# Molecular Dynamics

Simulation of the many-body system on the Heterogeneous cluster HybriLIT

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Kristýna Zoubková (CTU),
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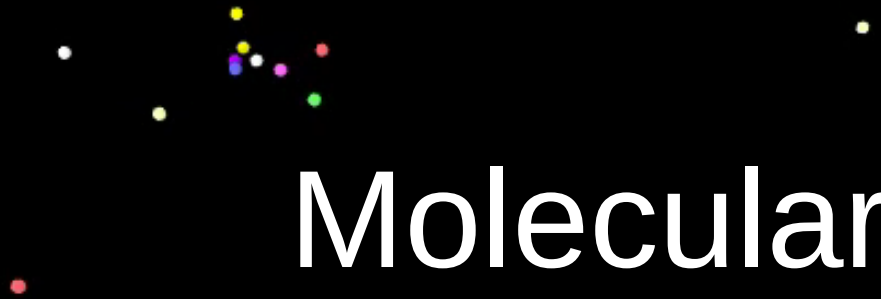

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# Introduction

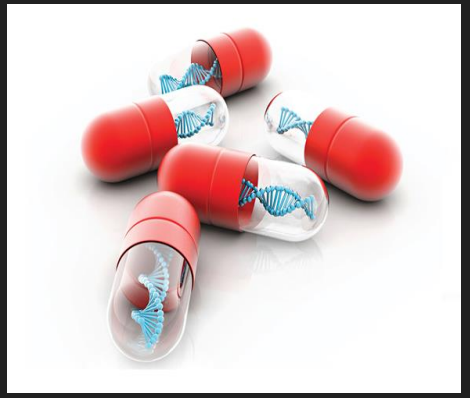
1. Molecular dynamics method
2. Application - Solar system model
3. Results
4. Other activities during practice

# History

- First introduced in 1950s by Alder and Wainwright
- First simulations
  - elastic collisions of spheres
  - radiation damage of copper
  - liquid argon

# Motivation

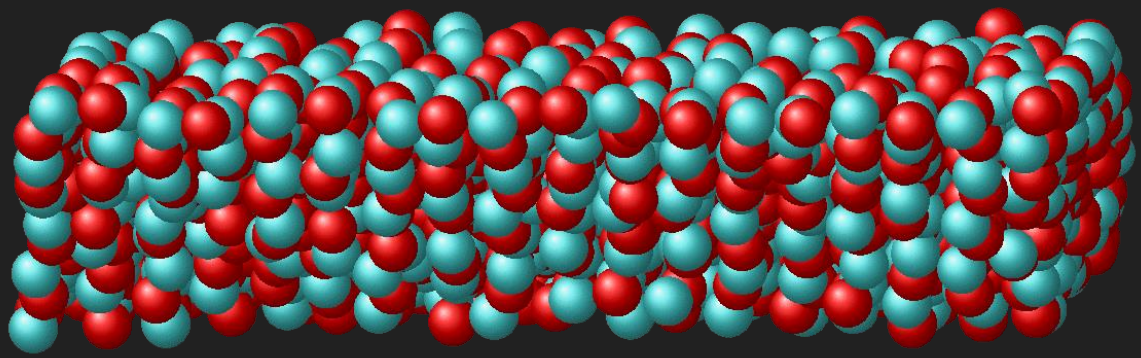
- Physic helps us to understand chemistry
- Bridge between microscopic and macroscopic world
- Bridge between theory and experiment
- Application - Synthesis, Fuels, Medicine

