this condition quickly leads to local heating of the atomistic region and destroys the simulation. In addition, the matching between the atomistic-continuum interface has to guarantee that large scale information is accurately transmitted in both directions.

The main purpose of the present talk is to introduce a new class of matching conditions between atomistic and continuum regions. These matching conditions have the property that they allow accurate passage of large scale (scales that are represented by the continuum model) information between the atomistic and continuum regions and no reflection of phonon energy to the atomistic region. These conditions can also be used in pure molecular dynamics simulations as the border conditions to ensure no reflection of phonons at the boundary of the simulation. As applications, we use our method to study the dynamics of dislocations in the Frenkel-Kontorova model, friction between crystal surfaces and crack propagation.

Joint work with Prof. Weinan E.

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Chebyshev Spectral Methods on Lattices

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Integration lattices have been used for many years for multidimensional integration. They are best applied to periodic functions with sufficient smoothness. For non-periodic integrands, periodization is usually forced. This article shows how one can use the Chebyshev expansion to take advantage of the smoothness of nonperiodic integrands. The error analysis shows how to choose good integration lattices for a class of smooth integrands. Numerical experiments illustrate how this method gives high convergence results.

An Adaptive Moving Mesh Algorithm for Finite Elements

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In this talk we will describe a moving grid method for generating finite element grids (meshes). This method is an extension of the deformation method that has its origin in differential geometry. Instead of forming the node velocity vector through a Poisson equation, we now obtain the velocity vector directly from a div-curl system, which is solved by a least square finite element method. Theoretical derivation shows that the Jacobian determinant of the grid mapping is equal to the (positive) monitor function, and thus, the grid will not tangle. In practice, the method should be combined with coarsening and refining steps to reduce excessive skewness if necessary. Numerical examples on triangular elements will be presented.

Revisit Convex ENO Schemes

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We study high-order convex ENO schemes for hyperbolic conservation laws and Hamilton-Jacobi equations.

This is a joint work with Xu-Dong Liu.

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Energy and Helicity Preserving Scheme

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We study the incompressible fluid equations with coordinate symmetry. With these symmetry, the flow reduces essentially to 2D problems. The incompressibility constraint is realized by introducing a generalized vorticity-stream formulation.

Moreover, with proper discretization of the nonlinear terms, we give a class of finite difference schemes that preserve both energy and helicity identities numerically. This is achieved by rewriting the non-linear terms (convection, vorticity stretching/geometric source, Lorentz force and electro-motive force) in terms of a Jacobian. Associated with these Jacobian $J(f, g)$, we introduce a permutation-triple $T(f, g, h)$ which satisfies certain permutation identities. These identities lead naturally to the conservation laws (all the first and quadratic moments including energy and helicity) in Navier Stokes equation and MHD. We then introduce the discretization of the nonlinear terms in various numerical schemes (finite difference, finite element, and spectral methods) that preserve these permutation identities and hence ensure that the solutions satisfy the physical conservation laws. This conservative property even holds true in the presence of the pole singularity for axisymmetric flows. Local mesh refinement near the boundary can also be easily adapted in this setting without extra cost.

A Numerical Method for Solving Variable Coefficient Elliptic Equation with Interfaces

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A new 2nd order accurate numerical method is proposed for solving the variable coefficient elliptic equation in the presence of interfaces where the variable coefficients, the source term, and hence the solution itself and its derivatives may be discontinuous. Jump conditions at interface are prescribed. The boundary and the interface are only required to be Lipschitz continuous instead of smooth, and the interface is allowed to intersect with the boundary. The method is derived from a weak formulation of the variable coefficient elliptic equation. Numerical experiments show that the method is 2nd order accurate in L^∞ norm.

Noise Removal Using Fourth-Order Partial Differential Equations with Applications to Medical Magnetic Resonance Images in Space and Time

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In this paper we introduce a new method for image smoothing based on a fourth order PDE model. The method is tested on a broad range of medical magnetic resonance images, both in space and time, as well as on non-medical test images. Our algorithm demonstrates good noise suppression with preservation of edges and contours and without destruction of important anatomical or functional detail, even at poor signal-to-noise ratios. We have also compared our method with a related second-order PDE model and find our method to perform overall better on the images being tested.

