Scientific Computing II

Molecular Dynamics Simulation

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Molecular Dynamics and N-Body Problems – An Introduction

- Micro and Nano Simulations
- Astrophysics
- Particle-oriented Numerical Methods
- Laws of Motion
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Micro and Nano Simulations
Astrophysics
Particle-oriented Numerical Methods
Laws of Motion
The Simulation Pipeline – What Did We Cover So Far?

phenomenon, process etc. → modelling

mathematical model → numerical treatment

numerical algorithm → implementation

simulation code → visualization

results to interpret

statement tool

embedding
The Seven Dwarfs of HPC – Dwarf # 4

“dwarfs” = key algorithmic kernels in many scientific computing applications

P. Colella (LBNL), 2004:
1. dense linear algebra
2. sparse linear algebra
3. spectral methods
4. **N-body methods**
5. structured grids
6. unstructured grids
7. Monte Carlo
Molecular Dynamics – Overview

- **modelling** aspects of molecular dynamics simulations:
  - why to leave the classical continuum mechanics point of view?
  - where appropriate?
  - which models, i.e. which equations?
- **numerical** aspects of molecular dynamics simulations?
  - how to discretize the resulting modelling equations?
  - efficient algorithms?
- **implementation** aspects of molecular dynamics simulations?
  - suitable data structures?
  - parallelisation?
# Hierarchy of Models

Different points of view for simulating human beings:

<table>
<thead>
<tr>
<th>issue</th>
<th>level of resolution</th>
<th>model basis (e.g.!)</th>
</tr>
</thead>
<tbody>
<tr>
<td>global increase in population</td>
<td>countries, regions</td>
<td>population dynamics</td>
</tr>
<tr>
<td>local increase in population</td>
<td>villages, individuals</td>
<td>population dynamics</td>
</tr>
<tr>
<td>man</td>
<td>circulations, organs</td>
<td>system simulator</td>
</tr>
<tr>
<td>blood circulation</td>
<td>pump/channels/valves</td>
<td>network simulator</td>
</tr>
<tr>
<td>heart</td>
<td>blood cells</td>
<td>continuum mechanics</td>
</tr>
<tr>
<td>cell</td>
<td>macro molecules</td>
<td>continuum mechanics</td>
</tr>
<tr>
<td>macro molecules</td>
<td>atoms</td>
<td>molecular dynamics</td>
</tr>
<tr>
<td>atoms</td>
<td>electrons or finer</td>
<td>quantum mechanics</td>
</tr>
</tbody>
</table>
Scales – an Important Issue

- length scales in simulations:
  - from $10^{-9}$ m (atoms)
  - to $10^{23}$ m (galaxy clusters)
- time scales in simulations:
  - from $10^{-15}$ s
  - to $10^{17}$ s
- mass scales in simulations:
  - from $10^{-24}$ g (atoms)
  - to $10^{43}$ g (galaxies)
- obviously impossible to take all scales into account in an explicit and simultaneous way
- first molecular dynamics simulations reported in 1957
More General: Particle-Oriented Simulation Methods

General Approach:

- "N-body problem"
  → compute motion paths of many individual particles
- requires modelling and computation of inter-particle forces
- typ. leads to ODE for particle positions and velocities

Examples:

- Molecular dynamics
- Astrophysics
- Particle-oriented discretisation techniques
Lab-on-a-chip, used in brewing technology (Siemens)
Flow through a nanotube (where the assumptions of continuum mechanics are no longer valid)
Protein simulation: actin, important component of muscles (overlay of macromolecular model with electron density obtained by X-ray crystallography (brown) and simulation (blue))
Applications for Micro and Nano Simulations

Protein simulation: human haemoglobin (light blue and purple: alpha chains; red and green: beta chains; yellow, black, and dark blue: docked stabilizers or potential docking positions for oxygen)
Applications for Micro and Nano Simulations

Material science: hexagonal crystal grid of Boronitrid
HPC Example – Gordon Bell Prize 2005

- Gordon-Bell-Prize 2005 (most important annual supercomputing award)
- phenomenon studied: solidification processes in Tantalum and Uranium
- method: 3D molecular dynamics, up to 524,000,000 atoms simulated
- machine: IBM Blue Gene/L, 131,072 processors (world’s #1 in November 2005)
- performance: more than 101 TeraFlops (almost 30% of the peak performance)

(Streitz et al., 2005)
HPC Example – Millennium-XXL Project

- \( N \)-body simulation with \( N = 3 \cdot 10^{11} \) “particles”
- study gravitational forces
  (each “particles” corresp. to \( \sim 10^9 \) suns)
- simulates the generation of galaxy clusters
  served to “validate” the cold dark matter model

