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Short-Interval Energy Measurements for Algorithm Selection in Particle Simulations

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Motivation

- Improving the energy efficiency of large simulations is becoming increasingly important.
- Particle simulations offer many algorithmic configurations (ACs) that may be optimal for different scenarios, and the optimal AC may vary within the same simulation.
- Dynamic Voltage and Frequency Scaling (DVFS) allows modern CPUs to reduce frequency and voltage during less compute-intensive phases to save energy. This introduces a non-linear relationship between runtime and energy consumption, potentially leading to different optimal ACs for each metric.

The main goal of this study is to demonstrate that **energy measurements at the iteration level can be used to select the most energy-efficient AC** in short-range particle simulations. We use the simulation of a heating sphere as a motivating example from Molecular Dynamics (MD) using the AutoPas library [1].

Results

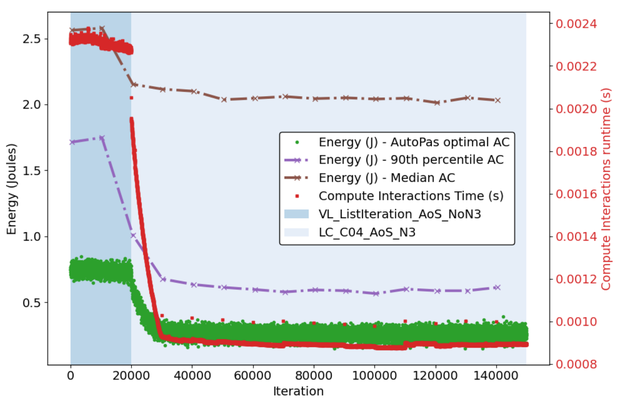

Figure 3 Runtime and energy consumption averaged over 10 iterations for pairwise interaction computations in the Heating Sphere scenario. The shaded area represents the currently optimal AutoPas configuration; median and 90th-percentile energy consumption values from the tuning phases are included for comparison.

- The optimal AC changes from `VL_ListIter_AoS_NoN3` at the start of the simulation to `LC_C04_AoS_N3` during the simulation.
- Dynamically selecting the optimal AC leads to approximately a **15.6% reduction in energy consumption and a 13.5% reduction in runtime** compared to a single-AC run for computing pairwise interactions.
- Full-Search was used because it guarantees an optimal AC, and establishes whether dynamic algorithm selection for minimizing energy makes sense.
- The tuning overhead arising from trialing suboptimal ACs in Full-Search was not considered here in order to demonstrate the potential gains from algorithm selection. This overhead would be significantly reduced when using smarter tuning strategies.

Methodology

AutoPas is a node-level library that dynamically selects the optimal AC to minimize the time or energy consumption of a particle simulation. Minimizing energy consumption using AutoPas relies on two main aspects:

- **Energy measurement**, as energy serves as the minimization function for our optimization problem. We utilize the Power Measurement Toolkit (PMT) [2], a lightweight, high-level library that enables the collection of power measurements on CPUs and other architectures. We require energy measurements at the iteration level, which may correspond to **time scales on the order of a few milliseconds**, very close to the frequency at which RAPL counters are updated, and can lead to erroneous samples.
- **Algorithm selection** technique (referred to as tuning strategy) [3] to select optimal AC directly or candidate ACs to be tested to find the optimal.

