MSA for Polymer Simulations: Optimizing GPU and CPU Simulations of MExMeMo

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Motivation and Introduction

MExMeMo: Combine continuum and particle dynamic methods to create a super-simulation using Modular Supercomputing Architecture (MSA).

- Particle dynamic methods: tracking individual particles → ***high-accuracy***; however, computationally demanding, limited scalability!
- Continuum methods: averaged results → ***efficiency and scalability***; however, loss of accuracy.

⇒ Couple both methods for best of both worlds!

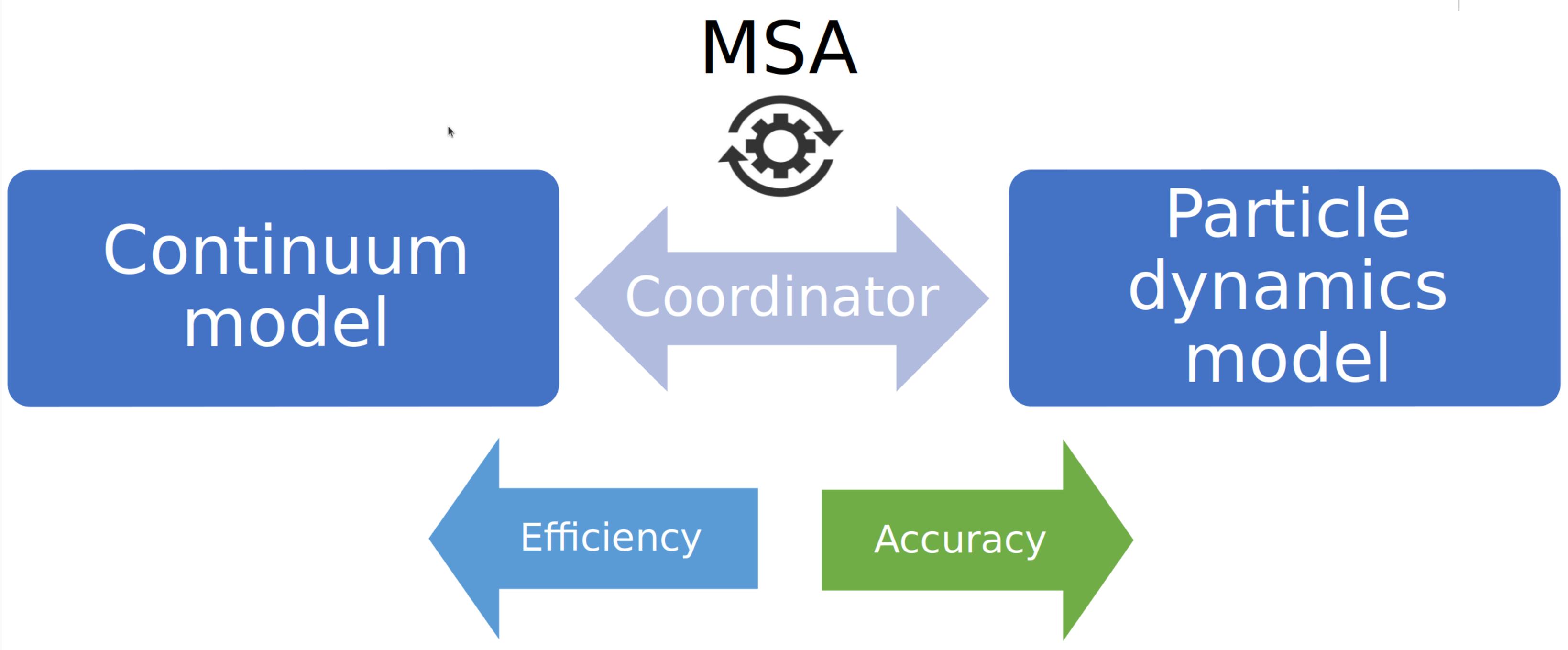
- Providing a digital twin for the fabrication and optimization of polymers.

JSC: Enable workloads on heterogeneous architecture, build ***coordinator***

SOMA Particle dynamic method, uses GPUs, JUWELS Booster.

DCAT Continuum model, uses the CPUs, JUWELS Cluster.

⇒ Optimize the different applications; enable standard data exchange protocol for coupled applications.



