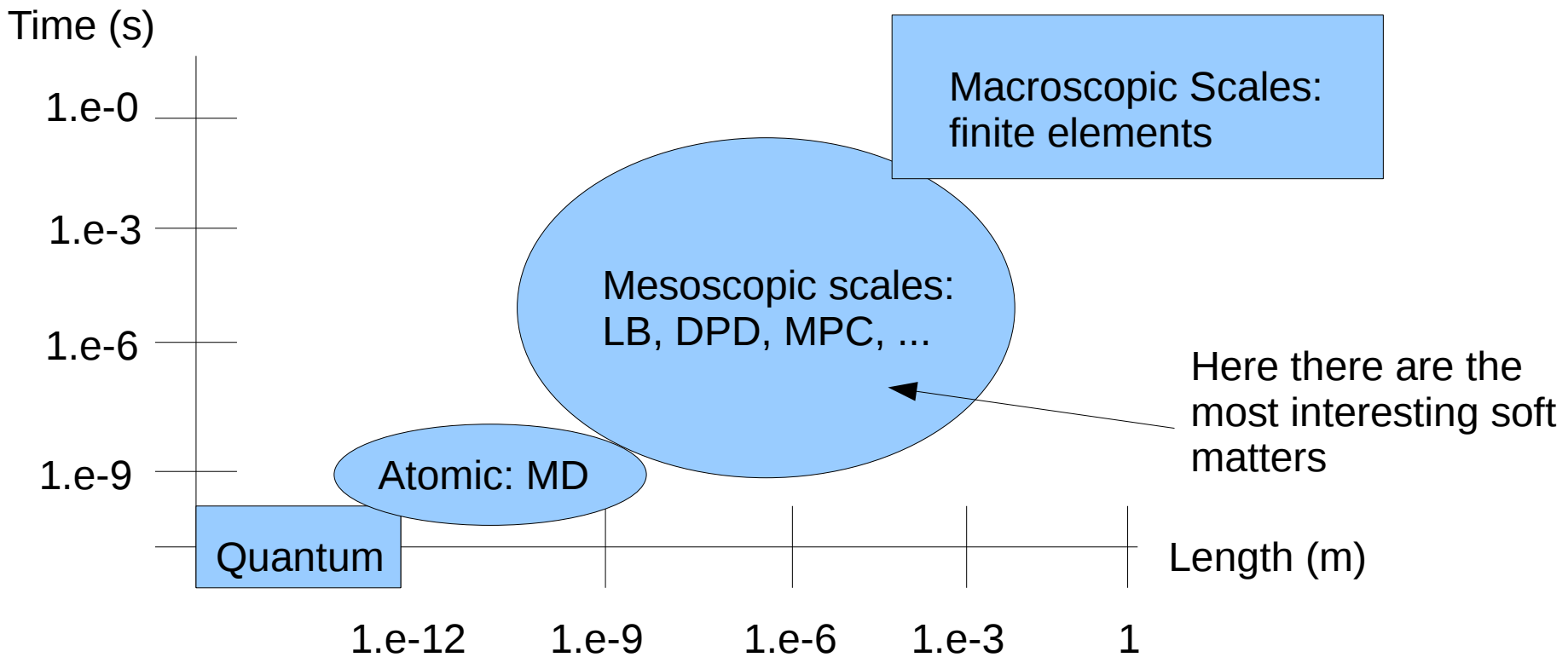
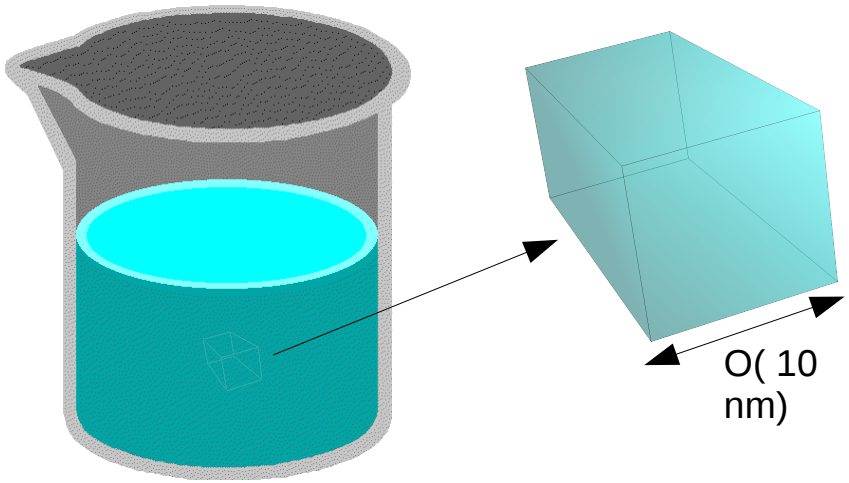
MESOSCOPIC METHODS

