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Microscopic Simulations of Complex Hydrodynamic Phenomena
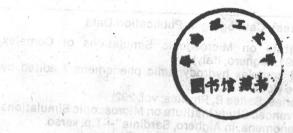
Microscopic Simulations of Complex Hydrodynamic Phenomena

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SPECIAL PROGRAM ON CHAOS, ORDER, AND PATTERNS

This book contains the proceedings of a NATO Advanced Research Workshop held within the program of activities of the NATO Special Program on Chaos, Order, and Patterns.

SPECIAL PROGRAM ON CHAOS, ORDER, AND PATTERNS

PREFACE

This volume contains the proceedings of a NATO Advanced Study Institute which was held in Alghero, Sardinia, in July 1991.

The development of computers in the recent years has lead to the emergence of unconventional ideas aiming at solving old problems. Among these, the possibility of computing directly fluid flows from the trajectories of constituent particles has been much exploited in the last few years: lattice gases cellular automata and more generally Molecular Dynamics have been used to reproduce and study complex flows. Whether or not these methods may someday compete with more traditional approaches is a question which cannot be answered at the present time: it will depend on the new computer architectures as well as on the possibility to develop very simple models to reproduce the most complex phenomena taking place in the approach of fully developed turbulence or plastic flows. In any event, these molecular methods are already used, and sometimes in an applied engineering context, to study strong shock waves, chemistry induced shocks or motion of dislocations in plastic flows, that is in domains where a fully continuum description appears insufficient. The main topic of our Institute was the molecular simulations of fluid flows.

The project to hold this Institute was made three years ago, in the summer of 1989 during a NATO workshop in Brussels on the same subject. It was felt by the participants that it would be profitable to have a longer and more tutorial meeting. We decided to organize it in the form of a summer school where all methods for computing flows from molecular modelling could be taught and, to some extent, confronted. However, we did not want to restrict ourselves to the technique's aspects and we enlarged the spectrum of the lectures by including the study of fundamental problems as well as of physical applications. It is a pleasure to acknowledge the encouragement we received from all members of the scientific committee. A non-negligible part of this encouragement is certainly due to the quality of the Parisian restaurant "Le Petit Zinc" where this project has been discussed.

The division and presentation of the articles of these proceedings has been made a posteriori by us. The first part is devoted to the Non-Equilibrium Molecular Dynamics studies. This contains articles which either discuss the theoretical foundation of the method or apply the method to specific non-equilibrium flows. Besides, Bill Hoover provided us with a personal view of the history of Non-Equilibrium Molecular Dynamics: this might give an opportunity to young researchers to realize that progress in Physics is often the result of controversies Applications to rheology (Ciccotti, Ryckaert, Pierleoni, Michopoulos), Shock waves (Holian, Carter), strong temperature gradients (Mansour) and convective instabilities (Rapaport) are the main subjects treated.

Lattice gas papers are the most numerous and this is an evidence of the excitement this technique has brought to the community of computational physicists. Theoretical foundations are explained in the basic introduction given by Ernst. Quite interesting also was the study by Levermore of the rigorous limits which lead to the hydrodynamic Navier-Stokes equations. Two articles deal with lattice-Boltzmann simulations (Mc Namara and Succi): the ability of

lattice-Boltzmann to reach high Reynolds number flow simulation has been also discussed during the (second) round-table discussion which is presented in the next chapter, after presentation of the DSMC method by its main author (Bird) and of the Brownian Dynamical simulation technique (Bossis).

Applications in lattice-gas simulations are numerous and they range from the study of diffusion in various lattice models (Cohen) to the flows in porous media (Rothman). Colloidal systems have been treated by a method which combines lattice-gas efficiency for the fluid motion and dynamics of the colloidal particles (van der Hoef): there is little doubt that the ability to mix different approaches on different time and spatial scales will be a key point in the success of the future methods proposed (see also Hoover). It is worth mentioning that a (more research oriented) workshop was held in Nice in June 91, just before our school, and that many papers were also presented at this conference: the proceedings of the Nice meeting are to be published as a special issue of the Journal of Statistical Physics: they are complementary to ours.

In the fourth part, a few fundamental problems are reviewed. The paper by Frisch is on a modern view of the Kolmogorov theory. Besides its historical interest, it also introduces into the delights of turbulence as seen from a modern point of view. Two other papers follow, which discuss the relation between Lyapunov exponents, characteristic of the chaotic behavior in phase space, and transport coefficients, expressions of the dissipative nature of fluids. This relation was also discussed in a round-table and we have tried to keep the lively character of the exchanges in the report. The discussions of this round-table as well as of the other one, were taperecorded, written down by Brigitte Herpigny (thank you Brigitte) and then sent to the authors for corrections.

