Third China-Sweden Workshop on Computational Mathematics

June 10–12 2002

Göteborg Sweden

School of Mathematical Sciences
Chalmers University of Technology
and Göteborg University

VETENSKAPSRÅDET
THE SWEDISH RESEARCH COUNCIL

The Wenner-Gren Foundations

Stiftelsen för Vetenskaplig Forskning och Utbildning i Matematik

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Background

The purpose of the workshop is to bring together leading experts in related areas from Sweden and China to exchange recent advances and ideas, and to promote research and collaboration.

The First China-Sweden Workshop on Computational Mathematics, was held in October 13–15, 1997, at Institut Mittag-Leffler, Djursholm, Sweden. It was organized by the Swedish Science Research Council (NFR) within the bilateral agreement between NFR and the National Science Foundation of China.

The Second China-Sweden Workshop on Computational Mathematics, was held in January 10–12, 2000, at Hong Kong University of Science and Technology.

Scientific Committee

Björn Engquist, Royal Institute of Technology

Bertil Gustafsson, Uppsala University

Mo Mu, Hong Kong University of Science and Technology

Zhong-Ci Shi, Chinese Academy of Sciences

Vidar Thomée, Chalmers University of Technology

Organizing Committee

Stig Larsson, Chalmers University of Technology

Axel Ruhe, Royal Institute of Technology

Venue

The workshop will take place in the Mathematics Center at Chalmers University of Technology, street address Eklandagatan 86 and Gibraltargatan 25. All lectures will be in lecture room MD9. Breakfast and coffee will be served as a buffe in room 5259. Computers are available on the bottom floor of the Mathematics Center. Participants will stay in the hotel "SGS veckobostäder", street address Utlandagatan 24, a short walk east of the Mathematics Center.

Sponsors

The Swedish Research Council

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Program

Monday June 10

7:30–9:00	Breakfast
	Chairman: Vidar Thomée
9:15–9:55	Zhong-Ci Shi, “Nonconforming rotated Q_1 finite element and applications.”
	Coffee
10:15–10:55	Bertil Gustafsson, “High order difference methods for wave propagation problems.”
11:00–11:40	Grafton W. H. Hui, “The water level formulation for shallow-water flow with bottom topograph.”
	Lunch
	Chairman: Grafton W. H. Hui
13:00–13:40	Claus Führer, “Construction of variable step size multistep schemes.”
13:45–14:25	Zhiming Chen, “Upscaling of well singularities of flow transport through heterogeneous media.”
14:30–15:10	Qiang Du, “Quantized vortices: theory and computation.”
	Coffee
	Chairman: Axel Ruhe
15:30–16:10	Per Lötstedt, “Anisotropic grid adaptation for Navier-Stokes’ equations.”
16:15–16:55	Pingwen Zhang, “The computational modeling of complex fluids.”
18:00	Dinner

Tuesday June 11

7:30–8:30	Breakfast
	Chairman: Chuan-Miao Chen
8:30–9:10	Stig Larsson, “A posteriori error analysis in the maximum norm for the time-dependent obstacle problem.”
9:15–9:55	Shuzi Zhou, “The convergence rate of domain decomposition methods for obstacle problems.”
	Coffee
	Chairman: Björn Engquist
10:15–10:55	Chuan-Miao Chen, “Numerical simulation of laser transmission and soliton.”
11:00–11:40	Anders Szepessy, “Convergence rates for adaptive finite element methods.”
	Lunch
	Chairman: Stig Larsson
13:00–13:20	Kyoung-Sook Moon, “Adaptive Monte Carlo algorithm of killed diffusion.”
13:25–13:45	Anders Logg, “Explicit time-stepping for stiff ODEs.”
13:50–14:10	Yubin Yan, “Finite element method for stochastic parabolic partial differential equations.”
	Coffee
14.30–	Excursion and dinner in the archepelago

