Hessian-free force-gradient integrators

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This talk deals with the framework of Hessian-free force-gradient integrators [1] for separable Hamiltonian systems of the form

$$H(p,q) = \frac{1}{2}p^\top M p + V(q).$$

Unlike traditional force-gradient integrators [2], the Hessian-free variants do not require the analytical expression of the force-gradient term, which includes the Hessian of the potential. Instead, the force-gradient update is approximated, effectively replacing the force-gradient term with an additional force evaluation. We examine the order conditions and discuss the geometric properties of the proposed numerical integration schemes. Moreover, we perform a linear stability analysis of (Hessian-free) force-gradient integrators and identify promising self-adjoint methods. Numerical experiments will be presented, highlighting the advantages and disadvantages of the Hessian-free variants.

References

1. *K. Schäfers, J. Finkenrath, M. Günther, F. Knechtli.* Hessian-free force-gradient integrators, *arXiv preprint*, 2024.

2. *I.P. Omelyan, I.M. Mryglod, R. Folk.* Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations, *Computer Physics Communications* 151.3, 272-314, 2003.

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