Introduction to Scientific Computing II

Molecular Dynamics Simulation (3)

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MD – Implementational Aspects
  - Verlet Neighbour Lists
  - Linked-Cell Algorithm
  - Linked-Cell – Data Structures

MD – Parallelisation
  - Shared Memory Parallelisation
  - Force Decomposition
  - Spatial Decomposition
  - Domain Decomposition
MD – Implementational Aspects
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Verlet Neighbour Lists

- every molecule stores its neighbours for a distance $r_{\text{max}} > r_c$
- every $n_{\text{upd}}$ time steps (dep. on $r_{\text{max}}$), the lists are updated
- the "buffer" has to be larger than the covered distance of a molecule for that time:

$$r_{\text{max}} - r_c > n_{\text{upd}} \Delta t v_m$$
Classical Linked-Cell Algorithm

molecules arranged in a lattice of cubic cells of side length $\sim r_c$

- hash table with "geometrically motivated" hash function
- "Binning" resp. "Bucketing"-techniques from "Computational Geometry"
- direct volume representation (voxel) of the influence region
Classical Linked-Cell Algorithm

molecules arranged in a lattice of cubic cells of side length $\sim r_c$

- runtime: $\mathcal{O}(n)$
- only half (point symmetry) of the neighbour cells are explicitly traversed (Newton’s 3rd law)
- erase and generate the data structure in each time step
Variable Linked-Cell Algorithm

- Lattice might be built up from cells of side length \( \frac{rc}{t} \) with \( t \in \mathbb{R}^+ \)
- Integer numbers are preferable for the divisor \( t \in \mathbb{N} \)
- For \( t \to \infty \), the examined influence volume will converge to the (optimal) sphere
Linked-Cell Algorithm – Data Structure I

- cells are stored as a one-dimensional array (vector)
- intrusive list for the cell molecules
- list to determine the processing sequence
• offset mask to determine the neighbours
• cache efficiency is influenced by the processing order (temporal locality)
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MD – Parallelisation

Profiling

Profiling seq. MD code (LJ 12-6)

→ force calculation is dominating
Shared Memory Parallelisation

- each process calculates one part ($\frac{N}{p}$) of the molecules (cells)
- availability of all relevant data (position) because of common memory
- “Shared Memory” algorithm: Velocity Störmer Verlet method
  1. parallel explicit Euler method $r, v$ (half step) for $\frac{N}{p}$ molecules
  2. parallel force calculations for $\frac{N}{p}$ molecules or the respective cells
     (force summation critical, respecting Newton's 3rd law: reduction; same with linked-cell algorithm)
  3. parallel implicit Euler method $v$ (half step) for $\frac{N}{p}$ molecules
Replicated Data I

- use shared-memory approach also for distributed memory architectures
- every node has to store all position data
- collective communication for the synchronization of redundant data
- result: "Atom Decomposition" algorithm:
  - Velocity Störmer Verlet method
    1. explicit Euler method $r, v$ (half step) for $\frac{N}{p}$ molecules
    2. distribute (gather-to-all) the $\frac{N}{p}$ position data for each PE to all other PEs
    3. force calculation for $\frac{N}{p}$ molecules
    4. possible distribution of partial forces to the appropriate PEs
    5. implicit Euler method for $v$ (half step) for $\frac{N}{p}$ molecules
Replicated Data II

- costs
  - calculation: \( \frac{N}{p} \)
  - communication partners per PE: \( p - 1 \)
  - memory requirements: \( N \) positions and \( \frac{N}{p} \) forces
Replicated Data II – Exploit Symmetry

- calculation: \( \frac{N}{2p} \)
- communication partners per PE: \( p - 1 \)
- memory requirements: taking advantage of Newton's 3rd law needs a vector for \( N \) (partial) forces and additional communication
Force Decomposition I

- each process calculates a part of the molecules and the force matrix
- on each node: position data of \(2 \frac{N}{\sqrt{p}}\) molecules
- communication: distribution of positions and calculated forces
- ”Force Decomposition” algorithm: Velocity Störmer Verlet method
  1. explicit Euler method for \(r, v\) (half step) for \(\frac{N}{p}\) molecules
  2. distribution of \(\frac{N}{p}\) position data per PE to \(2(\sqrt{p} - 1)\) PEs
  3. force calculation of a \(\frac{N}{\sqrt{p}} \times \frac{N}{\sqrt{p}}\) sub-matrix
  4. distribution of partial forces to \(\sqrt{p} − 1\) PEs
  5. implicit Euler method for \(v\) (half step) for \(\frac{N}{p}\) molecules
Force Decomposition II – Costs

- calculation: \( \frac{N}{p} \)
- communication partners per PE: 2 \((\sqrt{p} - 1)\)
Spatial Decomposition

- domain is decomposed into subdomains
- each processor handles one subdomain
- amount of molecules per processor is variable (molecules are moving!)
- overlapping buffer regions (halo, $r_c$) have to be synchronized
Spatial Decomposition

- overlapping buffer regions (halo, $r_c$) have to be synchronized
- point-to-point communication, dependent of
  - decomposition
  - molecule movement (flow velocity)
  - communication method: "x-y-z" vs. "direct"
Domain Decomposition: Cubes $\leftrightarrow$ Slices (1)

- assumption:
  - homogeneous molecule distribution
  - subdomains with $\frac{N}{p}$ molecules and volume $\frac{L^d}{p}$: $N \leftrightarrow L^d$
  - communication size proportional to halo volume

- slices:
  - 2 neighbour PEs
  - halo volume: $L^{d-1}2r_c = 2L^d\frac{r_c}{L}$
  - relatively easy to implement
  - bad scaling properties

- communication
  - amount: $2p$
  - ratio molecules to comm.: $\frac{L^d}{p} : 2L^d\frac{r_c}{L} = \frac{L}{2r_c p}$
Domain Decomposition: Cubes ↔ Slices (2)

- same assumptions
- cubes:
  - $3^d - 1$ neighbour PEs
  - side length: $l = \sqrt[d]{\frac{L^d}{p}} = \frac{L}{\sqrt[d]{p}}$
  - halo volume:
    \[
    (l + 2r_c)^d - l^d = \sum_{i=1}^{d} \binom{d}{i} l^{d-i} (2r_c)^i 
    \approx \binom{d}{1} l^{d-1} 2r_c 
    = 2d l^d r_c = 2d L^d p^{1-d-1} \frac{r_c}{L}
    \]
- communication
  - amount: $(3^d - 1) p$ (direct) or $2d \cdot p$ (x-y-z)
  - ratio molecules to comm.:
    \[
    \frac{\frac{L^d}{p}}{2d L^d p^{1-d-1} \frac{r_c}{L}} = \frac{p^2 L}{2dp^{1-d} r_c}
    \]