Introduction to Scientific Computing II

Molecular Dynamics Simulation (4)

Michael Bader – SCCS

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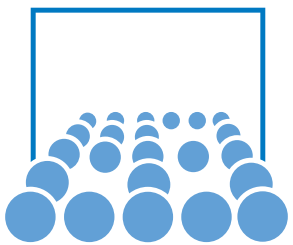

Numerical Methods for Long-Range Potentials

Introduction

Tree-Based Methods

The Barnes-Hut Method

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Numerical Methods for Long-Range Potentials

- so far: focus on **short-range potentials** such as Lennard-Jones, e.g.
  - resulting mutual interactions are restricted to particles in some local neighbourhood
  - facilitates numerical treatment and algorithmic organization: no quadratic complexity induced by an ”each-with-each” behaviour
- now: tackle **long-range potentials**, too
  - examples: Coulomb or gravitation potential
  - interactions between remote particles must not be neglected
  - simple cut-off not possible
  - nevertheless need for approaches that avoid quadratic complexity

Long-Range Potentials (2)

- what is long-range?
  - intuitively: potential function $U(r)$ does not decrease rapidly with increasing r
  - formally (one possibility): for $d > 2$, potentials not decreasing faster than r^{-d} for increasing r (criterion: integrability over $\mathbb{R}^d$)
- typical potentials in applications have both – a short-range part (to be dealt with according to the previous sections) and a long-range part,
  $\rightarrow$ represented as two additive components:

$$U(r) := U^{\text{short}} + U^{\text{long}}$$

Grid-Based Methods

- decompose U^{long} itself into a smooth but long-range and a singular but short-range part
- for the latter, use the linked-cell approach again
- for the first $\rightarrow$ so-called grid-based methods:
  - P^{3}M (Particle-Particle–Particle-Mesh) method
  - PME (Particle-Mesh-Ewald) method
  - SPME (Smooth-Particle-Mesh-Ewald) method)
- starting point: PDE-representation of the potential Φ

$$-\Delta\Phi(x) = \frac{1}{\epsilon_0}\varrho(x)$$

  - potential as solution of a potential (Poisson) equation
  - efficient solution with standard discretisation techniques (Finite Differences or Finite Elements, e.g.)
  - hence, feasible for the smooth long-range part and for homogeneous particle distributions

Hierarchical or Tree-Based Methods

- starting point: integral representation of the potential Φ

$$\Phi(x) = \frac{1}{4\pi\epsilon_0} \int \varrho(y) \frac{1}{\|y - x\|} dy$$

- advantageous especially for heterogeneous particle distributions (frequent in astrophysics, relevant also for molecular dynamics)
- examples:
  - panel clustering
  - Barnes-Hut method
  - (fast) multipole methods

Tree-Based Methods

- based on integral representation of the potential
- hierarchical decompositions of the domain of simulation
- adaptive approximation of the particle distribution
- widespread scheme: **octrees**
- allow for separation of **near-field** and **far-field** influences
- log-linear or even linear complexity can be obtained
- high flexibility with respect to more general potentials (as needed for special applications, such as biomolecular problems)

Series Expansion of the Potential

- general (integral) representation of the potential:

$$\Phi(x) = \int_{\Omega} G(x,y)\varrho(y)dy$$

(general kernel G, particle density $\varrho(y)$, and domain Ω)

- Taylor expansion of the kernel G (if sufficiently smooth apart from the singularity in $x = y$) in y around y_0:

$$G(x,y) = \sum_{\|j\|_1 \leq p} \frac{1}{j!} G_{0,j}(x,y_0)(y-y_0)^j + R_p(x,y)$$

(multi-index $j = (j_1, j_2, j_3)$, $j! = j_1!j_2!j_3!$, $G_{k,j}(x,y)$ mixed (k,j)-th derivative (k-th w.r.t. x, j-th w.r.t. y), remainder $R_p(x,y)$)

Series Expansion of the Potential (2)

- leads to expansion (and approximation) of the potential:

$$\Phi(x) \approx \sum_{\|j\|_1 \leq p} \frac{1}{j!} M_j(\Omega, y_0) G_{0,j}(x, y_0)$$

with the so-called **moments**

$$M_j(\Omega, y_0) := \int_\Omega \varrho(y)(y - y_0)^j dy$$

Subdivision of the Domain

- separation of near-field and far-field for given x:

$$\Omega = \Omega^{\text{near}} \cup \Omega^{\text{far}}, \qquad \Omega^{\text{near}} \cap \Omega^{\text{far}} = \emptyset$$

