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MATHEMATICAL LIBRARY SOFTWARE FOR APPLICATIONS OF PARALLEL SUPERCOMPUTERS

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We have developed application software for a variety of advanced scientific problems on a variety of parallel supercomputer platforms -- IBM PVS, IBM SP1 and IBM SP2, Cray T3D, and Silicon Graphics Power Challenge. Applications of our work have ranged from micro-lithography to chemical kinetics to fluid turbulence. Significant breakthroughs have been accomplished, which include the first aerial image of a full-scale 4Mb DRAM chip, and in the development of parallel lattice gas methods, especially lattice BGK methods. In fluid turbulence, breakthroughs have included the first direct simulation of the Kolmogorov $k^{-5/3}$ inertial range spectrum and the development of hyperviscous simulation techniques that allow parallel calculation at Reynolds numbers that rival the highest Reynolds numbers observed in nature, namely geophysical flows.

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FINAL REPORT

AFOSR/DARPA Contract F49620-91-C-0059
Mathematical Library Software
for Applications of Parallel Supercomputers

I. OVERVIEW

In this work we have developed application software for a variety of advanced scientific problems on a variety of parallel supercomputer platforms. The supercomputer platforms used in this work include the IBM PVS, IBM SP1 and IBM SP2, Cray T3D, and Silicon Graphics Power Challenge. The IBM PVS, located in our research facility at Princeton University, has been used for many of the research studies reported herein. It has 32 processors and the demonstration of good scaling behavior on this system has been one of our primary achievements.

Applications of our work have ranged from micro-lithography to chemical kinetics to fluid turbulence. Among the significant breakthroughs accomplished with support of this contract include the first aerial image of a full-scale 4Mb DRAM chip (in fact, the IBM 4Mb memory chip) which initially required about one day on our IBM PVS to calculate but, with algorithmic improvements, can now be done in less than one quarter of that time. We have also made significant breakthroughs in the development of parallel lattice gas methods, especially lattice BGK methods, which enable natural-grid solution of complex problems. In fluid turbulence, breakthroughs have included the first direct simulation of the Kolmogorov $k^{-5/3}$ inertial range spectrum and the development of hyperviscous simulation techniques that allow parallel calculation at Reynolds numbers that rival the highest Reynolds numbers observed in nature, namely geophysical flows.

A variety of parallel application software has been developed and has been communicated to a broad variety of collaborators in industry, universities, and government laboratories.

In the remainder of this report, we give a list of the papers published with support of this contract and a brief summary of the results obtained in each of these papers.

Number of Students Participating in the AFOSR/DARPA and the Number of Degrees Awarded:

Graduate Students:	Degree:
A. V. Cheklov	Ph.D 4/95
A. S. Ghandi	Ph.D expected 6/96
R. W. Powell	Ph.D expected 8/96
S. A. Smith	Ph.D expected 8/95
M-L. Tan	Ph.D 5/95
Y. Zhang	Ph.D expected 8/95

II. BIBLIOGRAPHY

Papers Acknowledging Support of Contract F49620-91-C-0059

Interaction of Surface Waves with Turbulence: Direct Numerical Simulations of Turbulent Open-Channel Flow (Vadim Borue, Steven A. Orszag and Ilya Staroselsky, J. Fluid Mech. (1995), vol. 286, pp. 1-23.

We report direct numerical simulations of incompressible unsteady open-channel flow. Two mechanisms of turbulence production are considered: shear at the bottom and externally imposed stress at the free surface. We concentrate upon the effects of mutual interaction of small-amplitude gravity waves with in-depth turbulence and statistical properties of the near-free-surface region. Extensions of our approach can be used to study turbulent mixing in the upper ocean and wind-sea interaction, and to provide diagnostics of bulk turbulence.

Numerical Simulation of Weakly Compressible Kolmogorov Flow with Kinetic Model (Y. H. Qian and S. A. Orszag), Conference Proceedings & Lecture Notes in Physics, Vol. 1, "Second International Conference on Computational Physics," ICCP-2, Sept. 13-17, 1993, Beijing, China, International Press (1995).

Kolmogorov flow has been used to study the transition to turbulence. The motoviation of this paper is to investigate this flow with a simple kinetic scheme. We observe numerically the -5/3 law of inverse cascade of energy spectrum at low wavenumbers and a steeper than -3 law at high wavenumbers when the flow is forced at small scales.