1) MExMeMo Simplified Model

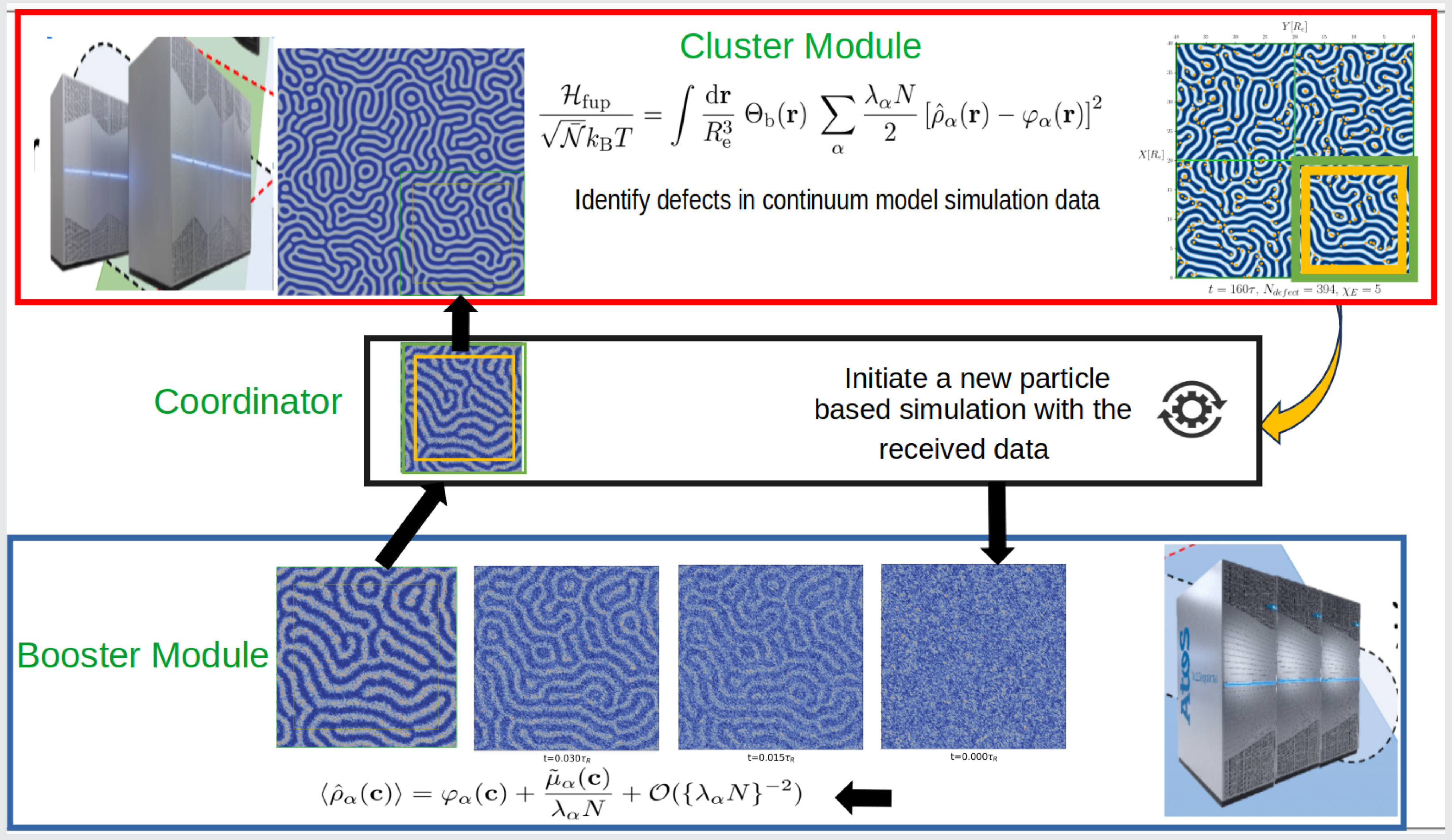


Figure 1: Basic MExMeMo model with one particle-based model instance on JUWELS booster.

