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Hessian-free force-gradient integrators and their application to lattice QCD simulations

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We present a novel class of Hessian-free force-gradient integrators \[arXiv:2403.10370\]. Unlike traditional force-gradient integrators, the Hessian-free variants do not require the analytical expression of the force-gradient term, which includes the Hessian of the potential. Instead, this term is approximated through an additional force evaluation.

We examine the order conditions and geometric properties of this new framework. Additionally, we perform a linear stability analysis of (Hessian-free) force-gradient integrators and discuss the relevance of this analysis to interacting field theories.

Among all self-adjoint Hessian-free force-gradient integrators with up to eleven stages, we identify the most promising ones in terms of computational efficiency and stability.

Finally, we demonstrate the application of these integrators in the molecular dynamics step of the Hybrid Monte Carlo algorithm for four-dimensional gauge field simulations in lattice QCD with Wilson fermions, showcasing the efficiency of the new decomposition algorithms.

Primary author: SCHÄFERS, Kevin (University of Wuppertal)

Co-authors: KNECHTLI, Francesco (University of Wuppertal); FINKENRATH, Jacob; GÜNTHER, Michael (University of Wuppertal)

Presenter: SCHÄFERS, Kevin (University of Wuppertal)

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