Lattice BGK Models for Thermohydrodynamics (Y. H. Qian and S. A. Orszag), Conference Proceedings & Lecture Notes in Physics, Vol. 1, "Second International Conference on Computational Physics," ICCP-2, Sept. 13-17, 1993, Beijing, China, International Press (1995).

Lattice BGK models are proposed for thermohydrodynamics. The theoretical values of the sound speed, the shear viscosity and the conductivity are verified by numerical simulations. One-dimensional shock-tube problems is used to test the models.

Pattern Formation in Phase Transition (Y. H. Qian and S. A. Orszag), Conference Proceedings & Lecture Notes in Physics, Vol. 1, "Second International Conference on Computational Physics," ICCP-2, Sept. 13-17, 1993, Beijing, China, International Press (1995).

The dynamics of liquid-gas phase transition is studied in this paper by using simple kinetic models. The analytical results are verified numerically in one, two and three dimensions.

Parallel Computation for Fluid Dynamics (Y.H. Qian and S. A. Orszag), Conference Proceedings & Lecture Notes in Physics, Vol. 1, "Second International Conference on Computational Physics," ICCP-2, Sept. 13-17, 1993, Beijing, China, International Press (1995).

There is a growing interest in parallel algorithms for computational fluid dynamics. In this paper, we describe some simple kinetic models which are capable of reproducing the hydrodynamic behaviours with a high efficiency.

Scalings in Diffusion-Driven Reaction A + B C: Numerical Simulation by Lattice BGK Models (Y.H. Qian and S. A. Orszag), Conference Proceedings & Lecture Notes in Physics, Vol. 1, "Second International Conference on Computational Physics," ICCP-2, Sept. 13-17, 1993, Beijing, China, International Press (1995).

We are interested in one application of lattice BGK models to the diffusion-driven reactive system A + B C, which was investigated by Galfi and Racz with an asymptotic analysis and by Chopard and Droz with a cellular automaton model. The lattice BGK model is free from noise and flexible for applications. We derive the general diffusion-reaction equations for the lattice BGK models under the assumption of local diffusive equilibrium. The 4th order terms are derived and verified by numerical simulations. The purpose of this paper is to compare the lattice BGK results with existing results before we apply the models to more complicated systems. The scalings concern the exponents a, b and the function G in the production rate of C component $R(x,t) = t^{-b}G(xt^{-a})$. We find the same values for a = 1/6 and b = 2/3 as Glfi and Racz found at long time limit. A *Gaussian* function for G is numerically obtained for the first time. Compared with the asymptotic analysis, lattice BGK is easy to apply to cases where no analytic or asymptotic results exist. Compared with the cellular automaton model, the lattice BGK model is faster, simpler and more accurate. The discrepancy of the results between the cellular automaton model and the lattice BGK models for the exponents come from the role of the intrinsic fluctuation. Once the time and space correlation of noise is given, we can incorporate a stochastic term in our models. The Schlogl model is also tested in this paper.

Recent Advances in Lattice Boltzmann Computing (S. Succi, Y. H. Qian and S. A. Orszag), submitted for publication, 1995.

Recent developments in the theory of the Lattice Boltzmann equation are presented, in particular, lattice BGK models are discussed in detail. Various applications are summarized.

Self-Similar Decay of Three-Dimensional Homogeneous Turbulence with Hyperviscosity (V. Borue and S. A. Orszag), Phys. Rev. E, 51, R856-R859 (1995).

Numerical simulations of the Navier-Stokes equations with hyperviscosity $(-1)^{h+1}\Delta^h$(h=8) show that periodic-box turbulence exhibits self-similar decay. The inertial-range energy spectrum has the scaling law $\varepsilon(t)^{2/3}/k^{5/3}$ where $\varepsilon(t)$ is the energy dissipation rate at time t. The total energy of the system decreases as $1/t^2$. The concept of constant Reynolds number decay is introduced, enabling us to perform long time averages and reliably measure higher order correlation functions. Comparisons are made with the case of forced turbulence reported earlier.

Numerical Studies of Three-Dimensional Kolmogorov Flow at High Reynolds Number (V. Borue and S. A. Orszag), submitted for publication.

