Chair for High Performance Computing
Philipp Neumann

**TaLPas: Task-Based Load Balancing and Auto-Tuning in Particle Simulations**
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**Disclaimer!**

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Recap: What is TaLPas?

- Investigation of thermodynamic states and properties of fluids → vapor-liquid systems, interfacial flows, complex fluids, ...
- Particular computational challenge: problems such as equation of state sampling, rare events, ...
  → many inter-dependent MD runs, each with different compute requirements
  → Similar problem settings: UQ, parameter identification, ...
Recap: Goals of TaLPas

- Hardware-independent acceleration of particle simulations → Node level auto-tuning library AutoPas
- Self-adapting performance-optimal distribution of work load → workflow manager, incorporating scheduler, performance predictor, particle sampling algorithm
- Resilience for particle systems
- Integrated (in-situ) visualization
Outline

• AutoPas
• Workflow Manager
• Performance Prediction
• In-Situ Visualization

1 Auto-Tuning: The AutoPas Library
2 Workflow Manager and Performance Prediction
3 In-Situ Visualization
4 Summary
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AutoPas

1 Gratl et al. AutoPas: Auto-Tuning for Particle Simulations. IPDPS proc. (iWAPT workshop), 2019
2 Tchipev et al. TweTriS: Twenty Trillion-atom Simulation. IJHPCA 33(5):838-854, 2019

(a) DirectSum
(b) LinkedCells
(c) VerletLists

• Data structures: SoA vs. AoS
• 7 containers: Direct sum, linked cells, Verlet lists, cluster lists
• 17 (OpenMP) traversals: coloring, slicing, etc.
• Auto-Tuning on data structures+containers+traversals
• Integration in ls1 mardyn
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AutoPas\(^1\)

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AutoPas¹

- Improve on “Brute-Force” testing due to outgrowing number of combinations → not a nice add-on, but a necessity!
  → work in progress: ML, Bayesian methods
- Data structures: SoA vs. AoS
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- work in progress: ML, Bayesian methods
- CUDA & Kokkos support

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AutoPas: Machine Learning for Auto-Tuning

- Based on classification via neural network
- Test only five configurations that are deemed best
- Finds (equivalent to) optimal configuration with probability of 99%
- Relies on training data
  → currently, it takes days to train...
  → hardware-dependent training
- Results from a recent evaluation:
  Full search: duration: 22.79s  # iterations: 27, 0.84 s/it.
  ML-based: duration: 2.05s  # iterations: 5, 0.41s/it.
  → optimal configuration: 0.36s/it (detected by both approaches)
- This is work in progress :-(
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Workflow Manager

- Last time: Equation of state fitting and vapor-liquid-equilibrium envelope
- Current work: Sparse Grid-based Perf. Prediction, Adsorption processes
  - study of adsorption in dispersive systems
  - relevant parameters: temperature, pressure, solid density, interaction fluid-solid
  - 350 simulations

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Workflow Manager and Adsorption

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Workflow Manager and Adsorption

Influence of fluid-solid interaction

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Still some user interaction required
→ work in progress
Debugging: some SLURM scalability issues…
Performance Prediction with Extra-P: Higher-Dimensional Parameter Spaces

- **Extra-P**
  - Originally: \( N \) parameters \( \rightarrow 5^N \) data points to generate performance model normal form

\[
f(r_1, r_2, \ldots, r_q) = \sum_{k=1}^{n} c_k \cdot \prod_{l=1}^{q} r_l^{i_{kl}} \cdot \log^{j_{kl}}(r_l)
\]

- Idea: Select subset of data points without degrading accuracy \( \rightarrow \) reinforcement learning approach
Performance Prediction with Extra-P: Higher-Dimensional Parameter Spaces

- Extra-P
  - Originally:
    \[ f(r_1, r_2, \ldots, r_q) = \sum_{k=1}^{n} c_k \cdot \prod_{l=1}^{q} r_{i_{kl}}^{i_{kl}} \cdot \log^{j_{kl}}(r_l) \]

- Idea: Select subset of data points without degrading accuracy
  → reinforcement learning approach
  → example: 3 params, 5% noise
Performance Prediction with Sparse Grids

- SG=Efficient hierarchical discretization for high-dimensional problems
- Method: Sparse grid regression with local mesh refinement
- Example: Molecular dynamics
  - Particle density $\rho \in [0.3; 0.9]
  - \# particles $N \in [10^3; 10^5]
  - Cut-off radius $r_c \in [1.2; 4.5]
  - Blocksize $b \in [10; 10^3]
  - \# MPI procs $p \in \{1, 2, 4, 8\}

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4 P. Neumann. Sparse Grid Regression for Performance Prediction Using High-Dimensional Run Time Data. Euro-Par Workshops (PMACS) 2019. Accepted
In-Situ Visualization

- MegaMol: Integration in ls1
- Data exchange via shared memory
- Different MPI worlds → if visualization fails, simulation continues

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Resilience

- Checkpointing-based
- Future work: evaluation of quality for molecular films
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Summary

- **AutoPas**
  - Integration in Is1, first application-relevant tests
  - Work in progress: improved tuning procedure, CUDA support
- **Workflow Manager**
  - New scenario: adsorption processes
    → first (hand-steered) workflow solution using Is1
  - Work in progress: Scheduling with performance prediction, integration of components, scalability
- **Performance Prediction**
  - New methods for high-dimensional parameter spaces (Extra-P, Sparse Grids)
  - Work in progress: Integration with Workflow Manager
- **In-Situ Visualization**: Integration of MegaMol and Is1

P. Neumann and colleagues acknowledge funding by the Federal Ministry of Education and Research, grants 01IH16008, project TaLPas.
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• ISC HPC 2020: Project Posters, Submission Deadline: 12 Feb 2020
• (If you know someone who’s) Interested in a PhD/Postdoc on HPC, multiscale flow simulation, molecular dynamics, performance prediction, etc.
  → contact me, philipp.neumann@hsu-hh.de :-)

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