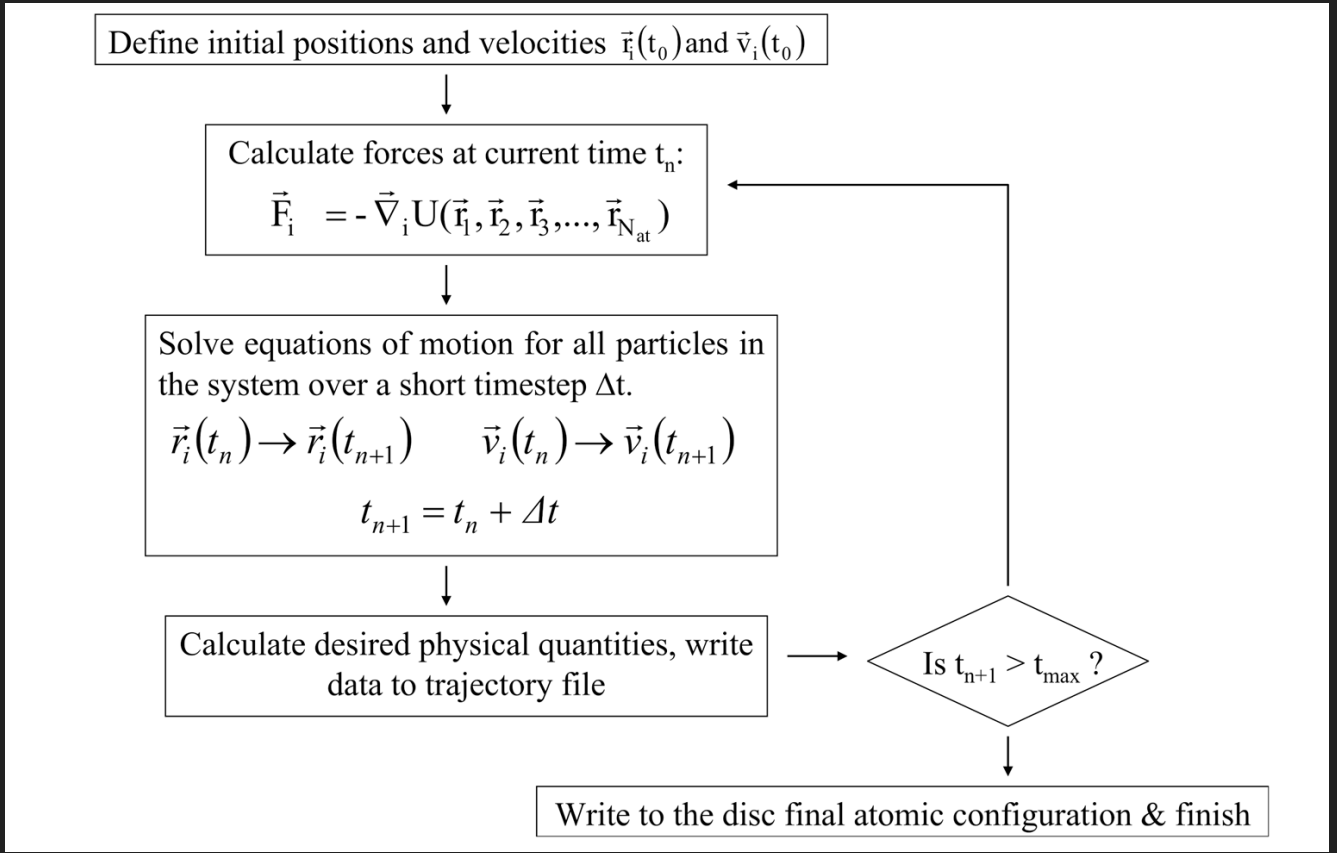
# Molecular dynamics method

- Simulation method for many body systems
- Used to observe movement of molecules or atoms
- Utilizes Newton's second law to predict motion

$$m_k \ddot{\vec{x}}_k(t) = F_k\left(\overrightarrow{x_1}(t) \dots \overrightarrow{x_n}(t)\right) = -\nabla_{\vec{x}_k} U\left(\overrightarrow{x_1}(t) \dots \overrightarrow{x_n}(t)\right)$$



# Algorithm


Define initial positions and velocities $\vec{r}_i(t_0)$ and $\vec{v}_i(t_0)$
Calculate forces at current time $t_n$:
$\vec{F}_i = -\vec{\nabla}_i U(\vec{r}_1, \vec{r}_2, \vec{r}_3, ..., \vec{r}_{N_{at}})$
Solve equations of motion for all particles in the system over a short timestep Δt.
$\vec{r}_i(t_n) \rightarrow \vec{r}_i(t_{n+1})$ $\vec{v}_i(t_n) \rightarrow \vec{v}_i(t_{n+1})$
$t_{n+1} = t_n + \Delta t$
Calculate desired physical quantities, write data to trajectory file
Is $t_{n+1} > t_{max}$ ?
Write to the disc final atomic configuration & finish