- decompose far-field into disjoint, convex subdomains:

$$\Omega^{\text{far}} = \bigcup_i \Omega_i^{\text{far}}$$

- note: decomposition depends on x, i.e. it is done for each particle position x
- each Ω_i^{far} has an associated point y_0^i
- how to choose the subdivision?

$$\frac{\text{diam}}{\|x - y_0^i\|} := \frac{\sup_{y \in \Omega_i^{\text{far}}} \|y - y_0^i\|}{\|x - y_0^i\|} \leq \theta$$

for some suitable constant $0 < \theta < 1$

Subdivision of the Domain (2)

resulting approximation for $\Phi(x)$:

$$
\begin{aligned}
\Phi(x) &= \int_{\Omega} \varrho(y) G(x,y)\,dy \\
&= \int_{\Omega^{\text{near}}} \varrho(y) G(x,y)\,dy + \int_{\Omega^{\text{far}}} \varrho(y) G(x,y)\,dy \\
&= \int_{\Omega^{\text{near}}} \varrho(y) G(x,y)\,dy + \sum_i \int_{\Omega_i^{\text{far}}} \varrho(y) G(x,y)\,dy \\
&\approx \int_{\Omega^{\text{near}}} \varrho(y) G(x,y)\,dy + \sum_i \sum_{\|j\|_1 \le p} \frac{1}{j!} M_j(\Omega_i^{\text{far}}, y_0^i) G_{0,j}(x, y_0^i)
\end{aligned}
$$

Error Estimates

- error characteristics for one fix particle position $x \in \Omega$:
  - local relative approximation error for one Ω_i^{far} can be shown to be of order $O(\theta^{p+1})$
  - global relative approximation error (summation over whole far-field) can be shown to be of order $O(\theta^{p+1})$
- this clarifies the role of θ:
  - allows to control the global approximation error in x
  - geometric requirement to the far-field subdivision: the closer Ω_i^{far} is located to x, the smaller it has to be to fulfil the θ-condition
- hence: a typical ”level of detail”
  - the closer, the higher resolved
  - cf. terrain representation in flight simulators

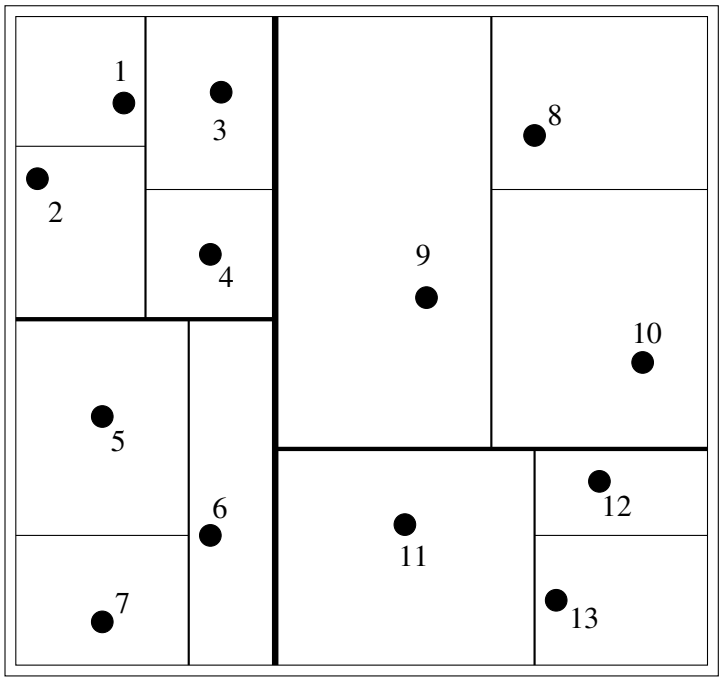
Tree Structures

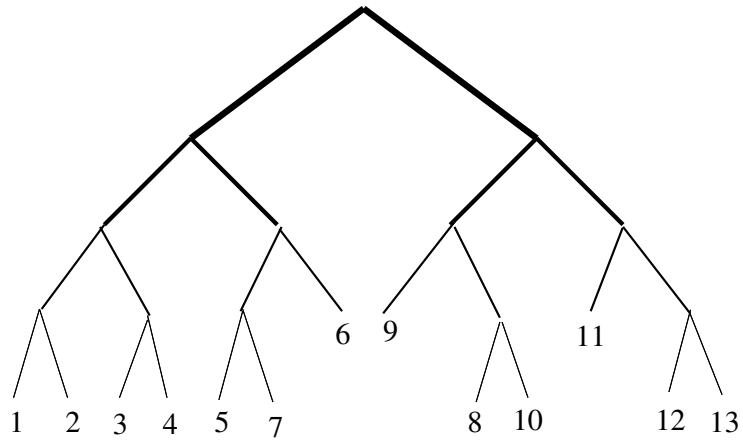
- central question: how can we construct all these necessary separations of near-fields and far-fields and subdivisions of far-fields in an efficient way?
- idea: recursive decomposition of Ω (a square in 2D, a cube in 3D – without loss of generality) in cells of different size, terminating the subdivision process if a cell is either empty or contains just one particle