(Springel, Angulo, et al., 2010)
Simulation Figures:

- $N$-body simulation with $N = 3 \cdot 10^{11}$ particles
- 10 TB RAM required only to store positions and velocities (single precision)
- entire memory requirements: 29 TB
- JuRoPa Supercomputer (Jlich)
- computation on 1536 nodes (each 2x QuadCore, i.e., 12 288 cores)
- hybrid parallelisation: MPI plus OpenMP/Posix threads
- execution time: 9.3 days; ca. 300 CPU years
Example – Gordon Bell Prize 2010

- direct simulation of blood flow
- particulate flow simulation (coupled problem)
- Stokes flow for blood plasma
- red blood cells as immersed, deformable particles

(Rahimian, . . . , Biros, 2010)
Example – Gordon Bell Prize 2010 (2)

Simulation – HPC-Related Data:
- up to 260 Mio blood cells, up to $9 \cdot 10^{10}$ unknowns
- fast multipole method to compute Stokes flow (octree-based; octree-level 4–24)
- scalability: 327 CPU-GPU nodes on Keeneland cluster, 200,000 AMD cores on Jaguar (ORNL)
- 0.7 Petaflops/s sustained performance on Jaguar
- extensive use of GEMM routine (matrix multiplication)
- runtime: $\approx$ 1 minute per time step

Article for Supercomputing conference:
http://www.cc.gatech.edu/~gbiros/papers/sc10.pdf
Example – Smoothed Particle Hydrodynamics

- approximate functions using kernel functions $W$:

$$f(x) \approx \int_{V} f(r') W(|r - r'|, h) \, dV'$$

- for $h \to 0$: $W \to \delta$ (Dirac function)

- approximation of derivatives → integration by parts:

$$\nabla f(x) \approx \int_{V} f(r') \nabla W(|r - r'|, h) \, dV'$$
Example – Smoothed Particle Hydrodynamics (2)

• approximate integrals at particle positions:

\[ f(r_i) \approx \sum_{j=1}^{N} \frac{m_j}{\rho(r_j)} f(r_j) W(|r_i - r_j|, h) \]

• in particular for the density

\[ \rho(r_i) \approx \sum_{j=1}^{N} m_j W(|r_i - r_j|, h) \]

• similar for derivatives:

\[ \nabla f(r_i) \approx \sum_{j=1}^{N} \frac{m_j}{\rho(r_j)} f(r_j) \nabla W(|r_i - r_j|, h) \]

• leads to N-body problem (based on Navier-Stokes equations, e.g.)
Laws of Motion

- force on a molecule: \( \vec{F}_i = \sum_{j \neq i} \vec{F}_{ij} \n\)
- leads to acceleration (Newton’s 2nd Law):

\[
\ddot{r}_i = \frac{\vec{F}_i}{m_i} = \frac{\sum_{j \neq i} \vec{F}_{ij}}{m_i} = -\sum_{j \neq i} \frac{\partial U(\vec{r}_i, \vec{r}_j)}{\partial |\vec{r}_{ij}|} m_i
\]  

(1)

- system of \( dN \) ODE (2nd order)
  (\( N \): number of molecules, \( d \): dimension),
- reformulated into a system of \( 2dN \) 1st-order ODEs:

\[
\vec{p}_i := m_i \dot{r}_i \\
\dot{\vec{p}}_i = \vec{F}_i
\]  

(2a)  

(2b)
Example: Hooke’s Law

- "harmonic potential": $U_{\text{harm}}(r_{ij}) = \frac{1}{2} k (r_{ij} - r_0)^2$
- potential energy of a spring of length $r_0$ when extended or compressed to length $r_{ij}$
- resulting force:

1D: $\vec{F}_{ij} = -\nabla U(r_{ij}) = -\frac{\partial U}{\partial r_{ij}} = -k (r_{ij} - r_0)$

allg.: $\vec{F}_{ij} = -k (r_{ij} - r_0)$
Example: Gravity

- attractive force due to the mass of two bodies (planets, etc.)
- gravity potential: \( U_{\text{grav}} (r_{ij}) = -g \frac{m_i m_j}{r_{ij}} \)
- resulting force:

\[
1D : \quad \vec{F}_{ij} = -\text{grad} U (r_{ij}) = -g \frac{m_i m_j}{r_{ij}^2}
\]
Example: Coulomb Potential

- attractive or repulsive force between charged particles
- Coulomb potential: \( U_{\text{grav}} (r_{ij}) = \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{r_{ij}} \)
- resulting force:
  \[
  1D: \quad \vec{F}_{ij} = -\nabla U (r_{ij}) = \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{r_{ij}^2}
  \]