High resolution numerical simulations (up to 256^3 modes) are performed for the three-dimensional flow in a periodic box of size $L = 2\pi$ driven by the large scale force $f_y = F cos(x)$ (Kolmogorov flow). High Reynolds number is attained by solving the Navier-Stokes equations with the hyperviscosity $(-1)^{h+1}\Delta^h$ (h = 8). It is shown that the mean velocity profile of the Kolmogorov flow is practically independent of Reynolds number and has the "laminar" form $\alpha V \cos(x)$ with nearly constant eddy viscosity. Nevertheless the flow is highly turbulent: the turbulent kinetic energy is nearly equal to the mean flow kinetic energy. The turbulent intensities, the energy dissipation rate and different terms in the energy balance equations have very simple structure of coordinate dependences $a + b\cos(2x)$ (here a, b are some constants). This makes Kolmogorov flow a good testing case for studying turbulent transport models. At large scales the flow is anisotropic, although at high Reynolds number it becomes isotropic at small scales. The problem of local isotropy is systematically studied by measuring longitudinal and transverse components of energy spectra and cross-correlations of different components of velocity. It is shown that pressure plays the crucial role in making flow locally isotropic. It is demonstrated that nearly a decade in wave-number space is required before anisotropic large scale flow may be considered locally isotropic.

Forced Three-Dimensional Homogeneous Turbulence with Hyperviscosity (V. Borue and S. A. Orszag), Europhysics Letters 29, 687-692 (1995).

High resolution numerical simulations (up to 256^e modes) are performed for the Navier-Stokes equations with hyperviscosity $(-1)^{h+1}\Delta$(h=8). With random white-in-time forcing, the inertial-range energy spectrum has the scaling law $1/k^{\alpha}$ with $\alpha \approx 1.85 \pm 0.05$ at small wave numbers k with a flatter region near the ultraviolet cutoff. The transitional region is characterized by a sharp change of the energy transfer mechanism. Spectra of fluctuations of higher order correlation functions are measured. At inertial range scales the system seems insensitive to the power h of the hyperviscosity.

Inverse Energy Cascade in Stationary Two-Dimensional Homogeneous Turbulence (V. Borue), Phys. Rev. Lett. 72, 1475-1478 (1994).

Direct numerical simulations with up to 1024^2 resolution are performed to study statistical properties of the inverse energy cascade in stationary homogeneous two-dimensional turbulence driven by small scale Gaussian white-in-time noise. The energy spectra for the inverse energy cascade deviate strongly from the expected $k^{-5/3}$ law and are close (somewhat flatter) to k^{-3}. The reason for the deviation is traced to the emergence of strong vortices distributed over all scales. Statistical properties of the vortices are explored.

Aerial Image of 3D Phase-Shifted Reticle -- 3D FAIM (E. Barouch, U. Hollerbach, and S. A. Orszag), Proc. SPIE 2197, 442, 1994.

As is well know, the mask in projection printing is a thin (about 1 μm thick) object, composed of numerous variable domains. The various domains contain different complex refractive indices. These refractive indices form a discontinuous "mask function", appearing as a coefficient in the Maxwell-Material (MM) equation that describes the transmission of the electric field through the 3D mask domain. The right-hand side of this equation involves the gradient of the dot-product of the electric field with the gradient of the log of the refractive index. Within each feature, the refractie index is a constant. Therefore its gradient vanishes, and the resulting local MM equation is the wave equation. However, at a feature boundary (chrome-quartz, phase-1 -- phase-2, etc.) the complex refractive index is discontinuous, resulting in a highly singular delta-function-like coefficient. The trailing components of the field display the standard Maxwell disoontinuity conditions, resulting in two very singular terms, i.e. a derivative of a delta function and a product of two delta functions. Such a source term, with such a remarkable oscillation, will be the origin of extreme instability in the numerical solution of the equations, no matter which direct solution algorithm is employed. Accordingly, the derivation of a preconditioner, namely a function which contains most of the unpleasantness of the equation times a function to be found, is absolutely essential to obtain accurate solutions in a reasonable time. Through an elaborate uniformly asymptotic scheme and scale analysis, we have derived such a preconditioner. The solution of the direct MM equation was compared with the solution using the preconditioner, and it gave us the confidence that we were on the right track. It actually means that one wishes to find the mask's Green function which, when convolved with the electric field incident on the mask, yields the exiting field which then enters the imaging optical system. It is the purpose of this paper to demonstrate the results obtained thus far, as well as to illustrate its implications on defocus linewidth control.

Automated Determination of CAD Layout Failures Through Focus: Experiment and Simulation (C. Spence, J. Nistler, E. Barouch, U. Hollerbach, and S. A. Orszag), Proc. SPIE 2197, 302, 1994.

