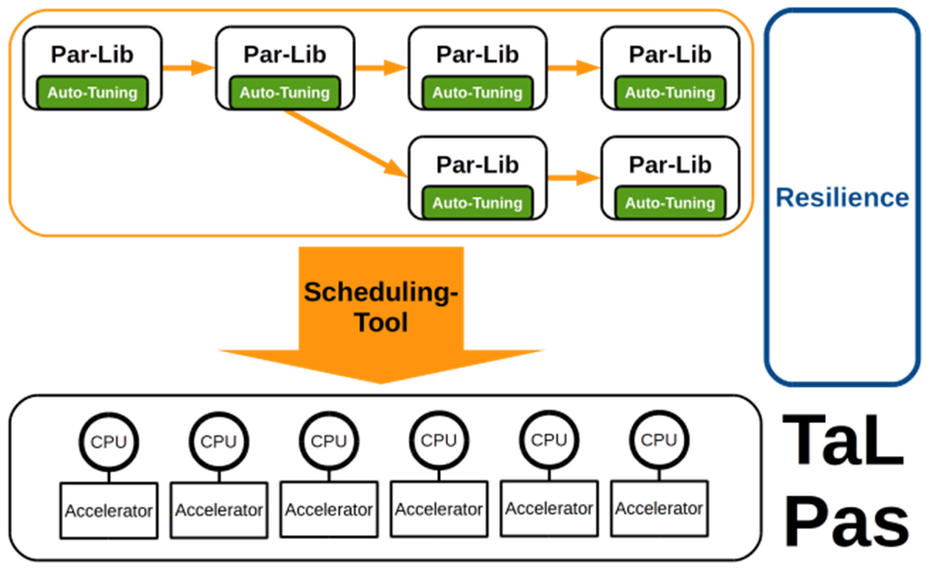
TaLPas

Task-Based **L**oad Balancing and Auto-Tuning in **Pa**rticle **S**imulations

Overview

Duration:	01.01.2017 – 30.06.2020
Coordination:	Helmut-Schmidt-Universität Hamburg, TU München
Partners:	High-Performance Computing Center Stuttgart/Universität Stuttgart Technische Universität Darmstadt Technische Universität Berlin Technische Universität Kaiserslautern



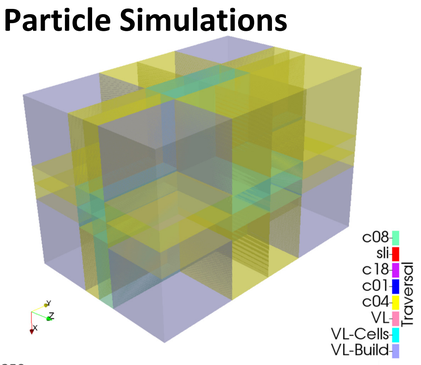
Objective and Methodology

TaLPas will provide a solution to fast and robust simulation of many, inter-dependent particle systems in peta- and exascale supercomputing environments. This will be beneficial for a wide range of applications, including sampling in molecular dynamics (rare event sampling, sampling of equations of state, etc.), uncertainty quantification (sensitivity investigation of parameters on actual simulation results), or parameter identification (fitting numerical model parameters to match experiments).
For this purpose, *TaLPas* targets

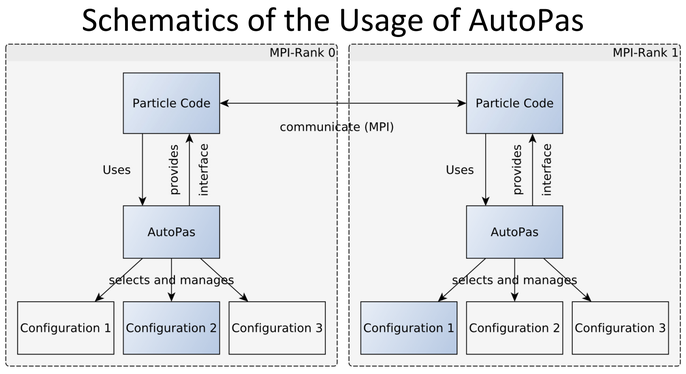
1. **the development of an auto-tuning based particle simulation library *AutoPas*** to leverage optimal node-level performance,
2. **the development of a scalable workflow manager** to optimally distribute inter-dependent particle simulation tasks on HPC compute resources,
3. **the investigation of performance prediction methods** for particle simulations to support auto-tuning and to feed the workflow manager with accurate runtime predictions,
4. **the integration of 1-3**, augmented by visualization of the sampling (parameter space exploration) and an approach to resilience. The latter will guarantee robustness at peta- and exascale.

