SPH-EXA: Optimizing Smoothed Particle Hydrodynamics for Exascale Computing

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hpc.dmi.unibas.ch/HPC/SPH-EXA.html

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1. Research Problem and Pursued Approach

How to perform Exascale-ready Smoothed Particle Hydrodynamics (SPH) simulations?

- **Interdisciplinary co-design** project between Computer Science, Astrophysics, and Computational Fluid Dynamics (CFD)
- **Assess the performance** of state-of-the-art Smoothed Particle Hydrodynamics codes
- **Understand their scalability limitations**
- **Design a mini-app** that synthesizes the characteristics of start-of-the-art SPH codes
- **Design and employ parallelization** methods and **fault-tolerance** mechanisms to sustain their scalability on massively parallel environments
- Employ state-of-the-art **dynamic load balancing** to address load imbalance

2. Methodology

- Comparative study of (parent) SPH production codes [2,7], shown in Table 1
- Performance analysis and optimization of parent SPH codes [7]. Their scalability is shown in Figure 1
- Design and development of the SPH-EXA mini-app [3]
  - Candidate for the SPEC HPC2020 benchmark suite
- Integration of state-of-the-art scheduling and load balancing methods [4], shown in Figure 2
- Development and integration of resilience techniques, such as selective replication [6]
- Development for reproducibility and portability via:
  - Continuous integration
  - EasyBuild
  - Containerization

Completed · Ongoing · Future

3. Achievements

Table 1: Differences and similarities between SPH-flow, SPHYNX, ChaNGa, and the SPH-EXA mini-app [3]

SPH Code	Code Version	Gradient Calculation	Kernel	Volume Elements	Mass of Particles	Time-Stepping	Neighbour Discovery	Self-Gravity
SPHYNX	1.4	IAD	Sinc	Generalized	Equal or Variable	Global	Tree Walk	Multipoles (4-pole)
ChaNGa	3.3	Kernel derivatives	Wendland	Standard	Equal or Variable	Individual	Tree Walk	Multipoles (16-pole)
SPH-flow	17.6	Kernel derivatives	Wendland	Standard	Equal or Variable	Global	Tree Walk	No
SPH-EXA mini-app	1.0	Kernel derivatives	Sinc, Wendland	Standard	Equal or Variable	Global	Tree Walk	Multipoles (16-pole)

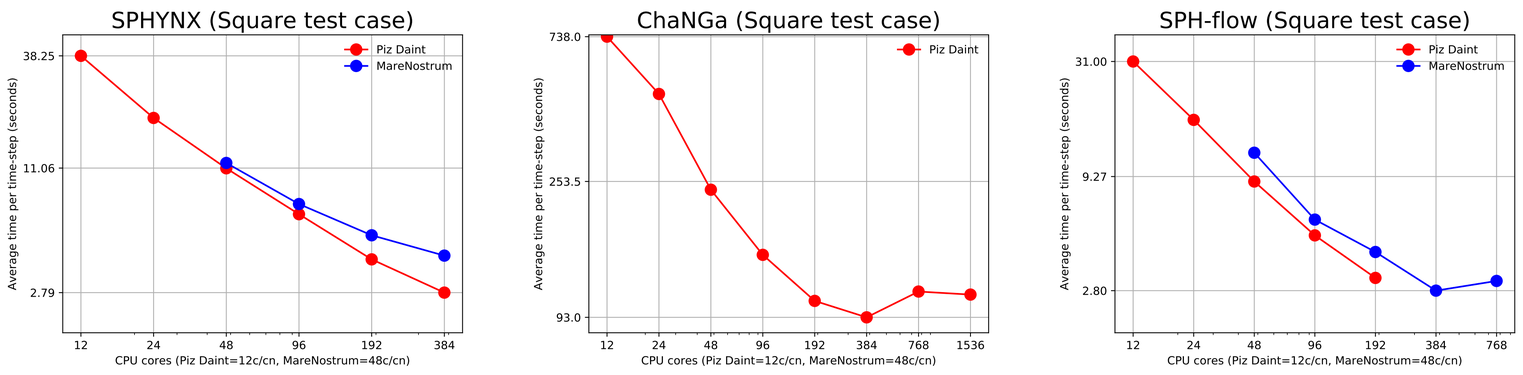

Figure 1: Strong scalability results of SPHYNX, ChaNGa, and SPH-flow, executing a rotating square patch test [3]