- MD, MC: microscopic description of the fluids or systems.
- But we need to go to higher sizes.



THE ROOT OF THE PROBLEM



- The limited power of current computers makes impossible simulate macroscopic systems.
- In small systems the ratio area vs volume is large and we have important surface effects.
- This surface effects prevent us of simulating correctly the behaviour of the bulk system by just considering the particles inside our cell.
-Furtheremore, due to the very small sizes accesible to us, the long-range component of the electrostatic interactions cannot be handled in an exact manner.

Distraction: Simulating 1cm^3 of H_2O aka 10^{23} atoms at 1/7/2006. Are we hopeless?

#1: Blue Gene DOE (USA) 367000 Gflop/s (#8: JUBL (Juelich) 45875 Gflop/s)

Flops required each step per atom	1	10	100	10^3	10^6	...	10^{23}
Calculate 1 step with current computer power (in years)	8.64	86.4	864	8640	8.6 millions	...	$8.6*10^{23}$ millions
Years to pass to be able to do the same in 1 second . Using Moore's law (double each 1.5 years).	42	47	51	57	72	...	156

AVAILABLE TOOLS:

* **BD – Brownian Dynamics:** solute is represented implicitly by random forces and frictional terms. Langevin equations. Problems: non conservation momentum, so diffusion but not hydrodynamics. You can put a tensor in Langevin equations and ..., but N very low.

* **SPH – Smoothed Particle Hydrodynamics**: (aka SPAM), you discretize the macroscopic partial differential equations like Navier Stokes in a irregular Lagrangian moving grid. One node can be considered one coarsened particle of fluid.

* **DMSC – Direct Simulation Monte Carlo**: for flow of diluted gases ok. Set of particles, alternating streaming (particles move ballistic) and collision steps (you choose particles to collide inside given "collision boxes"). Rules of collision according to the model you want, but always should respect M, p, E to be conserved.

* **LGA – Lattice gas automata**: the continuous is replaced by a set of particles that move from site to site in a regular fixed lattice. If two find themselves in a same lattice point, they collide and change their v following some rules. Better dt, and lengths than MD, but some problems ahoy: not Galilean invariant, no isotropy. Ways to solve it, but for systems with more than a phase or more complex fluids, difficult to solve, and not so appealing.

* **LB – Lattice Boltzmann**: improvement respect LGA. We use particle density distributions instead of single particles. We will see it later in detail.

AVAILABLE TOOLS (Cont):

* **DPD – Dissipative Particle Dynamics:** Fluid is described as N coarsened particles with continuous positions and velocities. Langevin equations to describe the movement. In the original DPD energy is not conserved (so restricted to isothermal systems) , but it can be fixed DPD+e. Problem Sc ~ 1.

* **MPC – Multiparticle Collision Dynamics (aka SRD – stochastic rotation dynamics)**: the youngest (1999). A variant of DSCM: collision (rotations all particles inside cells) + streaming (ballistic). You need random shifts of the cell to preserve Galilean invariance. You can hope to cope with a larger range of Sc numbers (the larger the Sc, more costly is the calculus). Very new, still room for testings and improvements.

Sc = Schmidt number ;
Sc = kinematic viscosity / Diffusion coefficient ← How important are Hydrodynamic effects?