Other applications describe the parallel between the statistical approach to turbulence and to fractures in solids (Chudnovsky), the simulation of membranes by phenomenological lattice models (Abraham) and the use of cellular automata-like models for the plastic flows in crystals (Pontikis) and of NEMD on granular flows (Thompson).

At the IUPAP meeting organized in Brussels in 1956, Berni Alder presented his first Molecular Dynamics studies of assemblies of hard spheres. As can be read in the proceedings of this meeting, Berni was then asked whether his new method could lead to a derivation of hydrodynamics from first principles: Berni replied that one could imagine computations of fluid flow in high-speed aerodynamics based on MD with the development of larger computing facilities. It is therefore quite natural that this Institute was held to honor Berni's 65th birthday: not only did his work set a high standard for subsequent work in the field of non-equilibrium fluids, but also it has been very important in the understanding of the connection between hydrodynamic modeling and microscopic motion. This book ends with the long-time tails story as it was told to us by its discoverer.

Our only hope is that the reports made accessible in these proceedings can give readers a little bit of the pleasure we had in participating to this school.

Michel Mareschal, CECAM (Orsay), and Brad Holian, Los Alamos

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FROM FLUID PARTICLES TO PHYSICAL PARTICLES: COMPUTING HYDRODYNAMICS

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INTRODUCTION

The Navier-Stokes equations of hydrodynamics are partial differential equations which result from the conservation properties in simple monoatomic or molecular fluids, when combined with linear constitutive relations. When appropriate boundary conditions are applied and initial values of the variables are specified, they predict the space- and time- dependant hydrodynamic fields, that is, the values of mass density ρ, fluid velocity $\mathbf{u}$, and energy density e in the fluid. The Navier-Stokes equations were written more than a century ago, and there seems to be now overall agreement that they contain sufficient physics to describe, for instance, the very complex and chaotic flows occurring in fully developed turbulence. There is little doubt that, if one were able to solve them, one could, to a very high degree of accuracy, reproduce or predict most of the flow problems that occur in physics, chemistry, and engineering applications.

It is also by now widely accepted that fluids are made of atoms or molecules. A fundamental description of fluids has however not yet been achieved, in the sense that rigourous derivation of the full non-linear Navier-Stokes equations from the basic microscopic equations of molecular motion in fluids is still missing. Intermediate steps however have been built during the course of time by mathematicians and physicists. In the case of dilute gases a kinetic equation has been derived by Ludwig Boltzmann, also more than a century ago, which describe the space time evolution of the velocity distribution function of the gas. The contraction from the full Boltzmann equation to the hydrodynamic subspace spanning the first moments of the one particle distribution function has been a central theme of research in kinetic theory: various methods have been developed which permit to recover the Navier-Stokes equations in a given limit, and eventually to estimate further approximations. The peculiarity of the molecular model only enters in the description through the value of the transport coefficients. This microscopic "derivation" of the Navier-Stokes equations also predict a loss of validity in the case of very dilute systems, when the mean free path becomes of the order of the length characteristic of the inhomogeneity. On the contrary, when the density is increased, it is believed that Navier-Stokes equations can be safely applied to liquids, compressible fluids, even with very large gradients.

Needless to say, solving the Boltzmann equation is far more complex than solving the Navier-Stokes equations. The complicated nature of the interactions between the particles results in a non-linear integro-differential collision operator in the Boltzmann equation. However, the non-linearity which makes Navier-Stokes equations difficult to solve comes from the so-called inertial term and has nothing to do with collisions between particles. It has therefore been argued that one also could study complex flows in gases by using a linearized collision operator in the Boltzmann equation. It is precisely the same type of arguments which has been used more recently: in order to reproduce complex flows, microscopic models, such as lattice-gas cellular automata (LGCA) or lattice Boltzmann simulations, have been proposed,

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which do not properly mimic the fluid on small scales, but appear to reproduce correctly the behaviour at large spatial and temporal scales.

This same point of view has been recently taken in statistical mechanics either to explore the general relationship between microscopic modelling and the Navier-Stokes equations or even to challenge traditional solvers of these equations on computers. The traditional approach of computational statistical mechanics applied to fluids has been to use molecular dynamics(MD), the computation of many-body trajectories, in the determination of transport coefficients from molecular interaction potentials. Since this problem does not require far from equilibrium states, it has been solved by computing equilibrium time correlation function, actually equilibrium thermal fluctuations, and by using fluctuation dissipation theorems. An alternative approach has been more recently developed, non-equilibrium molecular dynamics (NEMD). Instead of computing long equilibrium trajectories, fluid systems are simulated with external forcing which mimic thermodynamical forces. An interesting and, to some extent, unexpected result from these studies has been the fact that the linear relationship between forces and fluxes remain very robust in non-equilibrium states. Also, complex hydrodynamic behaviour has been reproduced at and out of equilibrium, leading to the establishment of the validity of the hydrodynamic model at small space and time scales even in far from equilibrium states.