Tree Structures

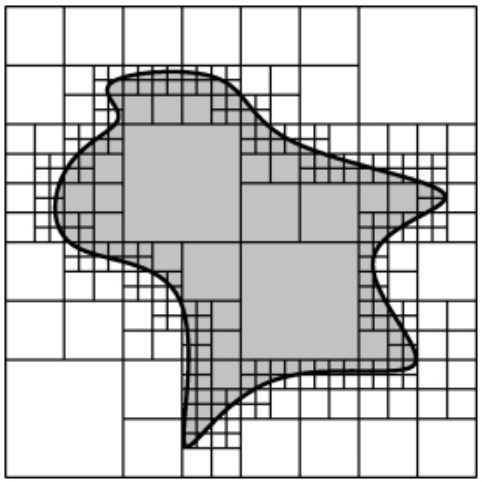
- concepts:
  - **kd-tree**: alternate subdivision in coordinate direction (x, y, and z), such that the separation produces two subdomains that roughly contain the same number of particles each
  - **quadtree** (2D) or **octree** (3D): subdivision into four congruent subsquares or eight congruent subcubes, respectively
- the following algorithms (Barnes-Hut etc.) use the octree approach

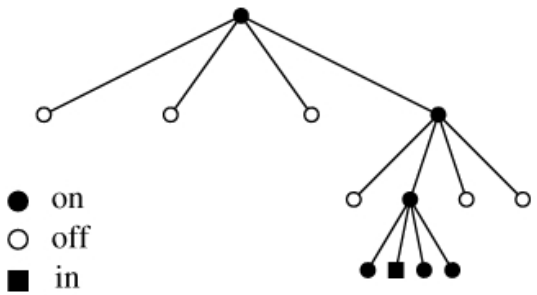
kd-Trees – Example

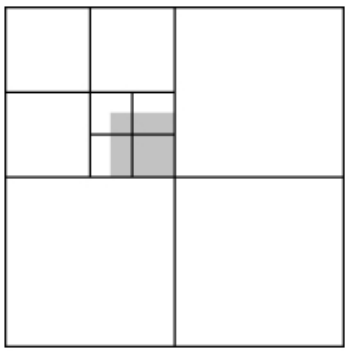


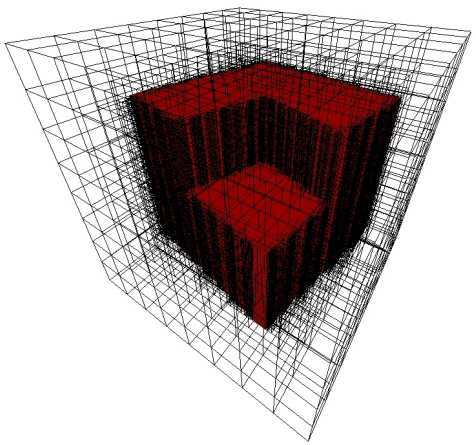


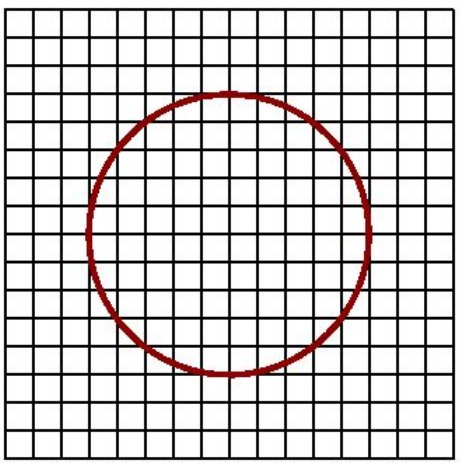
Quadtrees and Octrees – Examples

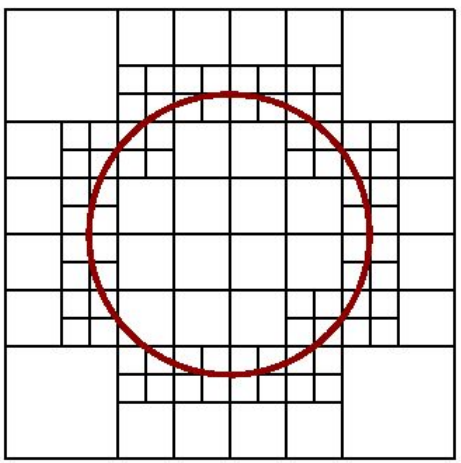












Recursive Computation of the Far-Field Subdivision

- create the octree corresponding to the set of particles
  - each node of the octree represents a subdomain of Ω or one **cell**
  - for each cell i, define some y_0^i (the centre point or the centre of gravity of all particles contained, e.g.) for doing the Taylor expansion
  - for each cell i, let the parameter diam just denote the diameter of the smallest surrounding sphere, e.g.
- objective: for each particle position x, use as few cells as possible (i.e. as big cells as possible) for fulfilling the diam-θ rule

Recursive Computation of the Far-Field Subdivision (2)

- hence: start from root node, check

$$\frac{\text{diam}}{\|x - y_0^i\|} \leq \theta \,,$$

  stop if fulfilled (no need for further subdivision) and proceed if not yet fulfilled
- note that for each x, we typically get a different subdivision
- but note also that all these subdivisions are just subtrees of our constructed octree

Recursive Computation of the Moments

- now: use this subdivision for the efficient calculation of the local moments $M_j(\Omega_i^{\text{far}}, y_0^i)$
- direct (numerical) integration or direct summation are not efficient
- therefore: use hierarchical tree structure to calculate all moments for all cells in one run and store them
- crucial property for that:

