Accepted Manuscript

Multi-stage splitting integrators for sampling with modified Hamiltonian Monte Carlo methods

Tijana Radivojević, Mario Fernández-Pendás, Jesús María Sanz-Serna, Elena Akhmatskaya

 PII:
 S0021-9991(18)30484-4

 DOI:
 https://doi.org/10.1016/j.jcp.2018.07.023

 Reference:
 YJCPH 8148

To appear in: Journal of Computational Physics

Received date:31 January 2018Revised date:21 June 2018Accepted date:12 July 2018



Please cite this article in press as: T. Radivojević et al., Multi-stage splitting integrators for sampling with modified Hamiltonian Monte Carlo methods, J. Comput. Phys. (2018), https://doi.org/10.1016/j.jcp.2018.07.023

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Highlights

- We introduce new multi-stage integrators for enhanced sampling with modified Hamiltonian Monte Carlo methods.
- The integrators are obtained from the minimization of the (expected) modified energy error introduced by numerical integration.
- We propose computationally efficient expressions for modified Hamiltonians of order 4 and 6 for the multi-stage splitting integrators.
- An outstanding improvement over Verlet observed for problems in which the potential function is (approximately) quadratic.

Download English Version:

https://daneshyari.com/en/article/6928563

Download Persian Version:

https://daneshyari.com/article/6928563

Daneshyari.com