

Sources

- [1] Michael Griebel, Stephan Knapek, and Gerhard Zumbusch. Numerical Simulation in Molecular Dynamics. Springer Berlin Heidelberg New York, 1st edition, 2007.
- [2] Bart Janssens. CXXWRAP.JL Julia and C++: a technical overview of CxxWrap.jl, 2020. URL <https://barche.github.io/juliacon2020-cxxwrap-talk/#/2/1>.
- [3] Honghui Shang, Li Shen, Yi Fan, Zhiqian Xu, Chu Guo, Jie Liu, Wenhao Zhou, Huan Ma, Rongfen Lin, Yuling Yang, et al. Large-Scale Simulation of Quantum Computational Chemistry on a New Sunway Supercomputer. arXiv preprint arXiv:2207.03711, 2022.
- [4] Jeff Bezanson, Stefan Karpinski, Viral B. Shah, and Alan Edelman. Julia: A fast dynamic language for technical computing. CoRR, abs/1209.5145, 2012. URL <http://arxiv.org/abs/1209.5145>.
- [5] Hans-Joachim Bungartz, Stefan Zimmer, Martin Buchholz, and Dirk Pflüger. Modell- bildung und Simulation: eine anwendungsorientierte Einführung. Springer-Verlag, 2nd edition, 2013.
- [6] Fabio Alexander Gratl, Steffen Seckler, Hans-Joachim Bungartz, and Philipp Neumann. N ways to simulate short-range particle systems: Automated algorithm selection with the node-level library autopas. Computer Physics Communications, 273:108262, 2021. doi: 10.1016/j.cpc.2021.108262.