$$M_j(\Omega_1 \cup \Omega_2, y_0) \;=\; M_j(\Omega_1, y_0) + M_j(\Omega_2, y_0)\,,$$

  if the point of expansion y_0 is the same

Recursive Computation of the Moments (2)

- in the (standard) case of different y_0^1 and y_0^2, there are simple conversion formulas:

$$M_j(\Omega_1, \hat{y}_0) = \sum_{k \leq j} \binom{j}{k} (y_0 - \hat{y}_0)^{j-k} M_k(\Omega_1, y_0)$$

  ($k \leq j$ component-wise, multiplicative binomial coefficients)
- this allows for a bottom-up calculation of the moments from the leaves to the root
- In the leaves:
  - if no particle present: zero
  - if one particle of mass m there in x: $m(x - y_0^i)^j$

Using these Building Blocks

still to be done for a numerical routine:

- how to construct the tree, starting from a given set of particles?
- how to store the tree?
- how to choose cells and expansion points?
- how to determine far-field and near-field?

several algorithmic variants to be discussed in the following

The Barnes-Hut Method

- oldest (dates back to 1986), simplest, and most widespread hierarchical tree-based approach
- original target applications: astrophysics (high particle numbers, very heterogeneous density distribution)
- particle-particle interaction via gravitation potential:

$$U(r_{ij}) = -G_{\mathrm{Grav}} \frac{m_i m_j}{r_{ij}}$$

- uses octrees: leaves of the tree represent empty cells or one particle, inner nodes represent clusters of particles or **pseudo particles**
- main underlying idea: gravitation (or other force) induced by many particles in one remote cell can be approximated by the influence induced by one pseudo particle of the accumulated mass in the cell's centre of gravity

The Barnes-Hut Method (2)

Three main steps:

- construction of the octree: refinement, until just one or no particle per cell (top-down recursion)
- calculation of pseudo particles: mass is just sum of the cell's particles' masses, associated point is the mass-weighted average of the particles' positions (bottom-up recursion)
- calculation of forces (N incomplete top-down traversals for N particles)