This paper describes a software program which compares the simulated aerial image of a mask pattern with the original, desired, mask pattern. The program uses the Fast Aerial Image Model (FAIM) to simulate the aerial image. A specific intensity contour is chosen and the distance from the contour to the desired design is calculated. Regions where the distance exceeds a specified tolerance are deemed failures and flagged. Corner-rounding errors are handled differently to line edge position errors. The threshold intensity used can be specified by the user, alternatively a 'critical feature' may be defined and the threshold set to the intensity value required to print it on size. In addition to describing the program, we also show examples of how the aerial image contour predictions compare with simulations of resist profiles and actual printed resist images for the case of an SRAM cell.

Spectral Exponents of Enstrophy Cascade in Stationary Two-Dimensional Homogeneous Turbulence (V. Borue), Phys. Rev. Lett. 71, 3967-3970, December 1993.

Direct numerical simulations with up to 4096^2 resolution are performed to address the question of universality of statistical properties of the enstrophy cascade in homogeneous two-dimensional turbulence driven by large-scale Gaussian white-in-time noise. Data with different Reynolds numbers are compared with each other. The energy spectrum is found to be very close to $1/k^3$. It is shown that the primary contribution to the enstrophy transfer function comes from wave-number triads with one small leg and two long ones, corresponding to wave numbers in the inertial range.

Reynolds Number Dependence of Isotropic Navier-Stokes Turbulence (Z-S She, S. Chen, G. Doolen, R. Kraichnan, and S. A. Orszag), Phys. Rev. Lett. 70, 3251-3254, May 1993.

Reynolds number dependence of turbulence energy spectra and higher-order moments of velocity differences is explored by numerical integrations of the incompressive Navier-Stokes equation. The simulations have spatial resolutions up to 512^3 and cover $15 \leq R_\lambda \leq 200$, where R_λ is the Taylor microscale Reynolds number. The energy spectra collapse when scaled by the wave number k_p of peak dissipation and also by the spectrum level at k_p . k_p varies with R_λ in accord with the 1941 Kolmogorov theory. High-order normalized moments of velocity differences over inertial-range distances exhibit an R_λ-independent variation with separation distance. Implications of these observations are discussed.

Far-Dissipation Range of Turbulence (S. Cheng, G. Doolen, J. Herring, R. Kraichnan, S. A. Orszag, and Z. S. She), Phys. Rev. Lett. 70, 3051-3054, May 1993.

Navier-Stokes turbulence at low Reynolds number ($R_\lambda \approx 15$) is studied by high-resolution computer simulation. The energy spectrum in the range $5k_d <$ $10k_d$ is well fitted by $k^a \exp(-ck/k_d)$, where k_d is the Kolmogorov dissipation wave number, $\alpha \approx 3.3$ and $c \approx 7.1$. High-order spatial derivatives of the velocity field exhibit strong intermittency, associated with gentle spatial variation of large-scale structure rather than with sparse, intense small-scale structures. Analysis by the direct-interaction approximation, which ignores intermittency, gives $\alpha = 3, c \approx 11$.

Vector Aerial Image with Off-Axis Illumination (E. Barouch, D. C. Cole, U. Hollerbach and S. A. Orszag), Proc. of the SPIE 1927, 686, 1993.

As the numerical aperture (NA) in optical projection systems increases, the vector nature of the projected electric and magnetic fields becomes more important. Recent advances in off-axis illumination, tilting condenser lenses, and applying spatial filters, as well as phase-shift masks, hold the potential of increased depth of focus. To simulate these techniques in the high-NA regime, we have developed new fast altorithms. The development reported here builds on our recent work [1] extending scalar aerial imaging. The systematic treatment of [1] has now been applied to account for the vector nature of light. The optical projection system examined here involves an aplanatic lens system with high NA and finite magnification as applied to both i-line and deep-UV, 4x and 5x, steppers. Our new algorithms owe their genesis to a variety of subtle mathematical properties of the scalar and vector aerial image formulae. These new algorithms are based on our high NA aerial image model juxtaposed with

Yeung's original ideas for the vector field image. This formulation, which involves non-uniform grid fast Fourier transform techniques, has resulted in a tremendous speedup of the aerial image simulation with uniform accuracy throughout a domain of 1000μ x 1000μ and beyond, with the potential to simulate an entire chip, thus providing a solution to the "grand challenge" of full-chip design.