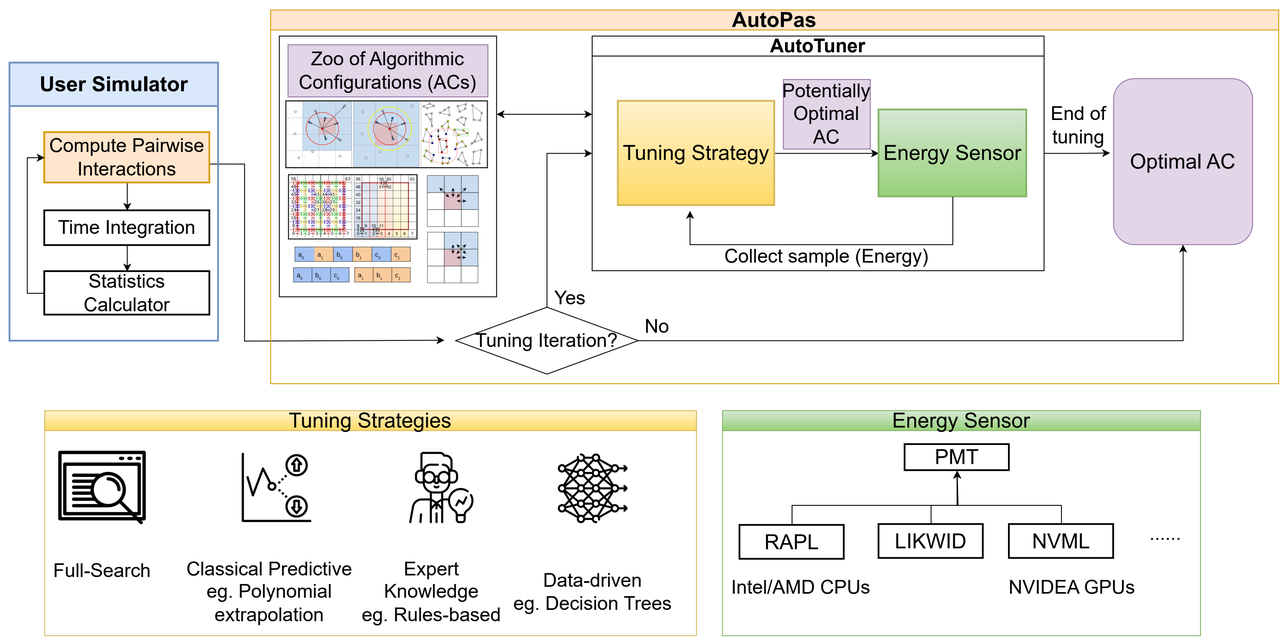

Figure 1 Flow chart showing how AutoPas internally selects the optimal AC at runtime while hiding the process from the user-simulator.

Example MD simulation:

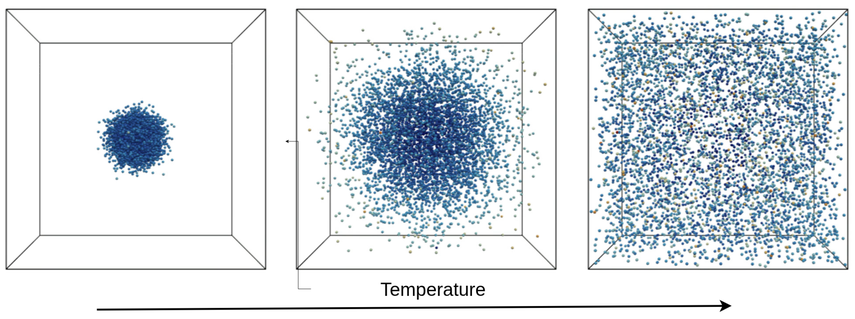

Figure 2 Heating Sphere scenario: An inhomogeneous system of Lennard-Jones particles arranged as a sphere becomes homogeneous as the temperature is gradually increased. The simulation was run with our in-house MD simulator `md-flexible`. The experiment was run on 1 node of HSUper [a] with 36 OpenMP threads.

[a] https://www.hsu-hh.de/hpc/en/hsuper/

Summary

- Algorithm Selection techniques in AutoPas can help reduce overall energy consumption and runtime in particle simulations.
- The current study presents energy as a viable metric for algorithm selection in particle simulations.
- The optimal **ACs obtained are the same as those obtained by minimizing runtime** [3], indicating that the effect of DVFS is negligible in this scenario.

Outlook

- Energy measurements are noisier than runtime measurements. The **impact of noise on algorithm selection** needs to be investigated in more detail.
- The **effect of DVFS leading to a different energy-optimal AC** should be investigated further in different scenarios.
- Future work will also explore scenarios in hybrid OpenMP–MPI settings, to understand the differences in energy and runtime costs of load imbalance.

References:

1. Gratl et al. 2021. N Ways to Simulate Short-Range Particle Systems: Automated Algorithm Selection with the Node-Level Library AutoPas. *Computer Physics Communications* 273 (2021), 108262. doi:10.1016/j.cpc.2021.108262
2. Corda et al. 2022. PMT: Power Measurement Toolkit. In *2022 IEEE/ACM International Workshop on HPC User Support Tools (HUST)*. 44–47. doi:10.1109/HUST56722.2022.00011
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