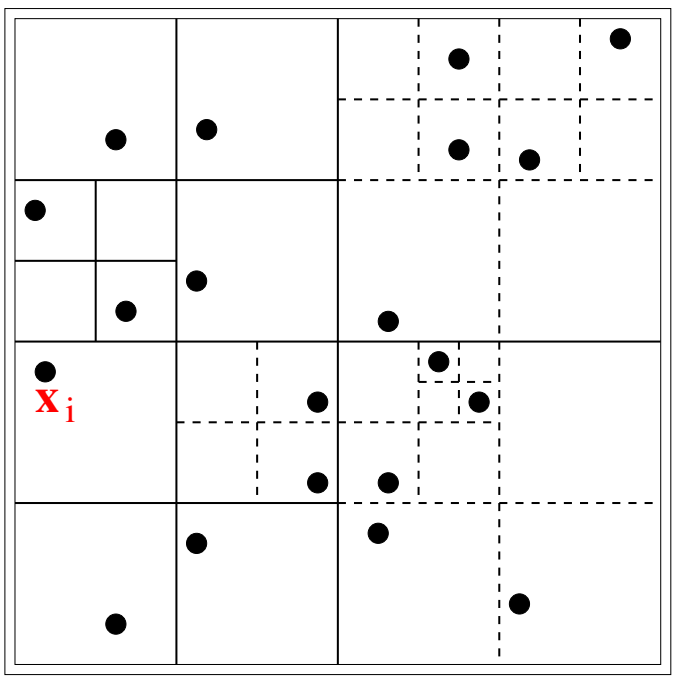
Calculation of the Forces

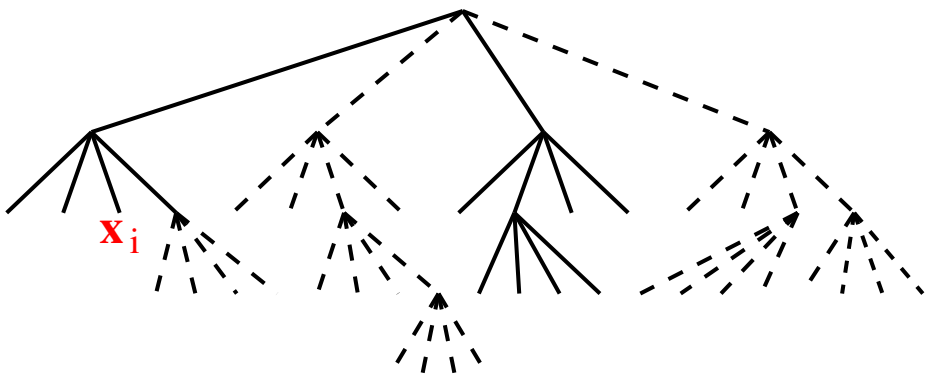
- remember: to be done for each particle
- assume a particle with position $x \in \Omega$
  - start in root node
  - proceed to son nodes, until the $\theta - \mathit{rule}$: $\frac{diam}{r} \leq \theta$ is fulfilled, where r denotes the distance of the corresponding pseudo particle to x
  - then, add the resulting interaction influence to the overall result
- implicit separation into near-field and far-field:
  - near-field: all leaves reached during this traversal (single-particle influence)
  - far-field: all inner nodes where the process stops, i.e. cells representing pseudo particles

Calculation of the Forces (2)

- several variants concerning the determination of the parameter diam
- Barnes-Hut method can be interpreted as a special case of the Taylor approximation discussed above for $p = 0$ (for the calculation of the pseudo particles, we just sum up masses, i.e. zero-th moments)

Example of the Tree Construction and Force Calculation





Accuracy and Complexity

- accuracy:
  - depends on control parameter θ
  - the smaller we choose θ, the larger gets the near-field and the smaller, hence, gets the error resulting from the corresponding far-field approximation
  - however, slow $O(\theta)$ convergence due to $p = 0$
- complexity:
  - increases for decreasing θ
  - for roughly homogeneous particle distributions:
    - number of active cells bounded by $C \log N/\theta^3$ for some constant C and N particles
    - overall cost of order $O(\theta^{-3} N \log N)$
  - for limit case $\theta \to 0$: method degenerates to the quadratic complexity of the original "each-with-each" approach without far-field approximation

Some Remarks on the Implementation

- use a standard data structure for each (pseudo) particle
- standard tree implementation with pointers:
  - each node contains one (pseudo) particle at most
  - subdomain corresponding to a node/cell can be either stored explicitly or calculated on-the-fly during a tree traversal
  - four (2D) or eight (3D) pointers from a node to its sons
- linearisation is possible, too (i.e. no need for pointers)
- tree traversal typically by recursion
  - pre-order (top-down)
  - post-order (bottom-up)

Some Remarks on the Implementation (2)

- tree construction:
  - successive insertion of particles
  - starting from the empty tree (i.e. the octree consisting of the root node only)
  - refine, when necessary (i.e. two particles in one node)
- calculation of pseudo particles:
  - bottom-up (post-order) traversal
  - sum of masses, weighted average of positions as described before
- calculation of forces:
  - outer loop: traversal visiting each leaf (to get the far-field approximation for each particle)
  - inner loop: top-down (pre-order) traversal until the θ-rule is fulfilled
  - parameter diam on-the-fly

Some Remarks on the Implementation (3)

- time integration: essentially as before, now as another tree traversal
- motion:
  - either via constructing a new octree
  - or via modifying the existing octree (generally preferred)