Lattice BGK Models for the Navier-Stokes Equation: Nonlinear Deviation in Compressible Regimes (Y. Y. Qian and S. A. Orszag), Europhys. Lett., 21(3), 255-259, 1993.

In this letter, a nonlinear deviation from the Navier-Stokes equation is obtained from the recently proposed LBGK models, which are designed as an alternative to lattice gas or lattice Boltzmann equation. The classical Chapman-Enskog method is extended to derive the nonlinear-deviation term as well as its coefficient. Their analytical expression is derived for the first time, thanks to the simplicity of the LBGK models. A numerical simulation of a shock profile is presented. The influence of the correction on the kinetics of compressible flow is discussed. A complete analysis of the thermodynamics including the temperature will be presented elsewhere.

Direct and Large-Eddy Simulation of Axisymmetric Wakes (A. G. Tomboulides, S. A. Orszag and G. E. Karniadakis), AIAA 31st Aerospace Sciences Meeting, Paper 93-0546, January 1993.

In this paper we present direct numerical simulations (Re = 25 - 1,000) and a large eddy simulation (Re = 20,000) for flow past a sphere, which is a prototype axisymmetric body. A new spectral element-Fourier method is implemented to discretize the incompressible Navier-Stokes in cylindrical coordinates, and a sub-grid model based on the renormalization group method (RNG) is used in the large eddy simulation. We identify two early bifurcations of the sphere wake, the first at Reynolds number 212 leading to a three-dimensional time-independent state, and the second at Reynolds number between 250 and 285 resulting in a time-periodic flow. A shear layer instability, observed in experiments, is also resolved accurately at Reynolds number 1,000. Our results from the large eddy simulation are in good agreement with experimental results both in terms of temporal response (frequency spectrum) as well as in terms of transport measures (drag coefficient).

Modes, Nodes, and Flow Codes (G. E. Karniadakis and S. A. Orszag), Physics Today, 34-42, March 1993.

The numerical simulation of high Reynolds number turbulent flows is a grand challenge problem that will tax supercomputing capability for decades to come. Massively parallel supercomputers seem the best hope for achieving progress on these fundamental problems with many practical applications.

Some Basic Challenges for Large Eddy Simulation Research (S. A. Orszag, I. Staroselsky, and V. Yakhot), in "Large Eddy Simulation of Complex Engineering and Geophysical Flows," Cambridge Univ. Press (ed. by B. Galperin and S. A. Orszag), pp. 55-78, 1993.

This paper reviews some of the basic features of LES and the techniques used to derive the LES equations. We discuss the conditions for self-consistency of LES. Then, review the RNG theory of the Navier-Stokes equations and the RNG-based derivation of a subgrid model for LES. We discuss the effect of rigid walls on LES and illustrate the problematics of the LES modeling of complex flows on the example of a subgrid-scale model for turbulent combustion.

On the Small-Scale Dynamical Behaviour of Lattice BGK and Lattice Boltzmann Schemes (S. Succi, D. d'Humieres, Y. H. Qian, and S. A. Orszag), J. Sci. Comp. 8, 219-230, 1993.

A quantitative assessment of the validity of the lattice BGK version of Lattice Boltzmann schemes is presented for the case of two-dimensional incompressible turbulence.

Eliminating Spurious Invariants in Lattice Models for Hydrodynamics (Y. H. Qian and S. A. Orszag), submitted to Complex Systems, to be published.

Most of lattice gas, lattice Boltzmann and lattice BGK models suffer from the existence of so-called spurious invariants which are usually scalar and transported by the dynamics. Their influence is shown in the pressure term. The presence of spurious invariants drives the solution of the system away from the Navier-Stokes equation's solutions. Though in lattice Boltzmann or lattice BGK models, the initial quantities of these spurious invariants can be set to zero in order to minimize their influence on dynamics, the production of such invariants by shock wave (strong gradients) or boundary conditions is not yet clear. We think that the existence of spurious invariants is one of the main sources of numerical instabilities. So it is important to remove the spurious invariants. In this paper, we will be able to eliminate some of such spurious invariants by replacing the propagation step by a smoothing procedure. We rederive the governing equations and obtain the transport coefficients. Some stagged invariants can be completely eliminated if the smoothing parameter Ω is set to 0.5. Numerical simulation does confirm the theoretical results. The consequence of removing small-scale spurious invariants is meaningful and useful for subgrid modelling, and we do believe that the smoothing procedure is very general and that unphysical behaviours can be reduced.