Wednesday June 12

7:30–8:30	Breakfast
	Chairman: Bertil Gustafsson
8:30–9:10	Vidar Thomée, “Maximum-norm estimate for the resolvent of a finite element discretization of the Laplacian.”
9:15–9:55	Mo Mu, “A networked PDE solving environment.”
	Coffee
	Chairman: Mo Mu
10:15–10:55	Mats G. Larson, “Discontinuous elements in least squares FEM.”
11:00–11:40	De-Hao Yu, “Hypersingular residuals and a posteriori error estimates in boundary element methods.”
	Lunch
	Chairman: Qiang Du
13:00–13:40	Johan Helsing, “Stress computations on multiply connected domains.”
13:45–14:25	Zhen-Huan Teng, “A novel exact boundary condition based on Kirchhoff-type formulae.”
14:30–15:10	Björn Engquist, “Heterogeneous multiscale methods.”
	Coffee
	Chairman: Zhong-Ci Shi
15:30–16:10	Olof Runborg, “Wavelet based numerical homogenization.”
16:15–16:55	Axel Ruhe, “Rational Krylov for large nonlinear eigenproblems.”
18:00	Dinner

List of speakers

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Abstracts

Numerical simulation of laser transmission and soliton

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Abstract. Laser transmission is described by nonlinear Schrodinger system. When dispersion $K > 0$, by use of a relative time $\tau = c(t - z/v)$, it becomes a canonical form

$$iu_z + \frac{1}{2}(u_{xx} + u_{yy} + u_{\tau\tau}) + |u|^2 u = 0. \tag{1}$$

There are five kinds of difficulty for its numerical solution: 1). High dimension; 2). Nonlinearity; 3). Unbounded domain; 4). Long time; 5). How choose a better initial value, if search its soliton. The computation of this problem is so compicated that no way to begin. Follow Y.Silberberg, we discuss the cases of sphere ($m = 2$) and cylinder ($m = 1$) symmetry, which are decreased to $1 + 1D$, but with a singular coefficient,

$$iu_z = \frac{1}{2}(u_{rr} + \frac{1}{r}u_r) + |u|^2 u = 0, u(0,r) = \phi(r), \quad u(z,0) = 1,\ u(z,\infty) = 0,\ z, r > 0. \tag{2}$$

By a model analysis, $u = U(r)exp(i\lambda z)$, it leads to a nonlinear eigenvalue problem

$$\frac{1}{2}(U_{rr} + \frac{m}{r}U_r) - \lambda U + U^3 = 0,\ U(r) > 0, U(0) = 1, U(\infty) = 0. \tag{3}$$

He has not explained how to solve it numerically, only given a few data and a sketch. In this paper, we shall propose an effective algorithm to calculate its soliton solution and then further study their properties. First, to solve (3), we adopt the following treatments:

1). Turn to discuss a corresponding initial value problem with $U(0) = 1, U'(0) = 0$ and different λ;

2). Use a continuous finite element method with weights r in $(0, 1)$ and r^m in $(1, \infty)$, so that the conservation for large r is retained.

3). Use the interpolated coefficient finite element method to treat the nonlinear term;

4). Adopt a new algorithm to choose the parameter λ, so that a desired solution $U(r,\lambda) \geq 0, U(R,\lambda) \approx 0$ in larger interval $(0,R)$ can be found.

Our numerical computations show that the desired eigenvalue λ and corresponding solution $U(r)$ are obtained and it is found that the solution $U(r)$ decreases exponentially in larger interval $(2,20)$, then $U' + bU = 0$, where the positive constant b is determined. In these computations, we found that the behavior of solution is very sensitive to the change of λ, and a lot of interesting phenomenon is observed.

Finally, we take fully discrete finite element scheme to solve (2) with the inital value $\phi = U(r)$ and artificial boundary values $u(z,0) = 1, u_r + bu = 0$ on $r = R$, where we can choose R a not large number. A long time computation show that $u(z,r) = U(r)exp(i\lambda z)$, and then $|u(s,r)| = U(r)$ is indeed a desired soliton solution.

Upscaling of well singularities of flow transport through heterogeneous media

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Abstract. There are three scales in the flow transport through heterogeneous media involving well singularities: the size of the well, the size of the heterogeneity of the media, and the size of the computational domain. In this talk, we are going to develop a multiscale coarse grid algorithm to solve such problems. Optimal error estimates are derived for the local periodic permeability. Numerical results will be reported.