It has not been the original purpose of NEMD to challenge the continuum approach. The cost of computing is many orders of magnitude greater when running full MD to model a typical flow than traditional Navier-Stokes solvers. Atomic models have however been extremely simplified: lattice gas cellular automata (LGCA) and lattice Boltzmann (LB) simulations have proved extremely efficient in computing flows. The achievements, limitations, perspectives of molecular simulations are the subject of these conference proceedings[1]. Various methods and results developed these last years are discussed in this volume. We would like to dedicate this introductory article to a presentation of the general framework which has witnessed these developments. After a general presentation of the Navier-Stokes equations in the first section, we will briefly discuss the kinetic approach and finally present the main results which have been obtained through the microscopic simulations of non-equilibrium fluids, mainly by molecular dynamics.

1. THE HYDRODYNAMIC EQUATIONS

The basic balance equations, in a simple monoatomic fluid, are mass, momentum and energy conservation equations[2,3,4]. Mass density being denoted by $\rho=\rho(\mathbf{R},t)$ and fluid velocity by $\mathbf{u}=\mathbf{u}(\mathbf{R},t)$, the mass conservation property implies

$$\frac{\partial \rho}{\partial t} + \mathbf{div} \cdot \{\rho\,\mathbf{u}\}= 0 \tag{1}$$

which is called the Continuity Equation. The momentum conservation equation reads

$$\frac{\partial (\rho\mathbf{u})}{\partial t} + \mathbf{div} \cdot \{\rho\mathbf{u}\mathbf{u}+\mathbf{P}\} =0 \tag{2}$$

where $\mathbf{P}$ is a second order tensor, the pressure tensor. The third equation is for energy conservation: given $e(\mathbf{R},t)$ the internal energy per unit mass and $\mathbf{J}_q$ the heat flux, one can write the exact conservation equation,

$$\frac{\partial (\rho(e+\frac{u^2}{2}))}{\partial t} + \mathbf{div} \cdot \{\rho\,\mathbf{u}\,(e+\frac{u^2}{2}) +\mathbf{P}.\mathbf{u} + \mathbf{J}_q\} =0 \tag{3}$$

These hydrodynamic equations are exact but not closed since they involve fluxes. In order to close them, relations between the quantities involved are needed. First, the <u>constitutive relations</u> which are phenomenological links between the fluxes $\mathbf{P}$ and $\mathbf{J}_q$ and the gradients (thermodynamic forces) of the variables themselves. These are the Fourier's law

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$$J_q = - \lambda \; \mathbf{grad} \; T \tag{4}$$

and Newton's law, which reads

$$P_{ij} = p \, \delta_{i,j} - \eta \, [\, \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \, \mathbf{div} \cdot \mathbf{u} \, \delta_{i,j} \,] - \zeta \quad \mathbf{div} \cdot \mathbf{u} \, \delta_{i,j} \tag{5}$$

These linear relations between fluxes and gradients involve the transport coefficients: λ, the thermal conductivity, η, the shear viscosity and ζ, the bulk viscosity, which in general depend on density and temperature, and therefore they cannot be considered as constant in space when the fluid is inhomogeneous.

The second set of relations needed to close the hydrodynamic equations is the relation between p, the hydrostatic pressure, and T, the temperature, with the variables ρ, $\mathbf{u}$ and e. This is provided by the local equilibrium hypothesis, which states that pressure and temperature are local equilibrium functions of the hydrodynamic fields e and ρ:

$$p = p(e, \rho), \qquad \frac{1}{T} = \left(\frac{\partial s}{\partial e} \right)_\rho \quad \text{with } s = s(e, \rho) \tag{6}$$

One can use these relations to express the equations obtained in various equivalent forms, depending on the variables chosen.

These equations can be solved when they are linearized around absolute equilibrium. For small deviations, one obtains a closed set of five equations which can be put under the form of "normal modes" solutions, the so-called hydrodynamic modes: two shear diffusive modes, two damped sound modes and an entropy diffusing mode. These solutions have been used to model the thermal fluctuations which spontaneously occur in equilibrium fluids and this has lead to the development of techniques measure transport coefficients through light scattering experiments[5].