Towards Front-Tracking Based on Conservation in Two Space Dimensions, Tracking Fronts on Cartesian Grid

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The main feature that distinguishes front-tracking methods from capturing methods is that discontinuities in front-tracking are treated as interior moving boundaries. Near the boundaries the solution is computed using schemes which simulates the boundary conditions, and away from the boundaries the solution is computed using schemes designed for smooth solution. Traditional front-tracking methods always uses lower dimensional grids, call fronts, to fit the moving boundaries; thus, the overall grid is adaptive. In two space dimensions, if the underlying grid is Cartesian, then away from the fronts the grid cells are rectangular, and near the fronts they are either triangular, trapezoidal, or pentagonal. Physical states, either pointwise values or cell-averages, are defined and computed on both regular and irregular grid cells. As working in this way, traditional front-tracking methods have, besides its obvious merit of high accuracy, the following drawbacks: 1) Algorithms are usually complex and hard to code, and an all-purposed algorithm is almost impossible. 2) So-called ‘Small-cell’ problem always troubles the methods, and often a great deal of algorithm is spent on dealing with this problem. Especially, when several fronts are close to each other, the situation will be even worse. 3) When apply the methods to the conservation laws, it is hard to maintain the conservation for the algorithm.

For many years, the author has been developing a new front tracking method for conservation laws in two space dimensions (see [1]). An important feature of the method is

that it does not use lower dimensional grids to fit the tracked discontinuities; the algorithm works just on Cartesian grid. The idea is as follows: As is well known, the movement of discontinuities can be described by certain evolution partial differential equation in a lower dimensional space. For examples, the movement of shocks, contact discontinuities and slip lines in 2D Euler equations can be described by the 2D Hugoniot conditions, which can be written as a PDE with t as the evolution variable and either with x an independent and y the dependent variable, i.e. the discontinuity positions, or vice versa. What we found is that by introducing ‘ghost’ physical states this PDE of movement can be written in terms of real and ‘ghost’ physical states, instead of discontinuity positions. And also the discontinuity positions can be recovered from given real and ‘ghost’ states. Because this new form of PDE is in the terms of physical states and in conservation form, it can be discretized on the Cartesian grid and the obtained difference scheme can be incorporated to the underlying scheme that computes the smooth solution. Once the real and ‘ghost’ states are computed, the numerical discontinuity positions can then be recovered from them. In doing this way, the above mentioned 2nd and 3rd drawbacks for traditional front-tracking methods are got rid off and the 1st one is eased. Numerical examples are presented to show the efficiency of the method.

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Capturing Material Interfaces with High Order Conservative Methods

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In this paper we consider a conservative model based on a level set equation introduced by Mulder, Osher and Sethian in [3], coupled to the Euler equations for gas dynamics to describe a two-component compressible flow in cartesian coordinates. It is well-known that classical shock-capturing schemes applied to conservative models are oscillatory near the interface between the two gases. Several authors have addressed this problem proposing either a primitive nonconservative algorithm, (Karni, [2]) or Lagrangian ingredients, (Ghost Fluid Method by Fedkiw, Aslam, Merriman and Osher, ([4])). We solve directly the conservative model by reformulating a flux-split algorithm, due to the first author, (see Donat and Marquina, [1]). We present various 1D numerical tests, showing the robustness and the accuracy of the algorithm. We compute different kind of waves generated from the shock-contact problems, for specific material interfaces. As the main application, we address a 2D simulation of the Richtmyer-Meshkov instability generated by a shock wave impinging a Helium-Air interface in mechanical and thermodynamical equilibrium. We will also study the shock-bubble interaction of a Helium cylindrical bubble in air with a Mach 1.22 shock wave, originally studied by Haas and Sturtevant, ([5]), and addressed by Quirk and Karni in ([6]), from the computational point of view by using a primitive nonconservative second order algorithm. We compare our numerical results with the Haas-Sturtevant experimental data, and getting good agreement with the Haas-Sturtevant data

for a simulation performed with our flux-split algorithm together with the WENO5 spatial reconstruction and the third-order accurate Runge-Kutta integration in time, due to Shu and Osher, see ([7]).

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Numerical Solution of Hyperbolic Partial Differential Equation Type Using Excel

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The paper shows that how powerful of Excel Spreadsheet in solving mathematical problems numerically. The numerical solution of an initial value problem with boundary conditions of hyperbolic partial differential equation type with an example using Excel is given, and the effect of changing the parameters of the equation is treated.