Quantized vortices: theory and computation

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Abstract. Quantized vortex, a well-known signature of superfluidity, was observed in superconductors half a century ago, and more recently, it has also been observed in the Bose-Einstein condensates, the so-called fifth state of matter.

In this talk, we will present some numerical algorithms for the computation of vortices in superconductors based on the phenomenological Ginzburg-Landau models and also vortices in the Bose-Einstein condensate in a rotating trap based on the Gross-Pitaevskii equations. Some striking similarities will be illustrated. A brief introduction to the physical background of these problems will be given. Some mathematical results concerning these equations as well as the computational challenges will be discussed. Numerical simulations and their physical interpretations will also be presented.

Heterogeneous multiscale methods

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Abstract. In many applications strong variations in temporal or spatial scales in the differential equations pose serious challenge to numerical simulations. We shall describe a framework for computations on the macroscale but where the forces and fluxes are computed on the microscale. This means that macroscale computations can be done without the knowledge of effective equations but also without the high computational complexity of a full microscale simulation. Examples will be given from homogenization theory for hyperbolic problems with oscillatory solutions.

Construction of variable step size multistep schemes

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Abstract. Multistep methods are classically constructed by specially designed difference operators on an equidistant time grid. To make them practically useful, they have to be implemented by varying the step-size according to some error-control algorithm. It is well known how to extend Adams and BDF formulas to a variable step-size formulation. In this paper we present a collocation approach to construct variable step-size formulas. We make use of piecewise polynomials to show that every k-step method of order $k+1$ has a variable step-size polynomial collocation formulation.

High order difference methods for wave propagation problems

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Abstract. It is well known that wave propagation problems over long time intervals require high order methods, and many such methods have been constructed. However, to keep high order accuracy also in time for problems with variable coefficients, the methods quickly become complicated. In this talk, we will consider acoustic wave propagation, and discuss a few finite difference methods for the wave equation in scalar form as well as in first order system form.

One way to achieve high accuracy in time, is to use the Numerov principle, based on substituting truncation errors in time by space derivatives. It turns out that the first order system form leads to less complicated approximations, while still keeping the conservation properties of the continuous formulation. We will show that the method works well even for discontinuous coefficients without any special procedures across the material interfaces.

Stress computations on multiply connected domains

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Abstract. The outstanding problem of finding a simple Muskhelishvili-type equation for the stress problem on multiply connected 2D domains is solved: we derive a Fredholm second kind integral equation with non-singular operators and where the unknown quantity is the interior limit of an analytic function. In a numerical application the stress field is resolved to a relative precision of 10^{-10} on a large, yet simply reproducible, setup containing 4096 holes and cracks. About 50 GMRES iterations are needed for full convergence. Comparison with previous results in the literature indicates that general purpose FEM software may perform better than many special purpose codes based on classic integral equations.

The present work is a part in a greater effort which aims at constructing fast and stable integral equation based software for fracture mechanics problems. Unlike most actors in this field we choose to base our algorithms solely on Fredholm equations of the second kind. This gives our algorithms superior stability. Standard practice in computational Solid Mechanics is work with Fredholm first kind equations. While such equations are simpler to derive than second kind equations they are more difficult to solve as they typically lead to system matrices whose condition number grow with the number of discretization points and as they often need numerical preconditioning – not unlike FEM.

I hope the talk will result in a discussion!

The water level formulation for shallow-water flow with bottom topograph

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Abstract. Shallow-water flow is traditionally formulated in terms of water depth and fluid velocity. This formulation enjoys great success for flow with horizontal bottom and no friction when the governing equations reduce to conservation laws. It, however, encounters difficulties in the presence of uneven bottom topography; in particular, it fails to replicate stationary flow. To overcome the difficulties, we formulate the problem of shallow-water flow in terms of water surface level and fluid velocity. The non-homogeneous equations are solved using the fractional step method together with a Godunov-type scheme for the homogeneous conservation law equations. The Riemann problem in this formulation is complicated but is readily solved with an approximation equivalent to coarsening the grid for bottom topography by doubling its size locally. Our method exactly replicates the stationary flow, and accurately computes quasi-stationary, steady, and unsteady flow. It has also been applied to compute the tidal bores on the Qiantang River on the East coast of China, producing excellent agreement with field observations.

