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INTERNATIONAL WORKSHOP ON PARALLEL PROCESSING AND ITS APPLICATIONS IN PHYSICS, CHEMISTRY AND MATERIAL SCIENCE
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PDE'S Cellular Automata and Parallel Computing

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These are preliminary lecture notes, intended only for distribution to participants.

PDE'S, CELLULAR AUTOMATA and PARALLEL COMPUTING

Federico Massaioli

CASPUR

Navier-Stokes Equations

$$\partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u} + \frac{1}{\rho}\boldsymbol{F}$$

$$\nabla\cdot\boldsymbol{u} = 0$$

- Generally difficult to solve
- Many established, highly efficient numerical techniques are available
- Many of these are not suitable to distributed memory parallel machines
- Treatment of flows in porous media or multiphase flows is difficult

Micro- and Macro-Dynamics

- N-S equations are a macroscopic description of a fluid

- The large scale behaviour of a fluid is a 'limit' of the dynamics on the molecular scale

- An arbitrary microdynamics can be simulated, as long as N-S equations are recovered in the macroscopic limit

- It is possible to choose the microdynamics of the system to ease parallel implementations and to support the description of highly heterogeneous media

Lattice Boolean Gases

(Frisch, d'Humières, ...)

- Regular lattice with every lattice site $\boldsymbol{x}$ connected to b neighbouring sites

$$\boldsymbol{x}+\boldsymbol{c}_i \quad i=1,\ldots,b$$

- The state of every site is encoded in b boolean variables n_i , evolving according to the rule

$$n_i(\boldsymbol{x}+\boldsymbol{c}_i,t+1)-n_i(\boldsymbol{x},t)=\Omega_i(n_j(\boldsymbol{x},t))$$

- The lattice and Ω_i must be chosen to recover N-S

- n_i encodes the presence of a particle with velocity $\boldsymbol{c}_i$

From Boolean to Real
(McNamara, Zanetti)

- Conventional computers are oriented toward floating point performance

- Boolean gases suffer from statistical noise, i. e. huge quantities of sites are needed

- In 3D, Ω_i is not expressible in a closed form

- The transformation from boolean to floating point ('mesoscopic' limit) solves the first two problems

$$n_i \quad \rightarrow \quad N_i = \langle n_i \rangle$$

The Last Steps

- Chapman-Enskog limit (Higuera, Jimenez):

$$\Omega_i = \sum_{j=1}^{b} A_{ij}(N_i - N_i^{eq})$$

with A_{ij} constructed from the boolean microdynamics

- Enhanced Collisions (Higuera, Succi, Benzi):
  A_{ij} can be derived from the conservation laws and the physical parameters, i.e. LBE is a model of hydrodynamics, unrelated to microdynamics of any type

The LBE Scheme

$$N_i(\boldsymbol{x}+\boldsymbol{c}_i, t+1) =$$

$$N_i(\boldsymbol{x}, t) + \sum_{j=1}^{b} A_{ij}\left(N_j(\boldsymbol{x}, t) - N_j^{eq}(\boldsymbol{x}, t)\right)$$

with

$$N_i^{eq} =$$

$$\frac{\rho_{eq}}{b}\left(1 + \frac{D}{c^2} u_\alpha c_{i\alpha} + \frac{D^2}{2c^4} \frac{b - 2\rho_{eq}}{b - \rho_{eq}} Q_{i\alpha\beta} u_\alpha u_\beta\right)$$

where

$$c = |\boldsymbol{c}_i|$$

$$Q_{i\alpha\beta} = c_{i\alpha} c_{i\beta} - \frac{c^2}{D} \delta_{\alpha\beta}$$

Hydrodynamic Behaviour

- FCHC 4D ($b = 24$) lattice projected down in 1, 2 or 3 D

- The collision matrix has 4 different eigenvalues: 0 (conservation laws), λ (viscosity), σ and τ (spurious ghost fields)

- Adiabatic limit:

$$\rho(\boldsymbol{x},t)=\sum_{i=1}^{b} N_i(\boldsymbol{x},t)$$

$$\boldsymbol{J}(\boldsymbol{x},t)=\rho(\boldsymbol{x},t)\,\boldsymbol{u}(\boldsymbol{x},t)=\sum_{i=1}^{b} \boldsymbol{c}_i N_i(\boldsymbol{x},t)$$

obey the N-S equations under some constraints on the collision matrix eigenvalues

LBE Pros

- Maintenance of a main, general purpose and optimized code
- Simple, quick and efficient SIMD and MIMD parallel implementations
- Easy boundary conditions
- Easy simulation of flows in grossly irregular geometries

LBE Cons

- Low Mach number
- Moderate Reynolds number
- Stability implies that on a lattice step $\Delta u/u < 20\%$

LBE Applications

- Turbulent Thermal Convection
- Flows in Porous Media
- Oil Reservoir Modelling
- Multiphase Flows

Recent Developments

- Unevenly Spaced Grids
- Compressible Flows
- Quantum Mechanics
- Lattice BGK Models

Future Developments

- Finite Volume LBE on Embedded Adaptive Grids