A Shock Instability Free FDS Scheme Based on Rotated Riemann Solvers

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This paper presents a robust flux-difference splitting scheme based on the rotated approximate Riemann solver. A general framework for constructing the rotated Riemann solver is described and a rotated Roe scheme is discussed in detail. It is found that the robustness of the rotated shock-capturing scheme is closely related to the way in which the direction of upwind differencing is determined. When the upwind direction is determined by the velocity-difference vector, the rotated Roe scheme demonstrates a robust shock-capturing capability and the shock instabilities (the odd-even decouplings and the carbuncle phenomena) can be eliminated completely. Several steady and unsteady test cases are presented to validate the proposed scheme.

Recent Advances in Strong-Stability-Preserving Runge-Kutta Methods

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It is common practice in solving time-dependent partial differential equations (PDEs) to first discretize the spatial variables to obtain a semi-discrete method of lines scheme. The subsequent ordinary differential equations can be discretized by an ODE solver. For problems with smooth solutions, a linear stability analysis is often adequate. For problems with nonsmooth solutions, however, such as solutions to hyperbolic conservation laws, a stronger measure of stability is often desired. In this talk we review and develop strong-stability-preserving high-order time discretizations for semi-discrete method of lines approximations of PDEs. We describe a new class of schemes that allows larger stable time step sizes and gives improved efficiency over methods currently available.

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Power ENO Methods: A Fifth Order Accurate Weighted Power ENO Method

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We introduce a new class of limiters used for second or higher order differences. We define new polynomial reconstruction procedures based on those limiters, following the original idea used before to design the ENO methods, introduced in [1]. We call those methods ‘Power ENO methods’, since the limiters are defined in terms of the exponent of a power, ([5]). The class of limiters includes as particular cases the minmod limiter of Van Leer and the harmonic limiter used for the PHM method, (see [3]). The main feature of this Power ENO methods is that improves the behavior near discontinuities, compared with the classical ENO methods. Indeed, the region of loss of accuracy near discontinuities is smaller than the one observed for the ENO methods. Previously, we used the harmonic limiter to design a fourth order accurate ENO method in [4], where the above feature was observed. We focus our attention here on a fifth order accurate weighted Power ENO method, constructed from a convex combination of three Power ENO parabolas, using a similar strategy than the one used by Jiang and Shu in [2], but with different optimal linear weights. The resulting method improves the behavior of the Jiang-Shu WENO5 near discontinuities.

Furthermore, we give analytical and numerical evidence of the good behavior of these methods used as reconstruction procedures for the numerical approximation by means of shock-capturing methods for scalar and systems of conservation laws in 1D and 2D in cartesian coordinates. We will present comparisons with PHM, ENO and WENO5 methods, (see [1], [6], [2]), discussing the advantages and disadvantages.

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Simulation of Fluid Interface Instability

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A new Ghost Fluid techniques is presented in this paper. When fluid field is multi-fluid, it is difficult to track the interface or capture it. Level Set method is used to capture the interface, and reinitialization skill is used to keep the level function keep distance function value. Three degree Runge-Kutta TVD time discretizing is used and five degree WENO scheme is used for space discretization, convex ENO scheme also used when we treat partial difference for special equation of states. As we know, any calculations will be asked for flux of points near interface. Physical quantities of other points across the interface will be used when we use numerical difference schemes. The Ghost Fluid method, suppose the total fluid field is the single fluid, so the numerical difference scheme can be used in whole fluid field, as if the interface does not exist. In Fedkiw's Ghost Fluid Method, pressure and normal velocity are copied from real physical quantities on Ghost point. This will not cause series problem when density of ratio of fluids is low, but when density of ratio of fluids is high, this will cause problem. A modification to the Ghost Fluid Method is presented in this paper, numerical simulation results support this modification.

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Advances in Snake Algorithms⁵

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Active contour model or Snake is a kind of image segmentation model which found wide applications including object recognition, computer vision, motion tracking, computer graphics and biomedical image processing. The original formulation involves the minimization problem

$$\min_{\nu(s)} = \int_{\Omega} \left(\frac{1}{2} (\alpha |\nu_s(s)|^2 + \beta |\nu_{ss}(s)|^2) - k_i |\nabla I(\nu)|^2 + E_{ext}(\nu(s)) \right) ds,$$

⁵This work was partially supported by a Hong Kong Baptist University faculty research grant: FRG/99-00/II-16

where $\nu_s(s)$ and $\nu_{ss}(s)$ represents the first and second order derivatives of the curve $\nu(s)$. By adjusting the weight of α and β , the relative importance of the corresponding terms, which represents internal tension forces and smoothness constraints, can be controlled; k_i adjusts the weight of the edge information as defined by the gradient term. $E_{ext}(\nu(s))$ is an optional external force supplied by the user for extra control.