The equation for the fluid velocity, in the case of an incompressible fluid of uniform temperature (the viscosity being constant) takes the form

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}.\mathbf{grad}) \, \mathbf{u} = - \frac{1}{\rho} \, \mathbf{grad} \, \{p\} + \frac{\eta}{\rho} \, \Delta \, \mathbf{u} \tag{7}$$

This equation only depends on the kinematic viscosity, $v = \eta / \rho$, and has a very rich variety of solutions. The central dimensionless parameter is the Reynolds number, $Re = uL/v$, where L is the characteristic length of the flow: this parameter appears as the ratio of the spatial derivative appearing in the left hand side ($ugradu \approx u^2/L$) to the one appearing in the right hand side ($v\Delta u \approx vu/L^2$). The scaling property of eq. (7) states that different flows in the same geometry can be related by a simple scaling relation if they have the same Reynolds number. For small Re, the right hand side of eq. (7) dominates and the dissipative terms smooth the flow. On the contrary, at high Re, the (non-linear) left hand side dominates and the fluid behaves as if it were inviscid.

Given precise boundary values for the velocity field, one may find in simple cases stationary solutions to eq. (7). These solutions exist for any value of the Reynolds number. However, for high values of Re, these solutions loose their stability in the sense that small perturbations like thermal fluctuations which take place in the fluid tend to grow. Actually there is a critical value of Re at which the fluid undergoes a bifurcation, with the appearance of a periodic motion added to the stationary solution. Increasing Re will induce more and more frequencies and phases, giving rise to a motion with more and more degrees of freedom (see reference 2). At very high values of Re, the number of degrees of freedom tend to infinity. Simplified models have been developed and studied these last years which aim at understanding the behaviour of the fluid at and near the transition point.

Although the turbulent behaviour observed in nature is probably well described by eq. (7), it is sometimes said that there is no theory of turbulence, except for the Kolmogorov approach: this is a theory which permit to predict local properties of turbulence by scaling arguments and it is presented in a modern perspective in Frisch's paper in this volume. This

absence of theory refers to the (up to now) impossibility to simplify the starting equation. One has to rely mainly on numerical solutions in order to compute the behaviour of the fluid in a given geometry. Many different numerical techniques have been developed these last years and many problems have been solved in this way[6].

A numerical solution is basically a transformation of PDE's into a finite set of algebraic equations[7]: in this sense, numerical simulations of Navier-Stokes equations only contain a finite number of degrees of freedom or modes and no method can pretend to give a full solution to the original equations. One has to discretize in space and time and in doing so, for example, one assumes that the evolution taking place on scales smaller than the grid size or the timesteps, being quickly damped, does not affect the subsequent fluid behaviour. Also, since one cannot resolve the small scales of turbulence in some regions, use has to be done of sub-grid turbulence models. Methods are mostly justified by their successes and limited by their failures when solutions are compared to experiments. A technique which has achieved successes in reproducing a 3D flow with Re ranging up to 10^6 cannot be straightforwardly applied in other geometries or conditions.

One sometimes also refers to the general name of Navier-Stokes equations to mention the complete set of the five equations in the general (compressible) case. This set of equations also leads to phenomena like bifurcations and loss of stability for stationary solutions in constrained systems: for example, in a fluid layer heated from below, at a critical value of the Rayleigh number, convection starts in the fluid and a stable structure is formed. While increasing the external forcing, and therefore the corresponding Rayleigh number, successive bifurcations will take place, with the appearance of new frequencies and phases, leading to the same very complex turbulent behaviour. Here also, scaling arguments, simplified models and numerical solutions have served as basic ingredients in order to understand non-equilibrium fluids. The study of fluid instabilities[8,9,10,11] has served as a paradigm to develop new conceptual tools which have served in many other areas of non-linear science, ranging from chemistry to quantum optics.

2. KINETIC THEORY

Three basic motivations have pushed the development of a more fundamental approach in the description of non-equilibrium fluids: first, one would like to have a justification of the constitutive relations and of the local equilibrium hypothesis based on physical grounds. Second, one is willing to have a theory which would describe the behaviour of fluids in conditions where the Navier-Stokes equations are no more valid: boundary layers and shock fronts are typical examples (fully developed turbulence could be also a possible case). Third, it is desirable to provide a link between the transport coefficients and the microscopic models in the same way that equilibrium statistical mechanics has given the tool to compute the equation of state from a hamiltonian.