# Solar system simulation

- Simulation for 61 bodies - planets, moons, dwarf planets etc.
- Initial conditions - real data from NASA and Caltech

  - https://ssd.jpl.nasa.gov/horizons.cgi

Simulation

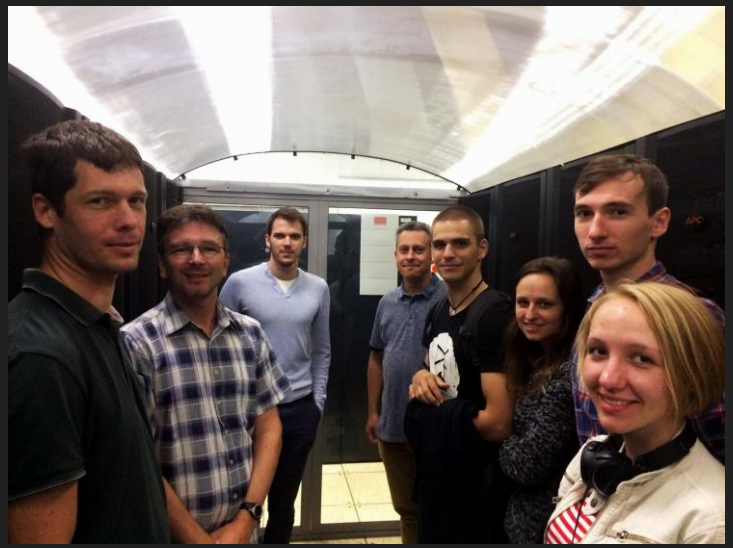
1. Solar system
2. Collision with another sun
3. Collision of two solar system

A. Stukowski Visualization and analysis of atomistic simulation data with OVITO - the Open Visualization Tool Modelling. Simul. Mater. Sci. Eng. 18 (2010), 015012 http://ovito.org/

# Other activities

International Conference “Mathematical Modeling and Computational Physics, 2017” (MMCP2017)

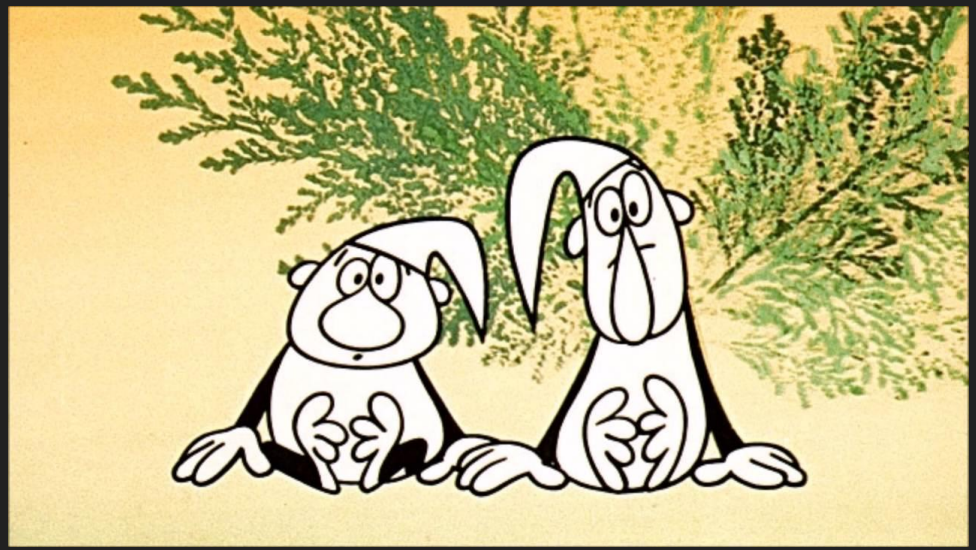
- Lectures
  - C/C++ programming
  - MPI parallel programming technology
  - OpenCL parallel programming technology
- Excursions
  - Heterogeneous cluster HybriLIT



# Heterogeneous cluster *HybriLIT*

- Computation component of a multifunctional center for data storage, processing and analysis
- Used for parallel programming technologies
- Nvidia graphic processors and Intel Xeon Phi coprocessors

Any questions?



# Thank you for your attention