Beating the Verlet integrator in Monte Carlo simulations

S. Blanes, F. Casas, and J. M. Sanz-Serna

Citation: AIP Conference Proceedings **1558**, 8 (2013); doi: 10.1063/1.4825407
View online: http://dx.doi.org/10.1063/1.4825407
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1558?ver=pdfcov
Published by the AIP Publishing

Beating the Verlet Integrator in Monte Carlo Simulations

S. Blanes*, F. Casas† and J.M. Sanz-Serna**

*Instituto de Matemática Multidisciplinar, Universitat Politècnica de Valéncia, E-46022 Valencia, Spain. Email: serblaza@imm.upv.es
†Institut de Matemátiques i Aplicacions de Castelló and Departament de Matemátiques, Universitat Jaume I, E-12071 Castellón, Spain. Email: Fernando.Casas@uji.es
**Departamento de Matemática Aplicada e IMUVA, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain. Email: sanzsern@mac.uva.es

Abstract. We propose a new methodology for constructing integrators to simulate Hamiltonian dynamics within Hybrid Monte Carlo and related algorithms. The algorithms based on the new approach are minor modifications of the standard Verlet integrator that nevertheless provide very substantial savings in computational cost.

Keywords: Verlet integrator, Monte Carlo methods, Hybrid Monte Carlo
PACS: 02.70.Ns, 02.70.Uu

INTRODUCTION

The Hybrid Monte Carlo method and related algorithms [2] require the numerical simulation of Hamiltonian dynamics

$$\frac{d}{dt}q = \nabla T(p), \qquad \frac{d}{dt}p = -\nabla V(q), \tag{1}$$

by means of a volume-preserving, time-reversible integrator. The Verlet integrator is the method of choice. In its position version, each step $i \to i+1$ includes three substeps given by

$$\begin{aligned} q &\leftarrow q_i + \frac{h}{2}\nabla T(p_i), \\ p_{i+1} &\leftarrow p_i - h\nabla V(q), \\ q_{i+1} &\leftarrow q + \frac{h}{2}\nabla T(p_{i+1}), \end{aligned}$$

where subindexes refer to time-levels and h is the step-length. The literature contains many attempts to improve on the Verlet method. For instance, one may consider more sophisticated algorithms that concatenate in a palindromic way *five* substeps

$$\begin{aligned} q &\leftarrow q_i + a_1 h\nabla T(p_i), \\ p &\leftarrow p_i - b_1 h\nabla V(q), \\ q &\leftarrow q + a_2 h\nabla T(p), \\ p_{i+1} &\leftarrow p - b_1 h\nabla V(q), \\ q_{i+1} &\leftarrow q + a_1 h\nabla T(p_{i+1}), \end{aligned}$$

seven substeps, etc. Each substep corresponds to a symplectic (and therefore volumen preserving) transformation in (p,q) space and the palindromic structure ensures time-reversibility [3]. Furthermore such concatenations are as easy to code as the Verlet algorithm.

The standard practice in the design of numerical integrators is to determine the coefficients a_j, b_j by trying to boost the *order* of accuracy. For instance seven substeps make it possible to achieve order 4. Once the target order has been achieved, any remaining free coefficients are chosen so as to minimize the size of the error constants. The idea of

11th International Conference of Numerical Analysis and Applied Mathematics 2013
AIP Conf. Proc. 1558, 8-10 (2013); doi: 10.1063/1.4825407

order of accuracy and error constants relate to Taylor expansions in the limit $h \to 0$, but provide no information on the performance of the method for a fixed value of h.

In [1], we show, analytically and experimentally, that such a methodology may not make much sense in Monte Carlo applications. It turns out that the sophisticated integrators suggested in the literature are more accurate than Verlet (once different methods are allowed the same amount of computational effort) *only* for values of h so small that the acceptance rate with Verlet is close to 100%. We therefore propose a new methodology based on analytical results that do not assume that $h \to 0$.

A NEW APPROACH

We consider the standard one-dimensional oscillator with kinetic and potential energy $T = p^2/2$, $V = q^2/2$. Over one time-step, a time-reversible, volume-preserving integrator is given by

$$\begin{bmatrix} q_{i+1} \\ p_{i+1} \end{bmatrix} = \tilde{M}_h \begin{bmatrix} q_i \\ p_i \end{bmatrix}, \qquad \tilde{M}_h = \begin{bmatrix} A(h) & B(h) \\ C(h) & A(h) \end{bmatrix},$$

for suitable real-valued functions $A(h), B(h), C(h)$, with $A(h)^2 - B(h)C(h) \equiv 1$. The average error in total energy $T+V$ over one step, i.e. the mathematical expectation of

$$\big(T(p_{i+1}) + V(q_{i+1})\big) - \big(T(p_i) + V(q_i)\big)$$

with respect to the Maxwell-Boltzmann probability density function $\propto \exp\big(-T(p) - V(q)\big)$, may be shown [1] to be bounded by the quantity

$$\rho(h) = \frac{\big(B(h) + C(h)\big)^2}{2\big(1 - A(h)^2\big)}.$$

(For stable values of h, the denominator is > 0.) Our suggestion is to ensure consistency and then to choose the remaining free parameters so as to minimize

$$\|\rho\| = \max_{0<h<r} \rho(h),$$

where r denotes the number of evaluations of the force $-\nabla V$ at each time-step. Thus the maximum value of h grows linearly with r to make up for the higher computational cost per step.

NEW METHODS

By following this procedure we identify [1] the following method that comprises five substeps (two force evaluations) per step:

$$a_1 = \frac{3 - \sqrt{3}}{6} \approx 0.21132, \quad b_1 = \frac{1}{2}, \quad a_2 = 1 - 2a_1.$$

With seven substeps (three force evaluations) the optimal choice turns out to be [1]

$$a_1 = 0.11888010966548, \quad b_1 = 0.2961950426112569, \quad a_2 = 1/2 - a_1, \quad b_2 = 1 - 2b_1,$$

while with nine substeps (four force evaluations) one finds

$$\begin{aligned} a_1 &= 0.071353913450279725904, \\ a_2 &= 0.268548791161230105820, \\ b_1 &= 0.191667800000000000000, \\ b_2 &= 1/2 - b_1, \\ a_3 &= 1 - 2a_1 - 2a_2. \end{aligned}$$

Numerical experiments involving different Hamiltonian functions $H = T + V$ show [1] that the new methods clearly outperform the Verlet integrator. The benefits become more marked for larger numbers of degrees of freedom, where the saving in computational time may be very high.

ACKNOWLEDGMENTS

The authors have been supported by projects MTM2010-18246-C03-01 (Sanz-Serna) and MTM2010-18246-C03-02 (Blanes y Casas) from Ministerio de Ciencia e Innovación, Spain.

REFERENCES

1. S. Blanes, F. Casas, and J.M. Sanz-Serna, *Numerical Integrators for the Hybrid Monte Carlo Method*, to appear.
2. S. Duane, A.D. Kennedy, B. Pendleton, and D. Roweth, *Phys. Lett. B.* **195** 216–222 (1987).
3. J. M. Sanz-Serna and M. P. Calvo, *Numerical Hamiltonian Problems*, Chapman and Hall, London, 1994.