Discontinuous elements in least squares FEM

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Abstract. Least Squares Finite Element Methods have several appealing properties including a very general formulation, stability, and suitability for multigrid. However, there are disadvantages too, for instance, strong regularity requirements on the exact solution. In particular, the regularity requirements lead to difficulties when solving problems on nonconvex polyhedral domains. In this work we investigate Least Squares Methods based on discontinuous approximation spaces which allow nonconvex polyhedral domains. Applications include first order system formulations of second order elliptic problems and the div-curl problem.

A posteriori error analysis in the maximum norm for the time-dependent obstacle problem

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Abstract. We consider finite element approximation of the parabolic obstacle problem. The analysis is based on a penalty formulation of the problem where the penalization parameter is allowed to vary in space and time. We estimate the penalization error in terms of the penalty parameter and the data of the equation. The penalized problem is discretized in space and time by means of a discontinuous Galerkin method. We prove an a posteriori error estimate in the space-time maximum norm involving a residual and the stability property of a linearized adjoint problem. The talk is based on joint work with D. A. French, R. H. Nochetto and M. Boman.

Explicit time-stepping for stiff ODEs

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Abstract. We present a new strategy for solving stiff ODEs with explicit methods. By adaptively taking a number of stabilising small explicit time steps when necessary, a stiff ODE system can be stabilised enough to allow for time steps much larger than what is indicated by classical stability analysis. For many stiff problems the cost of the stabilising small time steps is small and so the improvement is large. We illustrate the technique on a number of well-known stiff test problems.

Anisotropic grid adaptation for Navier-Stokes' equations

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Abstract. Navier-Stokes' equations are discretized in space by a finite volume method. Error equations are derived which are approximately satisfied by the errors in the solution. The dependence of the solution errors on the discretization errors is analyzed in certain flow cases. The grid is adapted based on the estimated discretization errors. The refinement and coarsening of the grid are anisotropic in the sense that it is different in different directions in the computational domain. The adaptation algorithm is applied to laminar, viscous flow over a flat plate, in a channel with a bump, and around a cylinder and an airfoil.

Adaptive Monte Carlo algorithm of killed diffusion

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Abstract. I will present an adaptive algorithm for weak approximations of stochastic differential equations by Monte Carlo Euler method. The goal is to compute expected values of functions of the solution depending on the first exit time from a given domain. In particular, I will explain why killed diffusions are good examples where adaptive methods are very useful.

The algorithm is based on the error expansion with a posteriori leading order term introduced in [A. Szepessy, R. Tempone, and G. Zouraris, Comm. Pure and Appl. Math., 54, 1169-1214, 2001] with almost optimal convergence rate proven in [K-S. Moon, A. Szepessy, R. Tempone, and G. Zouraris, preprint, `http://www.nada.kth.se/~szepessy/sode.ps`].

Finally, I will show numerical results from computations of barrier options in financial mathematics.

A networked PDE solving environment

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Abstract. PDE.Mart is a problem solving environment (PSE) for solving partial differential equations (PDEs) on computer networks. PDE.Mart consists of a web browser enabled graphical user interface (GUI), a server system (PDE Server) for building computational engines and providing the PDE solution services, and a distributed library (LIB).

The GUI provides a variety of functionality for users to easily and efficiently browse information, specify PDE problems, select solution methods, build solvers, control the computation, visualization, analysis, and I/O, etc. The implementation of the GUI is a combination of different network technologies including JAVA, CGI and HTML, depending on the invoke (interactive or batch) modes as well as network security and efficiency considerations. The core part of the GUI – the Interactive PDE GUI – is a Java applet. It consists of Domain Editor, PDE Editor, Mesh Editor, Discretization Editor, Solver Editor, and Solution Analyzer.

