AutoPas & ls1 mardyn: Enabling Auto-Tuning in MPI+X Load-Balanced Molecular Dynamics Simulations

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Barcelona, 29th October 2019
Motivation
Outline

AutoPas

ls1 mardyn

Experimental Results
AutoPas
AutoPas: Overview

- Node-Level C++ library
- User defines:
  - Properties of particles
  - Force for pairwise interaction
- AutoPas provides:
  - Containers, Traversals, Data Layouts, ...
  - Dynamic Tuning at run-time
- Black Box container
  ⇒ General base for $N$-Body simulations

https://github.com/AutoPas/AutoPas
AutoPas Interface

MPI-Rank 0

Particle Code

Uses

provides

interface

AutoPas

selects and manages

Configuration 1
Configuration 2
Configuration 3

MPI-Rank 1

Particle Code

Uses

provides

interface

AutoPas

selects and manages

Configuration 1
Configuration 2
Configuration 3

communicate (MPI)
AutoPas Interface

• One common interface for the AutoPas class and all its containers.
• Interface is compatible to neighbor list approaches:
  – Update container structure only every N time steps (reuse of neighbor lists).
  – Move particles between ranks only every N time steps.
  – Halo particle update still needed at every time step.
  – Add skin radius.
ls1 mardyn
ls1 mardyn

- ls1 mardyn is an MD simulation package.
- Actively used in chemical engineering.
- Supports AutoPas as underlying particle container.
ls1 mardyn – MPI Adapations

- Diffusive load balancing via library developed at JSC.
- Neighbor communication was adapted to AutoPas interface – allows efficient use of Neighbor lists.
Experimental Results
Conclusions

- AutoPas is a black box $N$-Body container.
- Dynamic tuning enables optimal performance for changing scenarios.
- Achievable for users without expert knowledge.
- Easy to integrate in existing codes.

... and future work:

- Add more advanced auto-tuning strategies.
- More / optimized algorithms.
- Tuning for more parameters.
- Search space reduction.
Backup Slides
Molecular Dynamics

- Here: small rigid molecules
- Simulation of movement of molecules
- Computation of pairwise forces
- Newton’s Laws of Motion
- $N$-Body problem $\Rightarrow O(N^2)$
Short Range Interactions: Lennard-Jones Potential

\[
U(x_i, x_j) = 4\varepsilon \left( \left( \frac{\sigma}{||x_i - x_j||_2} \right)^{12} - \left( \frac{\sigma}{||x_i - x_j||_2} \right)^6 \right)
\]  

(1)

- Characteristics of molecule type:
  - \(\varepsilon\): Potential well
  - \(\sigma\): Zero crossing
- Cutoff \(r_c\)

Figure: LJ-Potential for \(\varepsilon = 1\) and \(\sigma = 0.9\)
Challenges

- Total number of particles
- Particle density
- (In-)Homogeneity
- Systems changing over time
- Many possible algorithms

Overall goal:
Minimize time to solution!
Container Options

Direct Sum

Linked Cells

Verlet Lists

Memory Overhead

Computational Overhead
Container Comparison

- Every container has advantages
- Linked Cell benefits most from SoA
  \[ \Rightarrow \] best in dense scenarios
Linked Cells Parallelization Options

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c08

sliced
Hardware Comparison / Threads

- Traversals:
  - c08: 8-way domain coloring
  - sliced: regular 1D domain partitioning
Hardware Comparison / Data Layout

• Vector Instructions:
  - Magny: SSE4, 128
  - Haswell: AVX2, 256
  - KNL: AVX512, 512

⇒ Optimal data layout dependent on hardware
AutoPas in Is1 mardyn

- Uses Lennard-Jones functor from AutoPas
- New particle class
  - Inherits from AutoPas and Is1 mardyn particle interface.
  - Acts as coupler
- New particle container class
  - Only wrapper around AutoPas main interface.
Auto-Tuning Process

- Common interfaces for containers, traversals, etc ⇒ Strategy pattern
- Repeated periodically
- User can restrict testing space
Scenario: Spinodal Decomposition

- 4,008,960 particles
- Block size: $240 \times 240 \times 240$
- Periodic boundary conditions
- Cutoff = 2.5
- Sub-critical temperature
- Rapid and drastic change in homogeneity
  ⇒ Interesting target for tuning!
Tuning Behavior

- Tuning switches as expected
- Misclassification can happen
- Tuning and manual switching equally fast.
  \[ \Rightarrow \text{No overhead from tuning!} \]
- Tuning faster than static configuration.
- Faster than original ls1 mardyn, even in Reduced Memory Mode.