From Molecular Dynamics towards a Node-Level Auto-Tuning Library for N-Body Simulations

Fabio A. Gratl[†], Nikola Tchipev[†], Steffen Seckler[†], Philipp Neumann[‡], Hans-Joachim Bungartz[†]
f.gratl@.tum.de, n.tchipev@tum.de, seckler@in.tum.de, philipp.neumann@uni-hamburg.de, bungartz@in.tum.de, [†] Technical University of Munich, [‡] Universität Hamburg

Molecular Dynamics (MD) Simulations

Applications:

Chemical Engineering: cavitation, surface tension, gas separation, etc..

Goals:

- High node-level performance in arbitrary scenarios.
- Minimize time to solution.

Main Challenges:

- Drastic impact of simulation variables on time to solution.
- Performance depends on many variables that can change during runtime.

ls1-mardyn

Highly parallel MD Code

- Language: C++.
- Small rigid, multi-centered molecules
- Double, single and mixed precision
- Implemented Interactions:
  - 12-6 Lennard-Jones
  - Coulomb
  - Charge
  - Dipole
  - Quadrupole
- Highly efficient reduced memory mode enabling largest known MD simulation: $2 \cdot 10^{13}$ molecules.

Node-Level Challenges

Factors affecting performance

- Number of particles
- Particle density distribution
  $\Rightarrow$ Can change over time!
- Number of Lennard Jones centers
- Cutoff radius
- Heterogeneous Hardware

Can change time to solution and performance by orders of magnitude!

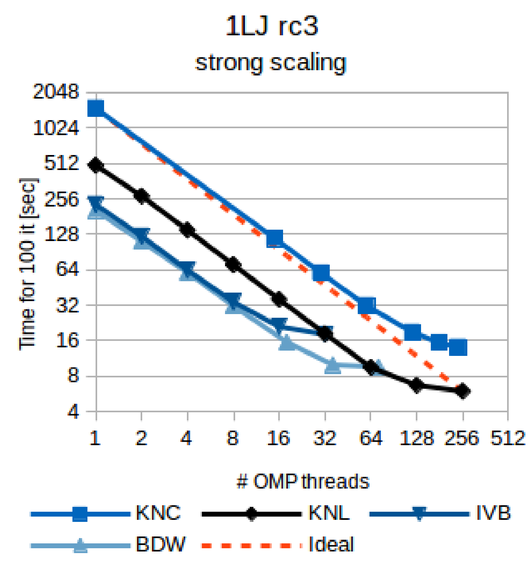
Potential Solutions

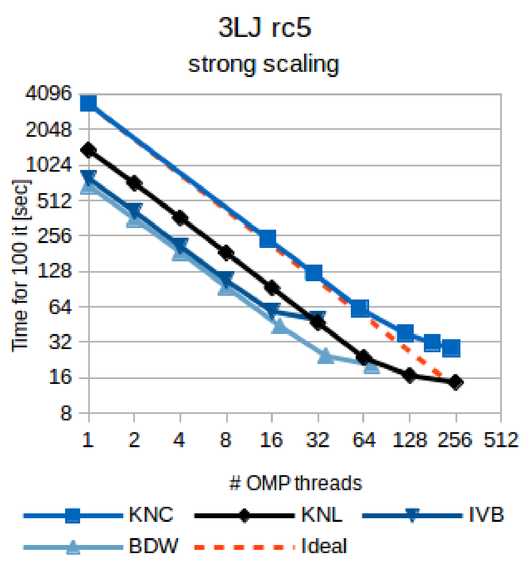
- Vectorization of Kernels
- Container (Linked Cells, Verlet Lists)
- Traversal patterns

Results

Homogeneous Scenario

- Large scenario: 1.3 million molecules
- Homogeneously distributed
- OpenMP with 8-way coloring scheme
- Different platforms





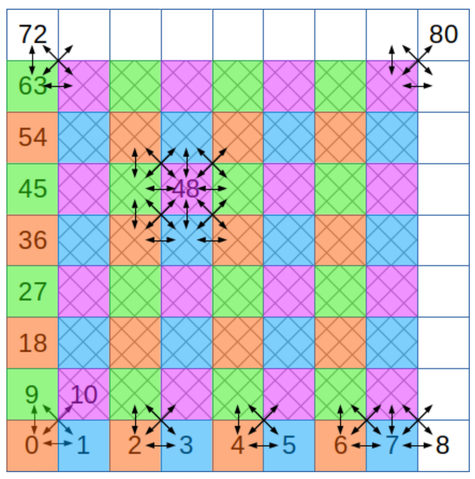
Available Traversal Options

c08

- 8-way coloring scheme (3D).