The PDE Server is a Java application running on the PDE.Mart host server. It communicates with the instances of the Interactive PDE GUI running on client machines in the client-server protocal via Java sockets. For each socket connection, the PDE Server creates a computational session for the client by the Engine Builder which takes the user's input from the GUI; creates and manipulates its domain object, PDE object, mesh object, discrete system object, and solution object; and sends the feedback to the corresponding client. The Engine Builder consists of Domain Creator, PDE Creator, Mesh Generator, Discretizer, and Solver. The computational engine is object-oriented, multi-threaded, and distributed. Each software part is viewed as an encapsulated object. High level distributed and parallel computing is realized through multiple threads and network sockets. There is, in fact, an intermediate interface between the GUI and Engine. It is a textual-based high level language mapped from the interactive GUI. The corresponding program file can be used to save and retrieve the status of the current GUI session for future work. Advanced users may also directly program on this level.

The LIB contains the supporting computational and utility software parts which may be local or remote, may be implemented in JAVA or other native languages such as C, C++, or FORTRAN. The LIB has a JAVA interface to the CP, a C/C++interface for the native methods in the JAVA interface, as well as a FORTRAN interface for the C++ implementation of the JAVA native methods corresponding to the FORTRAN

codes. Inside the LIB are a collection of JAVA, C/C++, FORTRAN codes that are either self-developed or ported from existing softwares with wrappers to encapsulate the local information and convert data structures. For the sake of efficiency, most of the computationally intensive software parts are implemented in native languages, and only the drive routines are wrapped and interfaced with CP through JAVA NATIVE INTERFACE (JNI).

PDE.Mart is an E-encyclopedia. Besides a PDE solving environment with powerful computing engines for both numerical and symbolic computation, it also provides comprehensive information related to PDE classification, mathematical and physical properties, useful links and search engines to related websites, solvers and remote servers.

As part of PDE.Mart, we have also developed a tool, WebInterfacer, for automatically generating a web browser enabled network interface for software developers to provide form based

services for using their softwares on their servers. Furthermore, the WebInterfacer system can be easily extended for generating other types of network interfaces.

The PDE.Mart project is led by Mo Mu at Hong Kong University of Science and Technology. One of our missions of the project is to investigate the impact and research issues of the rapidly growing network technologies in designing and developing networked PSEs for scientific and engineering applications.

Rational Krylov for large nonlinear eigenproblems

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Abstract. Rational Krylov is used to solve an eigenvalue problem that is nonlinear in the eigenvalue parameter. In each iteration, it gives an improved shifted and inverted Arnoldi factorization to a linearization of the original nonlinear problem.

The final eigensolution gives a latent pair of the nonlinear eigenproblem and a starting guess for the next latent pair. Purging of uninteresting directions reduces the size of the basis. Locking of already found latent vectors gives deflation. An inner iteration makes the residual orthogonal before the size of the basis is increased. One sparse LU factorization can be used to locate several latent pairs.

Results, taken from the thesis of Patrik Hager, are reported for three test examples coming from finite element approximations modelling viscously damped vibrating structures.

Wavelet based numerical homogenization

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Abstract. We consider the numerical solution of multiscale problems for PDEs. Typically, a direct discretization using a grid that resolves all scales will be too expensive, while using a coarse grid will give too inaccurate a discrete approximation. In analogy with classical homogenization theory, we derive an effective (discrete) coarse grid operator whose structure is similar to the one given by direct discretization, but with a locally altered stencil that takes the effect of subgrid scales into account. We show a general procedure for doing this, based on wavelet projections of the discrete fine grid operator followed by sparse approximation. We discuss some theoretical underpinnings of the method and show results from various numerical experiments.

Nonconforming rotated Q_1 finite element and applications

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Abstract. A detailed analysis of a newly appeared nonconforming rotated Q_1 finite element is presented. It is proved that this element is convergent on quadrilateral meshes for the general second order elliptic problem provided a condition on the mesh subdivision is imposed. Some optimal quadrature schemes to calculate the stiffness matrix are proposed, including a two-point scheme that excludes even a P_1 unisolvent set. Finally, the rotated Q_1 element is used to approximate the Reissner-Mindlin plate. A new locking free lowest order rectangular element is obtained.