2) Scalability of Continuum Model (DCAT)

- DCAT Large-scale simulation framework for polymer fabrication process (JUWELS Cluster).
- Enabling FMA instructions for FFT libraries.
- Generate training data for the machine-learning model.
- Using a standard format for exchanging data with the particle-based model.

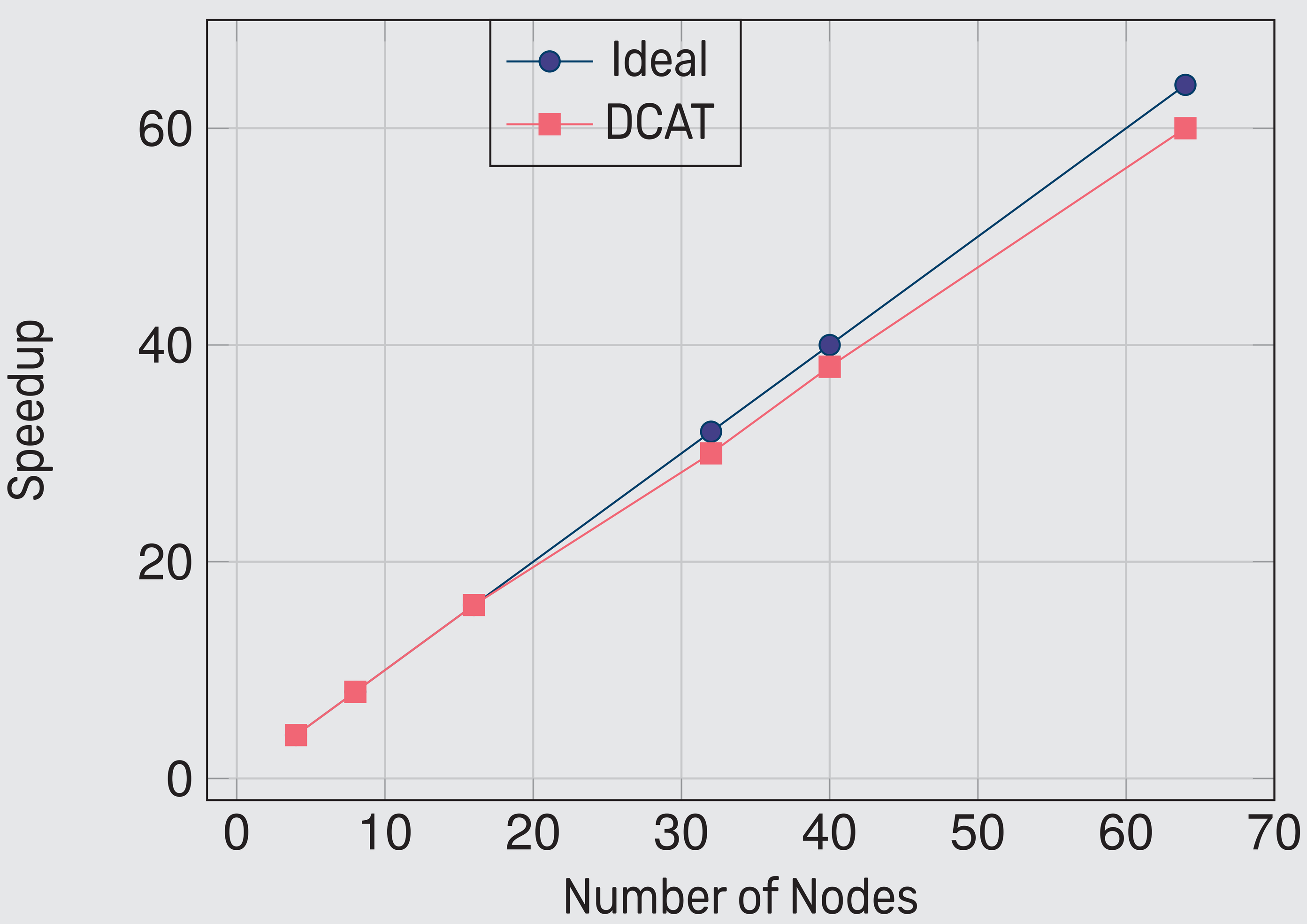


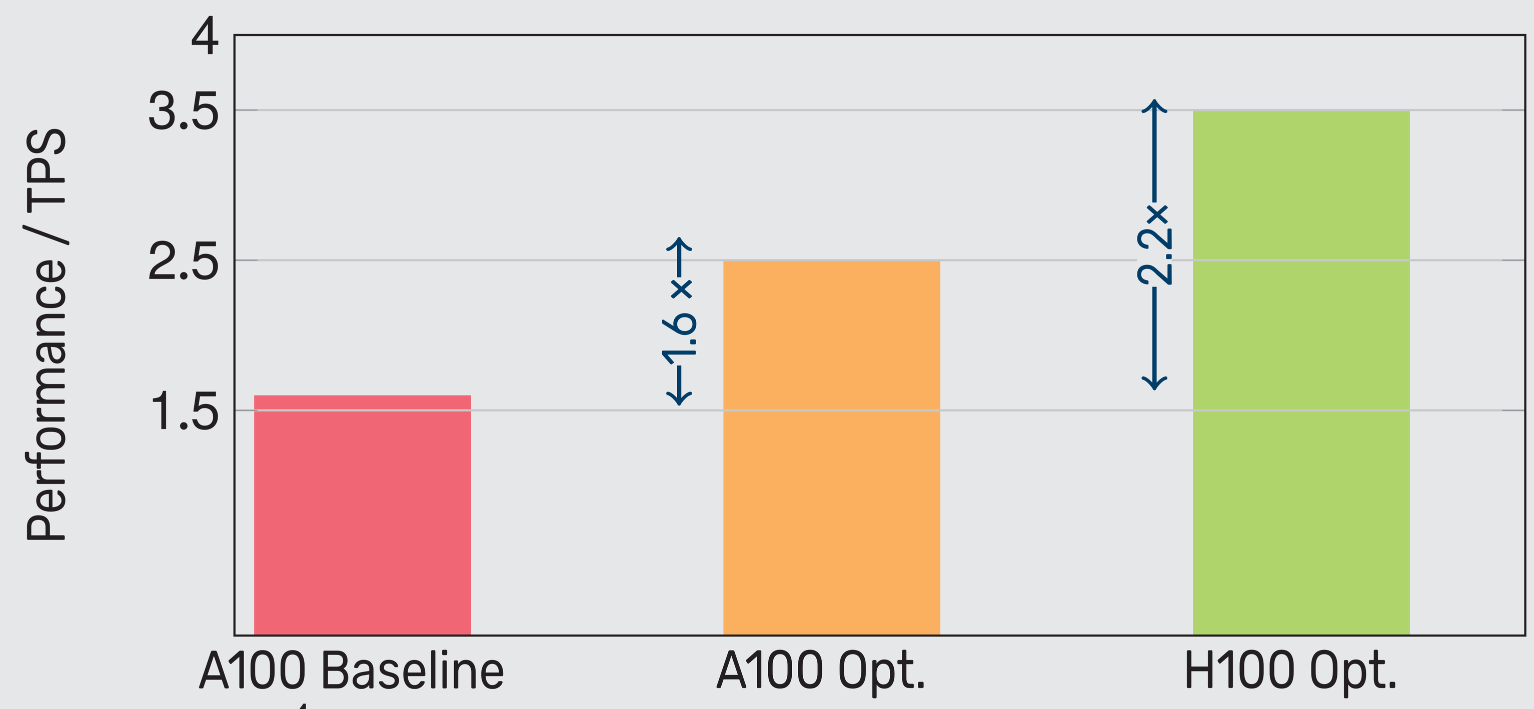
Figure 2: Good scalability of continuum model (DCAT) with number of nodes of JUWELS Cluster.