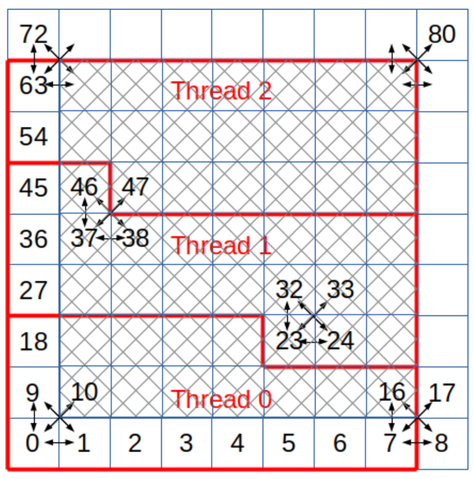
$\Rightarrow$ One barrier per color.

- Load balancing via OpenMP.



slice

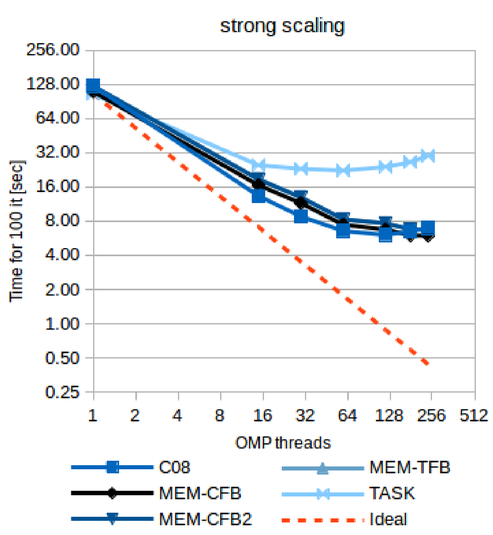
- One slice per thread.
- Only one lock per thread.
- No load balancing.



Comparison of OpenMP schemes: Towards Auto-Tuning

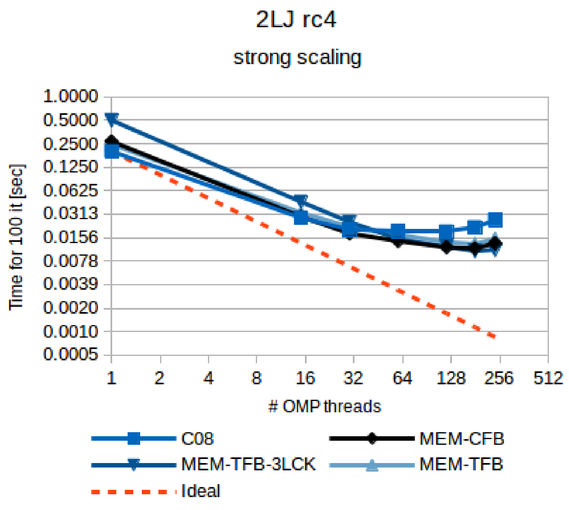
Inhomogeneous Scenarios

- Medium size: 40.000 molecules



Small Scenarios

- Small size: 1000 molecules



Library Goals

- **Optimal performance on arbitrary scenarios**
  - Simulation needs to be able to also handle domains with low particle count or inhomogeneous particle distributions.

$\Rightarrow$ Specialized approaches needed.