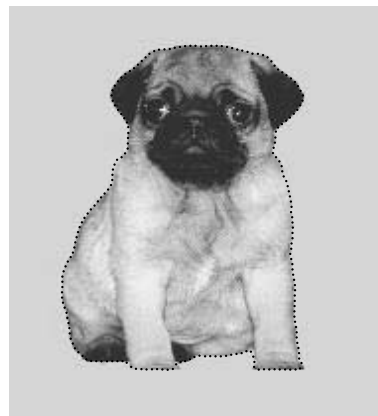
Although the original Snake algorithm is easy to implement and widely used, it suffers from the following limitations. Firstly, the solution of the algorithm is sensitive to the initial guess contour which is provided by the user and is usually required to be close to the object boundary. Secondly, the algorithm may easily overrun high curvature points like corners. Thirdly, the algorithm has difficulties to locate object boundary having non-convex regions. Lastly, the Snake curve can only move towards the object by shrinking, it cannot move towards the object by expansion. Although many attempts have been made to remedy such shortcomings, they are often rather complex and involve fine-tuning many additional parameters.

In this talk, we discuss new advances which modified the original Snake algorithm based on conformal mapping. The essential idea is to apply mapping so that the non-convex regions becomes convex in a transformed domain in which the original Snake algorithm can be used effectively. Experiments showed that our method is able to locate non-convex regions as well as irregular objects with sharp corners successfully. Also, we have established some mathematical analysis to this new approach. Based on this analysis, our method can be further enhanced as well as providing the user the ability to control the curve to move either by expansion or shrinkage. This provides a higher flexibility for the user of boundary detection.

The structure of our algorithm is quite similar to the original Snake algorithm. This makes the computational cost of our method almost the same as the original Snake algorithm. Thus our technique of integrating a conformal mapping to the snake algorithm has drastically improved its performance efficiently. Moreover, our approach can be easily combined with other Snake algorithms to exploit their respective advantages.



a. Original Snake



b. Our method

FIGURE 1. Contour detection results

Essentially Nonoscillatory Multigrid Time Stepping Schemes

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Efficient numerical solutions for convection dominated problems have been an active research area in the field of iterative methods. The discretization matrices arisen are generally nonsymmetric. While multigrid methods have been widely used as fast solvers for diffusion dominated problems, one cannot simply apply the same techniques for convection dominated problems since the hyperbolic nature of the equations exhibit completely different characteristics. In the numerical solution of hyperbolic equations, the concept of total variation (TVD) has been playing an important role in the design of nonoscillatory schemes. However, it has not been exploited much in the context of multigrid. In this talk, we propose new multigrid algorithms which preserve monotonicity and are TVD.

We consider the steady state solution of the model equation:

$$\begin{aligned} -\epsilon \Delta u + a(x, y) u_x + b(x, y) u_y &= f && \text{in } \Omega \\ \alpha u + \beta \frac{\partial u}{\partial n} &= g && \text{on } \partial\Omega, \end{aligned}$$

where ϵ is a small diffusion parameter, the vector (a, b) represents the convection velocity, and α, β determine the inflow and outflow boundary conditions. The algorithms and analysis presented will be mainly in 1D and 2D, but extension to 3D is possible in most cases. We are interested in the convection dominated limit where $\epsilon \rightarrow 0$. In this case, standard relaxation methods may no longer smooth the high frequency errors, and more importantly, the coarse grid correction process may lead to oscillatory numerical errors if the solutions contain discontinuities common in shock problems which deteriorate convergence rate.

There are generally two approaches proposed in the literature for convection dominated problems. One approach is based on Gauss-Seidel smoothing with downwind ordering of unknowns, followed by an exact coarse grid solve as in standard multigrid. While effective in model 2D problems, tracking of flow directions, especially in 3D and systems of PDEs, can be complicated. Another approach is based on Runge-Kutta smoothing, followed by an inexact coarse grid solve done by a few smoothing steps. The idea is to propagate the error out of the domain boundary faster by using multiple coarse grids. While effective for entering flows, it can be slow for recirculating flows since errors keep recirculating in the domain.

Ultimately, one must understand the propagation property of multigrid. Using the framework of phase velocity analysis on the multigrid iteration matrix by a recent collaboration work with Tony Chan, we find that wave propagation approach is highly dispersive; the oscillations generated slow down convergence. Secondly, coarse grid correction using direct discretization as coarse grid operator and exact coarse grid solve has a constant phase error independent of mesh size which again leads to oscillations. Thirdly, coarse grid correction using Galerkin coarse grid operator essentially has no phase shift error and the coarse grid correction is third order accurate which yields fast convergence.