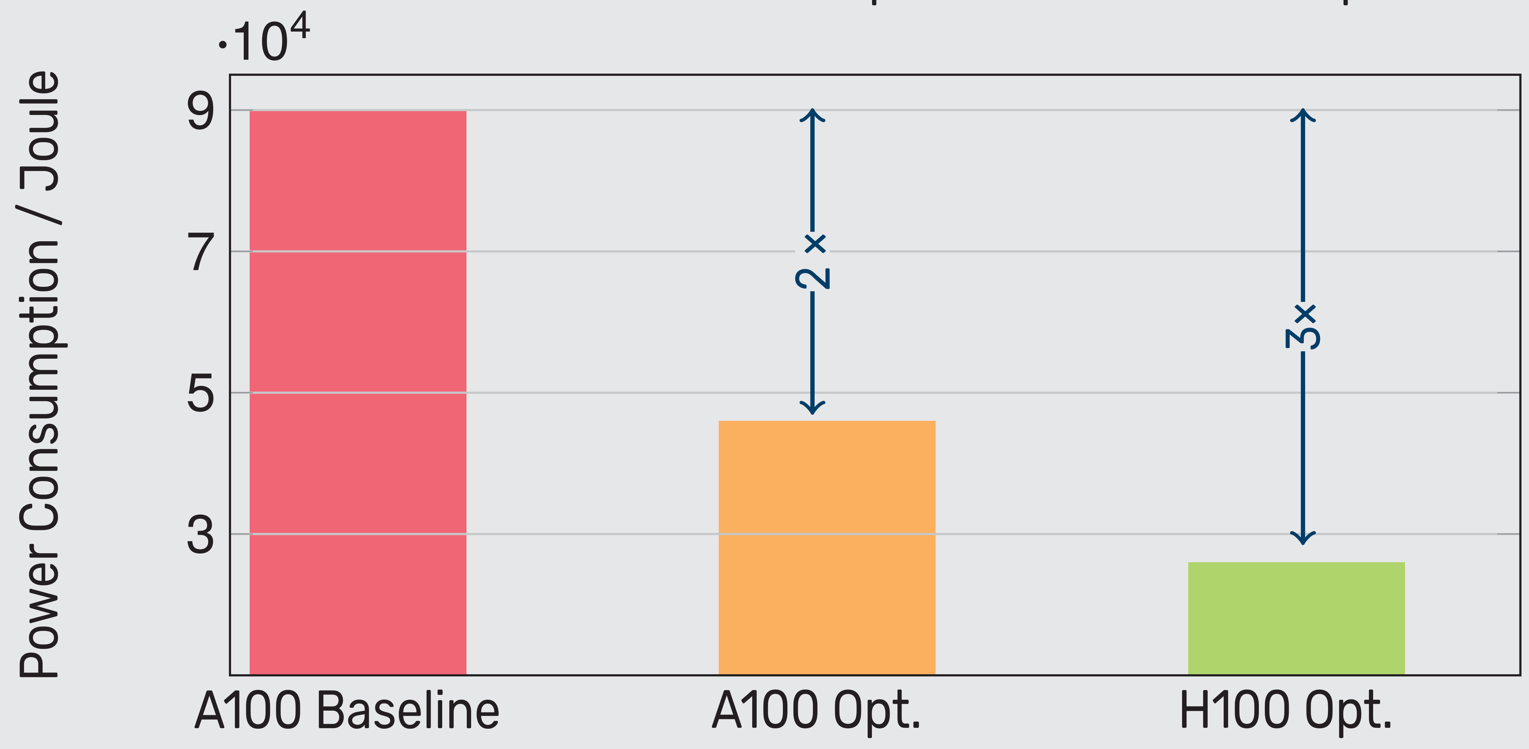
3) Performance Optimization of SOMA

SOMA GPU-based particle simulation developed at Uni Göttingen [1, 2]

- SOMA performance is limited by memory throughput, which we improved 2×.
- Time-to-solution improved 1.6× (**Timesteps per Second**, TPS).
- New hardware technology (H100): 2.2× (vs. SOMA baseline).
- Power consumption reduced 3×, 95 000 J → 26 000 J.

⇒ 18 TPS/MJ → 135 TPS/MJ (7.5×)





4) Future Road-map

- Design of a machine-learning solution for defects detection.
- Decision framework for scheduling and monitoring compute resources ⇒ Reduce time-to-solution/energy-to-solution.
- Vertical integration of simulation results with membrane fabrication.

Acknowledgment, References

MExMeMo is funded by the *Bundesministerium für Bildung und Forschung (BMBF)* under grant 16ME0660. BMBF receives funds by the European Union - NextGenerationEU.

(1) L. Schneider and M. Müller, *Comput. Phys. Commun.*, 2019, **235**, 463–476.
(2) M. Mueller and N. Blagojevic, *Bull. Am. Phys. Soc.*, 2023.