DTIC Information for AFOSR Task 2304CP Lattice-Gas Theory and Computation for Complex Fluid Dynamics

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1 Objective

Aid the Air Force modeling community by developing a "mid-level" approach to simulating the behavior of complex fluids, such as viscous incompressible fluids, hydrothermal fluids, inviscid fluids, multiphase fluids, and superfluids. Traditional approaches to complex fluid simulation include "low-level" molecular dynamics or "high-level" partial differential equation approximation schemes. MD suffers from insufficient spatial and temporal scales. The PDE schemes suffer from numerical instabilities and coarseness in the physical description. Lattice gases are a "mid-level" approach that achieves greater scales than MD while possessing unconditional stability due to its underlying physics-like microscopic dynamics while capturing in the macroscopic limit all relevant physics. A principle objective is to develop a general lattice theory and test its soundness and efficiency on novel fine-grained parallel computers architected along the lattice gas paradigm. Focused research objectives include: complex computation fluid dynamics, i.e. rheology of drops; multiphase/multicomponent fluids; discretized molecular dynamics of materials with complex transitions and structures; parallel fine-grained quantum computing; lattice-gas machines as a test-bed for ultra-fine-grained computations.

2 Approach

An early lattice-gas model studied transport coefficients near the critical point [1] by a simple extension of the Ising model with spins given a quantum of momentum. This model manifested sound waves, surprising fluid-like behavior given the model's simplicity and severe spacetime discretization. The transport properties of discrete classical gases were explored further in the 1970's [2]. The particles' momentum vectors are quantized in both magnitude and direction and a particle is just a single bit streaming through a spatial lattice. Particles arriving at the same space-time lattice point undergo collisional scattering which is handled by a "processor" at the lattice node. This is the essence of a lattice-gas computing architecture: a crystallographic lattice based array of simple processors, each simultaneously handling the collision and streaming of local particles. By the mid 1980's new possibilities had emerged: 1) recovery of the Navier-Stokes incompressible fluid equations [3]; and 2) low-cost, fast parallel architectures [4] with supercomputer like performance. A prototype desktop special-purpose machine, the cellular automata machine CAM-8 [5], offers lattice-gas simulation speeds comparable to large parallel supercomputer speeds [6, 7, 8]. It is now known lattice-gases can mimick a broad and ever expanding class of complex fluids, including microemulsions [9] and certain quantum fluids [10, 11]. The technique—which originally found applicability in modeling flow through porous media, two-fluid immiscible flow, multiphase flow, and reaction-diffusion systems—has more recently been applied to fine-grain quantum computing [12].

3 Progress

Progress in this AFOSR 2304CP project has been reported through more than two dozen publications.

3.1 Fiscal Year 1997

This year has been a landmark year for research finds. The theoretical foundations laid over the past several years of this project have culminated in several important discoveries: (1) a complete Hamiltonian based theoretical description of lattice gases; (2) a long-range multienergy lattice gas (lattice molecular dynamics) approach obeying semi-detailed balance in its collision transitions; (3) a quantum lattice gas for computational Navier-Stokes fluid dynamics; and (4) a refined integer lattice gas with markedly improved computational efficiency offering an unconditionally stable lattice Boltzmann scheme obeying detailed balance. The discovery of a lattice-gas Hamiltonian has allowed us to develop a complete statistical mechanics formulation of the lattice-gas system. For example, applied to lattice molecular dynamics models, it has allowed for a full diagrammatic Mayer cluster expansion for the emergent equation of state. The discovery of a quantum lattice gas for NS fluid flow offers an important new avenue for fine-grained quantum computing where the need for long-term quantum coherence is avoided altogether making the construction of a quantum computer more conceivable and practical. Finally, we now understand how entropy must be maximized in integer lattice gas collisions and how the associated statistical mechanics analysis predicts the same equilibrium particle distribution as obtained via the usual Chapman-Enskog analysis.

3.2 Fiscal Year 1996

Developed lattice gas/Boltzmann methods to model multiphase/multicomponent complex fluid behavior relating to the microphysics in aircraft contrails in the upper troposphere. Tested new computing architectures/strategies for lattice based parallel computation. Current codes capture hydrodynamic behavior at drop size scales, $L \sim 1$ millimeter. Experimented with lattice molecular dynamics: (1) using nonlocal interactions in an integer lattice gas restoring Galilean invariance in the emergent fluid dynamics; (2) semi-detailed balance lattice gases with nonlocal interparticle interactions, and (3) tested Monte Carlo/Metropolis implementation of a Hamiltonian based integer lattice gas obeying detailed-balance to recover the Cahn-Hilliard equation coupled to the Navier-Stokes equation; and (4) modelled binary fluids, colloids, and dipolar fluids. Results include: shear viscosity numerical measurements of an integer lattice gas compared to mean-field theory prediction; classifying droplet growth regimes; hydrothermal fluids to test the Rayleigh-Benard convective instability; and quantum lattice gases for parallel quantum computation.

3.3 Fiscal Year 1995

Two discrete fluid models are the lattice-gas automaton (LGA) and lattice-Boltzmann equation (LBE), each with advantages and disadvantages. Developed the integer lattice-gas to retain the advantages of both. The integer lattice-gases uses L bits to represent a particle count in each momentum state (the $L = 1$ case reduces to LGA). Like the LGA, the integer lattice-gas: (1) is exactly computed on a discrete spacetime lattice (all the additive conserved quantities, e.g. mass and momentum, are kept strictly fixed during the entire coarse of the calculation—there is no numerical round-off error); (2) microscopically obeys semi-detailed balance; (3) has a mesoscopic limit defined by ensemble averaging; and (4) acts like a fluid in the macroscopic limit (the usual Chapman-Enskog expansion is performed). Like the LBE, the integer lattice-gas: (1) recovers the correct fluid equations, with full galilean invariance; (2) achieves a reduction in viscosity; and (3) achieves a considerable noise reduction. We have carried out numerical experiments on parallel computers (CAM-8, CM-5, SP-2) to verify our theoretical analysis of the model. Completed two designs for a billion node massively-parallel lattice-gas computer (funded by two 6.2 SBIRs).

3.4 Fiscal Year 1994

Developed a finite-temperature lattice-gas liquid-gas—with a pressure, density, and temperature dependent equation of state—simple enough for a Maxwell construction to predict the complete liquid-gas coexistence curve. In a single-speed lattice-gas model there arises in the pressure a term depending upon the square of the bulk velocity. Completed a treatment of a multispeed lattice-gas showing velocity takes on a physical interpretation where the total internal energy partitions into a bulk motion term, or kinetic energy, and a fluctuating motion term, or random heat energy associated with gas temperature. Found a molecular dynamics technique using a lattice-gas with multiple long-range interactions–a fluid-solid transition emerges. Implemented lattice-gases on two parallel architectures: MIT's prototype CAM-8 and the CM-5. Implemented on the CAM-8 a 3D lattice-gas fluid with a highly symmetrical icosahedral lattice. Implemented lattice-Boltzmann models on the CM-5 and SP-2; Reynolds number of 50,000 obtained so far.

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