The phase velocity framework lays the foundation of new designs of multigrid methods for convection dominated problems. In particular, one must avoid numerical oscillations due to either dispersion or phase error. We will propose new multigrid time-stepping schemes which attempt to preserve monotonicity and in some cases, the total variation diminishing property for linear and nonlinear wave equations. In either case, the methods are nonoscillatory. The idea is to construct matrix-dependent interpolation and restriction, and to use a novel nonstandard coarse grid correction update formula. We prove that the proposed multilevel methods preserve monotonicity and are TVD in 1D. As a result, one step convergence for linear problems can be obtained if sufficiently many levels are used. We have also generalized the algorithms to nonlinear problems by constructing a nonlinear interpolation operator using local Riemann solvers.

The same principle can be applied to higher dimensions. However, pathological cases exist if standard coarsening is used. We will use multiple coarsening to overcome this difficulty. Numerical results in one and two dimensions for linear and nonlinear problems show that the convergence rate is independent of mesh size; furthermore, the convergence improves with increasing number of coarse grid levels.

Quasineutral Limit of Euler-Poisson System with and without Viscosity

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The quasineutral limit of Euler-Poisson system with and without viscosity in plasma physics in the torus \mathbb{T}^d is studied. That Quasineutral regimes are the incompressible Euler or Navier-Stokes equations is proven. In the mean time, long-time existence for large amplitude smooth solutions of Euler-Poisson system in torus $\mathbb{T}^d, d \geq 1$, with or without viscosity as the Debye length $\lambda \rightarrow 0$ is also obtained provided that the smooth solution of incompressible Euler or Navier-Stokes equations exists globally for nearby initial data. In particular, global existence of large amplitude smooth solutions of Euler-Poisson system in torus \mathbb{T}^2 with or without viscosity and with small Debye length is obtained. The proof of these results is based on a straightforward extension of the classical energy method, the modulated energy method, the iteration techniques and the standard compactness argument.

⁶Supported by the National Youth Natural Science Foundation (Grant No. 10001034) of China and the FWF-Projekt "14876-MAT" "Fokker Planck and Mittlere-Feld-Gleichungen" (Austria). I would like to thank Professors E. Feireisl, L. Hsiao, P. A. Markowich and Z. P. Xin for many useful discussions, with especial thanks to Prof. Xin for first introducing me this problem when I visited Institute of Mathematical Sciences, The Chinese University of Hong Kong. I also wish to express my gratitude to Professor P. A. Markowich. Without his help and friendly advice, this work would not have been possible.

A Jump Condition Capturing Scheme for Elliptic Interface Problems

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We propose a simple finite difference scheme for the elliptic interface problem with discontinuous diffusion coefficient using a body fitting curvilinear coordinate system. The resulting matrix is symmetric and positive definite and hence standard techniques can be applied in accelerating the inversion of the matrix. The main advantage of the schemes is its simplicity. It is a genuine finite difference scheme in the sense that the coefficient of the matrix are simply the centered difference 2nd order approximation of the metric tensor $g^{\alpha\beta}$. In addition, the interface jump conditions are naturally built into the elliptic operator. By patching local coordinate systems together, the scheme can also handle corner singularities of the interface. No interpolation/extrapolation process is involved in the derivation of the scheme. Both the solution and the flux are observed to have second order accuracy.

On Moving Contact Line Hydrodynamics of Immiscible Fluid

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Immiscible two-phase flow in the vicinity of the contact line (CL), where the fluid-fluid interface intersects the solid wall, is a classical problem that falls beyond the framework of conventional hydrodynamics. In particular, molecular dynamics (MD) studies have shown relative slipping between the fluids and the wall, in violation of the no-slip boundary condition. While there have been numerous ad-hoc models to address this phenomenon, none has been able to give a quantitative account of the MD slip velocity profile in the molecular-scale vicinity of the CL. We give a continuum formulation of the immiscible flow hydrodynamics, comprising the generalized Navier boundary condition, the Navier-Stokes equation, and the Cahn-Hilliard interfacial free energy. Numerical simulation of our hydrodynamic model yields near-complete slip of the contact line, with interfacial and velocity profiles matching quantitatively with those from the molecular dynamics simulations. This is a joint work with T.Z. Qian and P. Sheng.