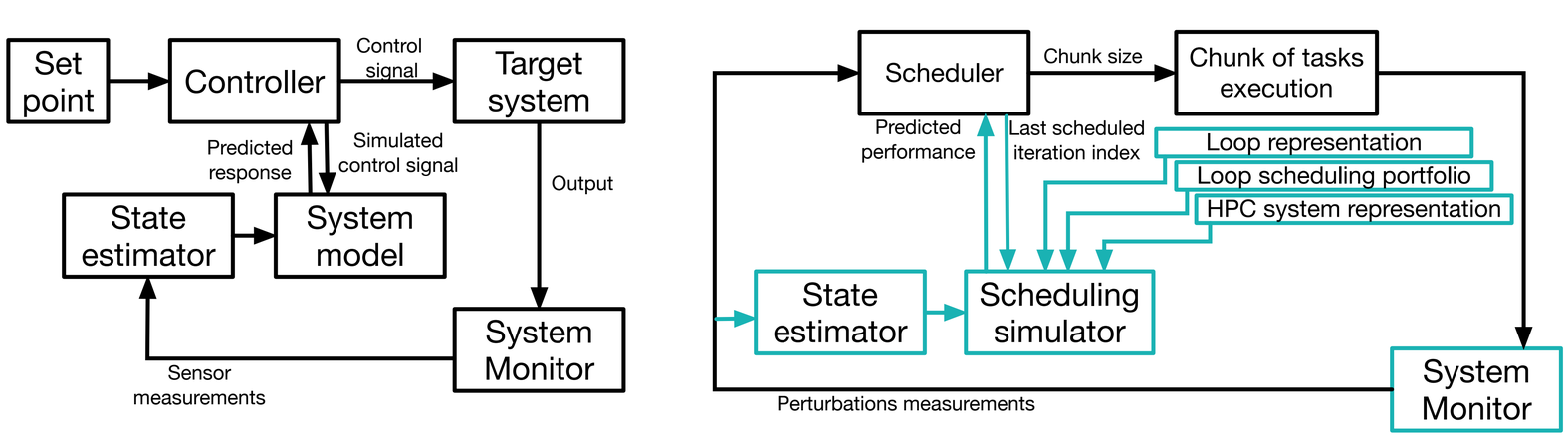

Figure 2: A generic control system (left) and the Simulator in the Loop (SiL) approach for loop scheduling [4] (right)

5. Acknowledgments

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4. Project Publications

[1] PASC SPH-EXA: Optimizing Smoothed Particle Hydrodynamics for Exascale Computing. *hpc.dmi.unibas.ch/HPC/SPH-EXA.html*

[2] R. M. Cabezón, K.-C. Pan, M. Liebendörfer, T. Kuroda, K. Ebinger, O. Heinimann, A. Perego, and F.-K. Thielemann Core-collapse supernovae in the hall of mirrors: A three-dimensional code-comparison project. In *Astronomy & Astrophysics*, Volume 619, November 2018, Article Number A118, November 13, 2018

[3] D. Guerrera, R. M. Cabezón, J.-G. Piccinali, A. Cavelan, F. M. Ciorba, D. Imbert, L. Mayer, and D. Reed. Towards a Mini-App for Smoothed Particle Hydrodynamics at Exascale. In *Proceedings of the 3rd International Workshop on Representative Applications (WRAp 2018) of the 20th IEEE Cluster Conference (Cluster 2018)*, Belfast, UK, September 10-13, 2018

[4] A. Mohammed and F. M. Ciorba SiL: An Approach for Adjusting Applications to Heterogeneous Systems Under Perturbations In *Proceedings of the International Workshop on Algorithms, Models and Tools for Parallel Computing on Heterogeneous Platforms (HeteroPar 2018) of the 24th International European Conference on Parallel and Distributed Computing (Euro-Par 2018)*, Turin, Italy, August 27-31, 2018

[5] D. García-Senz, R. M. Cabezón, and I. Domínguez Surface and Core Detonations in Rotating White Dwarfs. *The Astrophysical Journal*, Volume 862, Number 1, July 19, 2018

[6] A. Cavelan, F. M. Ciorba, and R. M. Cabezón Detection of Silent Data Corruptions in Smooth Particle Hydrodynamics Simulations Poster at the *30th ACM/IEEE International Conference for High Performance Computing, Networking, Storage and Analysis (SC 2018)*, Tier A, Dallas, Texas, USA, November 11-16, 2018

[7] D. Guerrera, F. M. Ciorba, R. M. Cabezón, A. Cavelan, L. Mayer, D. S. Reed, D. Imbert, and J.-G. Piccinali Towards an Exascale-Ready Mini-App for Smooth Particle Hydrodynamics. Poster at the *2018 Platform for Advanced Scientific Computing Conference (PASC18)*, Basel, Switzerland, July 2-4, 2018.

[8] D. Guerrera, A. Cavelan, R. M. Cabezón, D. Imbert, J. G. Piccinali, A. Mohammed, L. Mayer, D. Reed, and F. M. Ciorba. SPH-EXA: Enhancing the Scalability of SPH codes Via an Exascale-Ready SPH Mini-App. In Proceedings of the 2019 Spheric International Workshop, Exeter, UK, June 2019.

[9] A. Cavelan, R. M. Cabezón, J. H. Muller-Korndorfer, and F. M. Ciorba. Finding Neighbors in a Forest: A h-tree for Smoothed Particle Hydrodynamics Simulations. In Proceedings of the 2019 Spheric International Workshop, Exeter, UK, June 2019.