Convergence rates for adaptive finite element methods

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Abstract. There are numerous adaptive methods for partial differential equations, but the theoretical understanding of convergence rates for adaptive algorithms is not as well understood, with a good exception for the wavelet methods by Cohen, Dahmen and DeVore.

I will present a rigorous convergence result for a general adaptive finite element algorithm based on successive subdivision of the mesh: the algorithm decreases the maximal error indicator with a constant factor until it stops; the algorithm stops with the optimal number of elements, up to a problem independent factor; and the global error is asymptically bounded by the tolerance parameter, up to a problem independent factor, as the tolerance tends to zero.

The talk will answer how to measure the convergence rate (i.e. what is the optimal number of elements?), why the convergence of the error density for the error indicators is subtle and why this convergence is essential.

A novel exact boundary condition based on Kirchhoff-type formulae

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Abstract. A novel exact non-reflecting boundary condition based on Kirchhoff-type formulae is derived for exterior three-dimensional wave problems. The Kirchhoff-type non-reflecting boundary condition is originally proposed by L. Ting and M. J. Miksis and numerically tested by D. Givoli and I. Patlashenko for one-dimensional problems. The computational attractive merit is that their temporal non-locality is limited to a fixed amount of past information. However a long-time instability is exhibited in the testing numerical solutions. The novel boundary condition proposed in this talk eliminates the long-time instability and is reduced to the local non-reflecting boundary condition, proposed by B. Engquist and A. Majda, in one-dimension model. Three-dimension numerical tests are carried out on cubic domain with cubic surface artificial boundary condition.

Maximum-norm estimate for the resolvent of a finite element discretization of the Laplacian

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Abstract. We present a new logarithm free resolvent estimate in maximum-norm for the discrete Laplacian associated with a quasiuniform family of piecewise linear finite element spaces on a convex d-dimensional domain with smooth boundary. We discuss the relation of such an estimate, via semigroup theory, to stablity estimates for associated spatially semidiscrete and fully discrete finite element methods for parabolic equations. The result is joint work with N. Yu. Bakaev and L. B. Wahlbin.

Finite element method for stochastic parabolic partial differential equations

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Abstract. I will present our first attempts to prove error estimates for finite element approximations of a parabolic stochastic partial differential equation: $du + Au\,dt = dW$, where A is an elliptic operator and W is space-time white noise. Based on appropriate nonsmooth data error estimates for deterministic finite element problems, we obtain the error estimates in semidiscrete and fully discrete cases in both strong and weak norms. Our results are general and can be applied to several spatial variables.

Hypersingular residuals and a posteriori error estimates in boundary element methods

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Abstract. A reliable and efficient *a posteriori* error estimation plays a key role in the adaptive finite or boundary element methods. In this paper some *a posteriori* error estimates for boundary element methods, based on classical and hypersingular residuals, are discussed. The residuals are defined as the differences between two sides of the boundary integral equations when the exact solution is replaced by the approximate solution. Three kinds of the residuals are compared here. Numerical examples show some advantages of the hypersingular residuals, especially obtained from the natural boundary integral equations. It is a good *a posteriori* error indicator for some boundary element methods.

The computational modeling of complex fluids

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Abstract. Viscoelastic liquid have been known to display striking differences to Newtonian fluids in a variety of flow situation. It is a challenge priblem to understand the microstructural features of the viscoelastic fluid and interactions with fluid flow. A new molecular model for liquid crystalline polymers (LCP) that includes distortional stress and mass diffusion is built by us, which is used to simulate the disclinations of LCP. A new model of non-Newtonian flow is also constructed by using the new kinetic theory.

The convergence rate of domain decomposition methods for obstacle problems

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Abstract. A kind of additive or multiplicative space decomposition methods for obstacle problems are discussed. The convergence theorem and the geometrical rate (in quadratical functional case) or asymptotically geometrical convergence rate have been proved.