A Local Spectral Method for Scientific Computing

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There has been an ongoing interest in computational methodology by numerous researchers in every field of science and engineering. Most effort has been centered in developing either global methods or local methods for solving a variety of problems. Global methods, such as Fourier or Chebyshev spectral methods, are usually highly accurate. But local methods, such as finite element and finite difference methods, are much more flexible for handling complex boundaries and geometries. We introduce a local spectral method, i.e., discrete singular convolution, (DSC) for achieving global methods' accuracy and local methods' flexibility in solving problems with complex boundaries and geometries. The mathematical foundation of the proposed method is the theory of distributions. Example applications are discussed to fluid dynamics, electromagnetics, solid mechanics and nonlinear waves.

Gas-kinetic Schemes for Fluid Simulations

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Firstly, we will introduce a gas-kinetic scheme based on the Boltzmann equation for the compressible Navier-Stokes equations. Due to the implementation of initial nonequilibrium state and the use of the BGK solution, the gas-kinetic scheme solves the Navier-Stokes equations accurately in a wide range of the ratio between the particle collision time and the numerical time step. The scheme has been successfully applied to the viscous compressible flow simulations. Many numerical examples will be presented. In order to extend the above scheme to the rarefied gas regime, based on the gas-kinetic equation we will generalize the constitutive relation between the viscosity coefficient and other macroscopic flow variables, such as the temperature. The generalized viscosity coefficient will depend not only on the local macroscopic variables, but also on their gradients. With the implementation of a generalized particle collision time, the gas-kinetic scheme is used for the shock structure calculations, and the numerical results are compared with the experiments.

Applications of Ghost Fluid Methods to Instabilities of Fluid Interfaces and Synthetic Jet

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The ghost fluid methods, developed by Fedkiv and Osher et al in 1998, is an efficient numerical method for simulating complex flow problems. In the present work, we apply it to simulate interface instabilities and synthetic jet problems. The interface instability is a well known problem in the complex flow simulation aspect. In our work, Richtmyer-Meshkov and Rayleigh-Taylor instability problems with various initial and boundary conditions have been considered. The simulation results show that the ghost fluid method is suitable to simulate interface instability problems. The synthetic jet problem is a very interesting phenomenon in the complex flow field, which does not generate from any source. So, it is called as zero mass jet yet. It has been verified through fluid experiments some years ago. But, numerical simulation results have not been found up to now. In the present work, we apply the ghost fluid method to simulate this problem and the numerical result is satisfied.

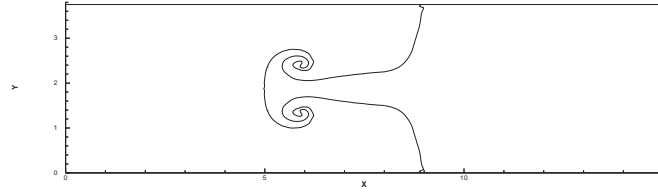


FIGURE 1. Richtmyer-Meshkov Instability with reflecting bottom boundary condition

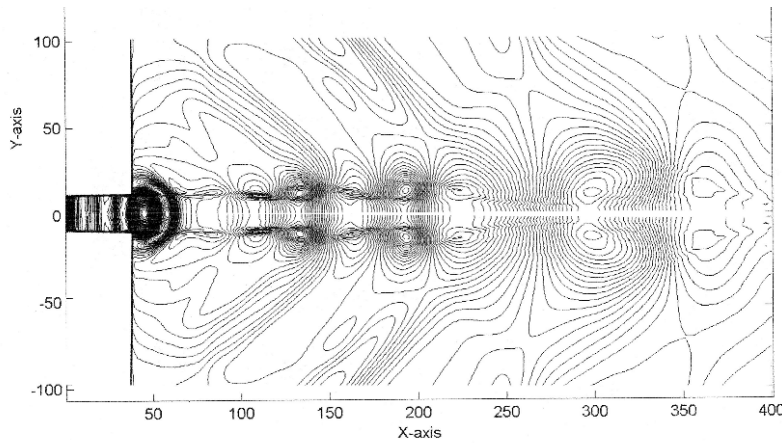


FIGURE 2. Zero mass jet problem, pressure contours

Co-authors with: Xiao Ming, Jiazun Dai, Jingui Lei and Yang Jiang

Some Iterative Solutions of Saddle-point and Saddle-point Like Systems⁷

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In this talk we shall discuss some recent developments in iterative solutions of saddle-point and saddle-point like systems, arising from the discretizations of Maxwell's equations, Navier-Stokes equations and optimizations.

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