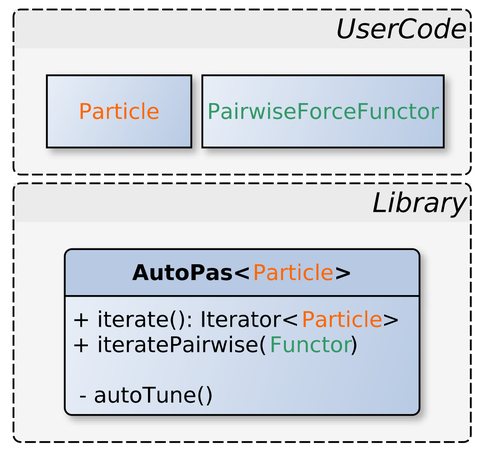
There is no silver bullet
$\Rightarrow$ We want to export containers, traversals and kernels to make them available as a library.

- **More modular code structure**
  - Since different scenario settings benefit from dedicated techniques, these need to be easily exchangeable.
  - Example: Cell traversal pattern (see above)
    - $\star$ Direct Sum, c08, slice, ...

$\Rightarrow$ **Auto-Tuning**

- Instead of the user, the code should find the optimal combination of techniques.
- Too many combinations possible to test all.
  $\Rightarrow$ Performance Modeling (e.g. automated empirical with ExtraP).
- Reevaluate combination during runtime and adapt appropriately.
- Provide flexibility through "strategy" software pattern.

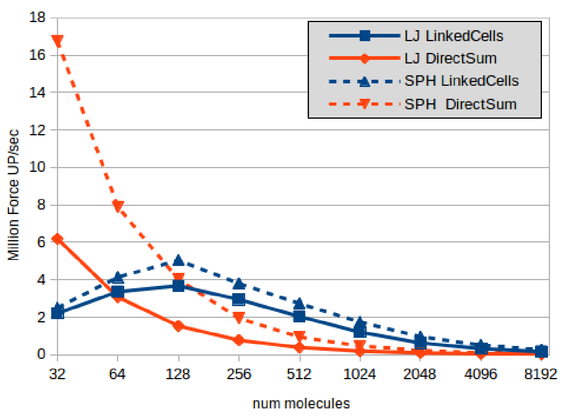
Outlook: AutoPas

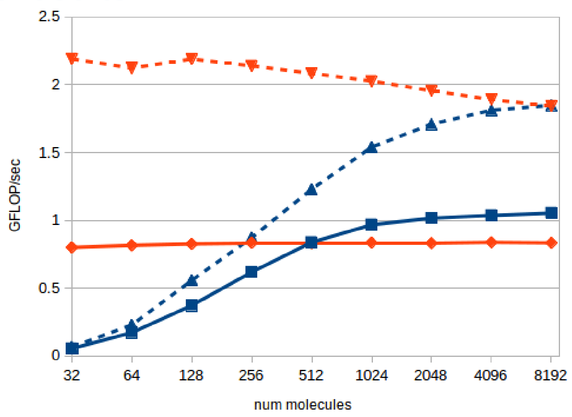


Vision

- Base to build full N-Body Simulations on top of.
- Manages node-level performance internally via Auto-Tuning with Performance Modeling.
- Modular C++ Template design to dynamically select optimal SIMD, OpenMP, Datastructures, etc. at runtime.

First results





References

[1] N. Tchipev, A. Wafai, C. W. Glass, W. Eckhardt, A. Heinecke, H.-J. Bungartz, and P. Neumann, "Optimized force calculation in molecular dynamics simulations for the intel xeon phi," in *European Conference on Parallel Processing*, pp. 774–785, Springer, 2015.

[2] N. Tchipev and et al., "Twetris: Twenty trillion-atom simulation." submitted, 2018.

[3] N. Tchipev, A. Costinescu, S. Seckler, P. Neumann, and H.-J. Bungartz, "Towards autotuning between openmp schemesfor molecular dynamics on intel xeon phi," 2017. SIAM CSE '17.

Bundesministerium für Bildung und Forschung

Intel® Parallel Computing Center TUM & LRZ

We thank the Intel Parallel Computing Center "ExScaMIC-KNL" and the Federal Ministry of Education and Research, Germany, project "Task-based load balancing and auto-tuning in particle simulations" (TaLPas), grant number 01IH16008 for financial support of this research.