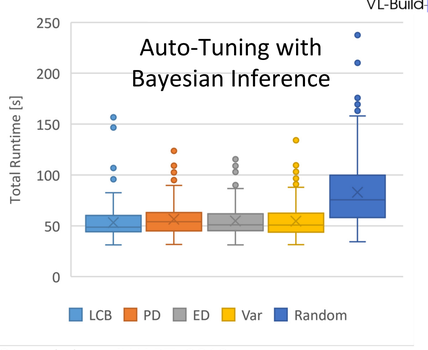
AutoPas[1] – Node-Level Auto-Tuning Library for Particle Simulations

- Short-range systems
- Allows selection of more than 30 algorithm configurations (data structures, traversals, …)
- Ready for use in MPI-parallel applications[2]
- Integrated into ls1 mardyn and lammps
- See https://github.com/AutoPas



Schematics of the Usage of AutoPas



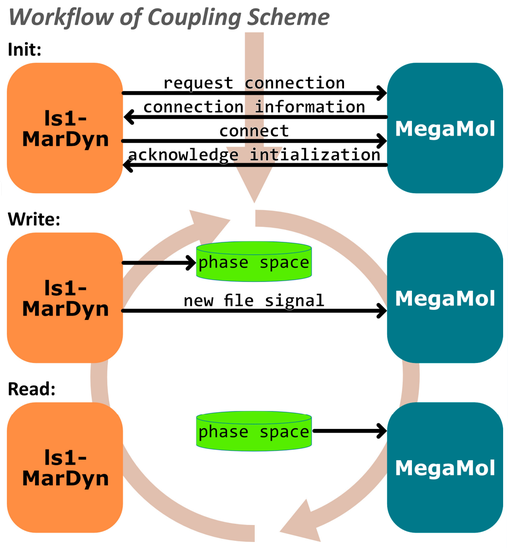


[1] F. Gratl, et al. *AutoPas: Auto-Tuning for Particle Simulations.* In Proc. of IPDPS, workshop iWAPT, 2019
[2] S. Seckler, et al. AutoPas in ls1 mardyn: Massively Parallel Particle Simulations with Node-Level Auto-Tuning. Submitted, 2020

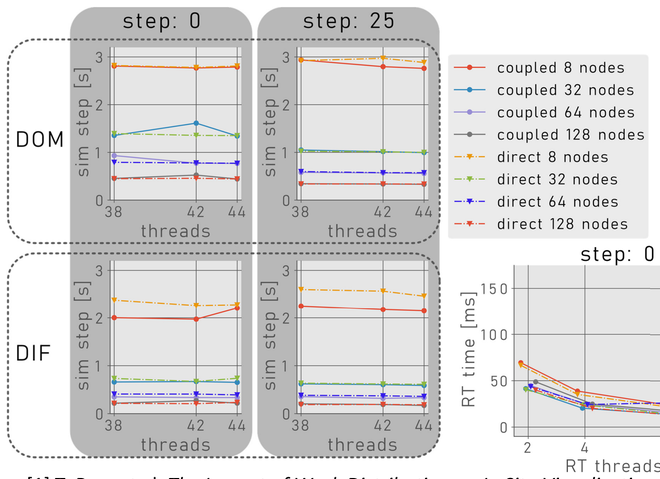
In Situ Visualization[1]

- Loose coupling scheme between ls1-MarDyn and MegaMol
  - Node-local phase space transported via shared memory
  - Signal to MegaMol scripting interface starts visualization of new data
- Small impact of visualization on simulation
- Visualization benefits from diffusion-based load-balancing

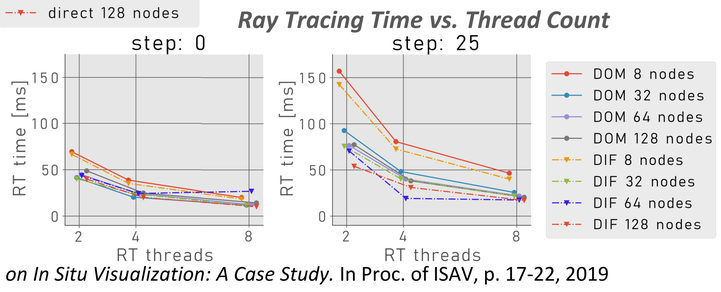
Workflow of Coupling Scheme



Simulation Time vs. Thread Count wrt. Static DOMain decomposition vs. DIFfusion-based load-balancing

