Simulation recipes from the Parrinello family cookbook

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Atomic-scale modeling of matter has made enormous progress over the past decades, increasing its accuracy with more efficient approximations of the electronic structure problem, and extending the time and length scales over which the statistical mechanics of defects and emergent phenomena can be sampled.

The recent incorporation of machine-learning approaches into modeling has opened up the problem, and opportunity, of combining physically-principled and data-driven algorithms into a coherent and effective modeling framework.

I will present a couple of "simulation recipes" that combine traditional and last-generation modeling techniques, showcasing the lasting impact of algorithmic developments in the atomistic modeling community and providing inspiration for its future research directions.

[1] E. Cignoni, D. Suman, J. Nigam, L. Cupellini, B. Mennucci, and M. Ceriotti, "Electronic Excited States from Physically Constrained Machine Learning", ACS Cent. Sci. **10**(3), 637–648 (2024).

[2] F. Bigi, M. F. Langer, and M. Ceriotti, "The dark side of the forces: assessing non-conservative force models for atomistic machine learning", in *Forty-Second International Conference on Machine Learning* (2025).

[3] F. Bigi, S. Chong, A. Kristiadi, M. Ceriotti, "FlashMD: long-stride, universal prediction of molecular dynamics", arXiv:2505.19350 (2025)