Chair of Scientific Computing in Computer Science
Univ.-Prof. Dr. Hans-Joachim Bungartz

Technische Universität München

Seminar Final Presentation

Algorithm Selection and Auto-Tuning in AutoPas

Manuel Lerchner
manuel.lerchner@tum.de

Advisors:
Manish Kumar Mishra, M.Sc. (hons)

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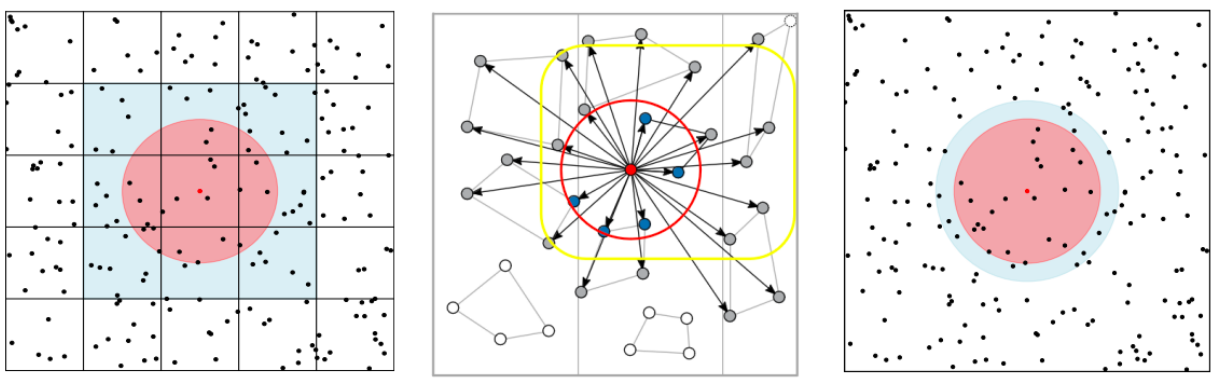
AutoPas

What is AutoPas?

- Library for arbitrary N-body simulations
- Optimal performance by switching implementations
  - **Container:** Finding neighboring particles
  - **Traversal:** Parallel force calculations
  - **Data Layout:** Memory access optimization
  - **Newton 3:** Force calculation optimization



[Newcome et al., 2024]

Structure of AutoPas

- Three main areas:
  - User Application
  - Algorithm Library
  - Tuning Strategies
- Algorithm Library:
  - Huge Search Space[1]
- Tuning Strategies:
  - Full Search
  - Random Search
  - Predictive Tuning
  - Bayesian Search
  - Rule Based Tuning

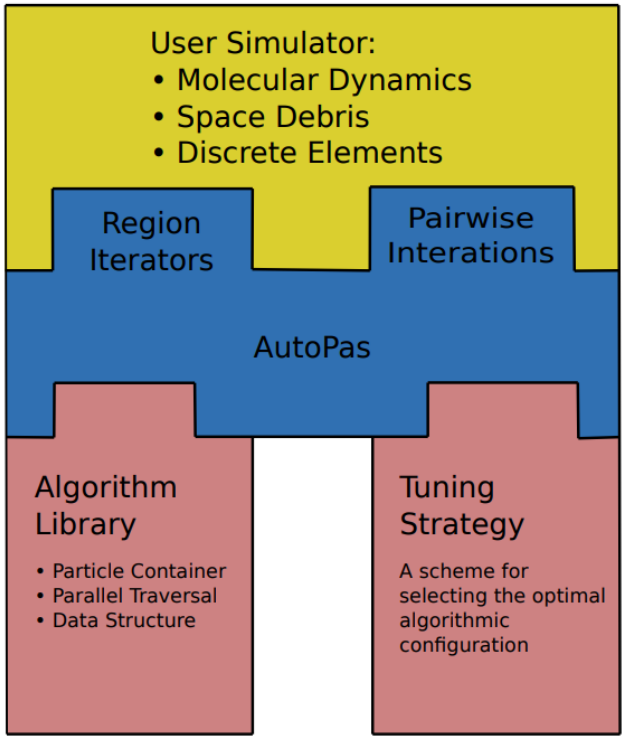


Figure: [Newcome et al., 2023]

[1] Container × Traversal × Data Layout × Newton 3 × Load Estimator × Cell Size Factor

Thank you for your attention!

Questions?

References I


Newcome, S. J., Gratl, F. A., Muehlhaeusser, M., Neumann, P., and Bungartz, H.-J. (2024).
Autopas: Dynamic algorithm selection in molecular dynamics for optimal time and energy.
In *SIAM Conference on Parallel Processing (PP24)*. SIAM.


Newcome, S. J., Gratl, F. A., Neumann, P., and Bungartz, H.-J. (2023).
Towards the smarter tuning of molecular dynamics simulations.
Amsterdam, The Netherlands.

Backup:

- A
- B