From these three basic goals, only the third one can be considered as really achieved: indeed the determination of transport coefficients from microscopic models can be done at equilibrium and in that case linear response can be safely used: one can derive (formal) microscopic expressions for the hydrodynamic modes, independently of any approximations, that is valid for every fluid density: the evaluation of these formal expressions however require involved computations and approximations. Let us only mention that the details of the potential of interaction between model particles do not seem to be very important for the values of the transport properties[12].

The first two objectives cited above are still the object of intense research. Much of the work done in this area has been based on the Boltzmann equation, the equation which determines the time dependence of the one particle distribution function in a dilute gas. It has also served as an example, a guide for dense fluids. However, successes in kinetic theory of liquids are limited either to formal results or to near equilibrium situations[13].

Let $f_1(\mathbf{R}, v, t)$ be the one particle distribution function. Its time evolution can be derived from the equation of motion of the particles which constitute the fluid: hard sphere particles which have no interaction energy but have an excluded volume, Lennard-Jones point particles or soft spheres are typical satisfactory models for atomic fluids. This leads to the so-called BBGKY hierarchy equations: the equation for f_1 involve f_2, the one for f_2 involve f_3 and so on up to the equation for the full phase space density f_N. The first equation of the hierarchy simplifies in the case of a dilute system ($nd^3 \rightarrow 0$, with n the number density and d a molecular size parameter): one then assumes that collisions are instantaneous in time and local in space

and that the two particle correlation function can be factorized as a product of one particle functions, the celebrated "stosszahlansatz", molecular chaos assumption[14]. Under these conditions, the Boltzmann equation follows: in the absence of external forces it reads,

$$\frac{\partial f_1}{\partial t} + v \cdot \frac{\partial f_1}{\partial R} = \int dv_1 \int d\Omega \; \sigma(\chi,g) \; g[\; f_1(R,v',t) f_1(R,v_1',t) - f_1(R,v,t) f_1(R,v_1,t)] \qquad (8)$$

The equation expresses the change of the density f_1 as due to the inertial term $(v \cdot \partial/\partial R)$ and a gain and loss balance: particles with velocity v at R collide with particles of velocity v_1 at R, with deflection angle χ and cross section σ: g is the relative velocity $|v_1-v|$ and the post-collision velocities are denoted with a prime.

This is not an exact equation. It is an approximate equation which has been shown to follow rigorously from dynamics for a finite time interval and in the so-called Grad limit: $n\rightarrow\infty$, $d\rightarrow 0$, nd^2 finite[15]. Existence theorems for solutions have been proven in specific cases. More important, this equation has an H-theorem which states that, if a solution exist, then it evolves in time in a monotonous way to the equilibrium distribution. Most of what we know on this solution is still based on the perturbative method devised by David Enskog and independently by Sydney Chapman.

This latter method is based on a theorem which is worth recalling since it leads to a kind of paradox[16]. This is Hilbert's theorem which states that f_1 can be expanded as a power series in a parameter δ, the Knudsen number, then its solution for positive times only depends on the initial value of the five first moments of f_1 which are precisely the conserved variables:

$$\rho(R,t) = m \int dv \; f_1(R,v,t) \qquad (9a)$$

$$\rho(R,t) \; u(R,t) = m \int dv \; v \; f_1(R,v,t) \qquad (9b)$$

$$\rho(R,t) \; e(R,t) = m \int dv \; m\frac{(v-u)^2}{2} f_1(R,v,t) \qquad (9c)$$

Note that the left hand side of eq. (8) is of order u/L, while the left hand side is of order $1/\tau_{coll}$. Dividing both sides by u/L, we find that the left hand side is of order $L/\Lambda \approx \delta^{-1}$, the inverse of the Knudsen number which is used as a smallness parameter. This leads to a singular perturbation problem, since the assumed expansion is singular in the limit $t\rightarrow 0$. However, the theorem suggests that for times larger than the collision time, there exist solutions which depend only on the first five moments of f_1 and not on the full f_1 at $t=0$: these are called normal solutions.

The Chapman-Enskog[17] method and a mathematically sounder method subsequently developed by Grad[18,19], the moment method, are explained at length in classical textbooks on kinetic theories. They lead to successive approximations of the equations for the conserved variables, the smallness parameter being the Knudsen number as shown on the table below

order in δ	$f_1 =$		transport equations	transports coefficients
zeroth	$f^{(0)}_{local\ equilibrium}[1+$		Euler	no
first	$\phi^{(1)}+$	$o(\frac{\partial}{\partial R})$	Navier-Stokes	λ,η,ζ
second	$\phi^{(2)}+...$	$o(\frac{\partial^2}{\partial R^2})$	Burnett	19
...			....	...

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