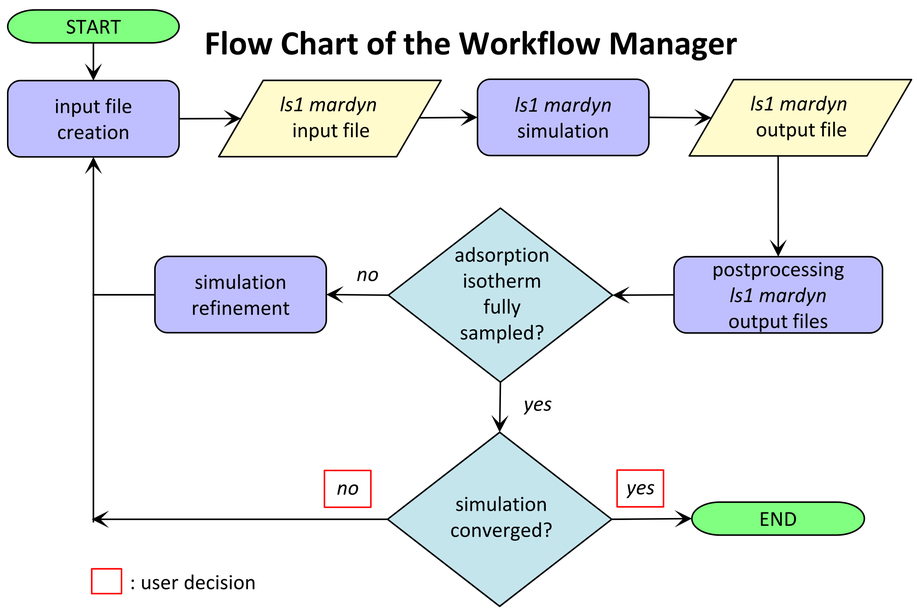


Ray Tracing Time vs. Thread Count

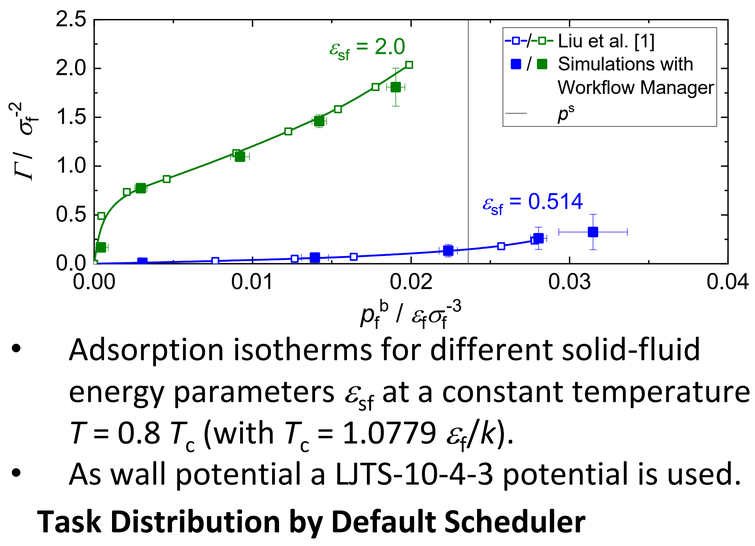


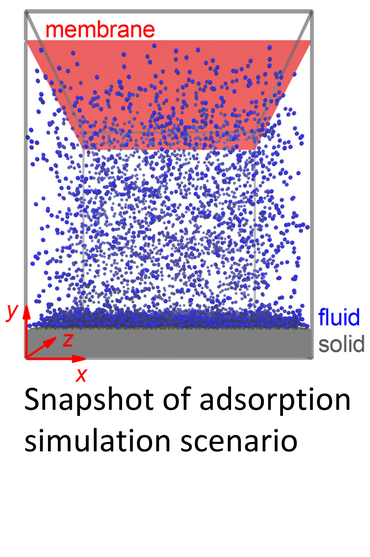
[1] T. Rau, et al. *The Impact of Work Distribution on In Situ Visualization: A Case Study.* In Proc. of ISAV, p. 17-22, 2019

Using the Workflow Manager for Adsorption Isotherm Sampling



Adsorption Isotherm Results

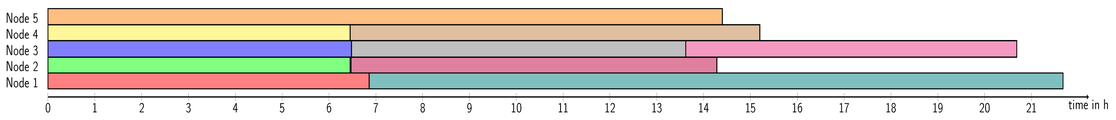




Snapshot of adsorption simulation scenario

- Adsorption isotherms for different solid-fluid energy parameters ε_{sf} at a constant temperature $T = 0.8\ T_c$ (with $T_c = 1.0779\ \varepsilon_f/k$).
- As wall potential a LJTS-10-4-3 potential is used.

Task Distribution by Default Scheduler



- Time distribution of tasks to nodes of adsorption isotherm simulations.
- Tasks distinguished by color.
- Work in Progress: Coupling with Extra-P for performance prediction
- TaLPas-supported developments of Extra-P yield an average 85% reduction in performance modeling cost, relevant particularly for higher-dimensional parametrizations

[1] J. Liu, et al. *Adsorption in Purely Dispersive Systems from Molecular Simulation, Density Gradient Theory, and Density Functional Theory*. J. Chem. Eng. Data. In press.

Contact: Prof. Dr. Philipp Neumann, Helmut-Schmidt-Universität Hamburg, philipp.neumann@hsu-hh.de
Website: www.talpas.de
This project has received funding from the Federal Ministry of Education and Research, grant numbers 01IH16008A-F.
SPONSORED BY THE Federal Ministry of Education and Research