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Adapted Nested Force-Gradient Integrators: The Schwinger Model Case

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Abstract. We study a novel class of numerical integrators, the adapted nested force-gradient schemes, used within the molecular dynamics step of the Hybrid Monte Carlo (HMC) algorithm. We test these methods in the Schwinger model on the lattice, a well known benchmark problem. We derive the analytical basis of nested force-gradient type methods and demonstrate the advantage of the proposed approach, namely reduced computational costs compared with other numerical integration schemes in HMC.

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1 Introduction

For the Hybrid Monte Carlo algorithm (HMC) [5], often used to study quantum chromodynamics (QCD) on the lattice, one is interested in efficient numerical time integration schemes which are optimal in terms of computational costs per trajectory for a given acceptance rate. High order numerical methods allow the use of larger step sizes, but demand a larger computational effort per step; low order schemes do not require such large computational costs per step, but need more steps per trajectory. So there is a need to balance these opposing effects.

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Omelyan integration schemes [11] of a force-gradient type have proved to be an efficient choice, since it is easy to obtain higher order schemes that demand a small additional computational effort. These schemes use higher-order information from force-gradient terms to both increase the convergence of the method and decrease the size of the leading error coefficient. Other ideas to achieve better efficiency for numerical time integrators are given by multirate or nested approaches. These schemes do not increase the order but reduce the computational costs per path by recognizing the different dynamical time-scales generated by different parts of the action. Slow forces, which are usually expensive to evaluate, need only to be sampled at low frequency while fast forces which are usually cheap to evaluate need to be sampled at a high frequency. A natural way to inherit the advantages from both force-gradient type schemes and multirate approaches would be to combine these two ideas.

Previously, we studied the behavior of the adapted nested force-gradient scheme for the example of the n-body problem [15] and would like to learn more about their usefulness for lattice field theory calculations. Due to the huge computational effort required for QCD simulations, it is natural to attempt an intermediate step first. We chose the model problem of quantum electrodynamics (QED) in two dimensions, the Schwinger model [12], since it is well-suited as a test case for new concepts and ideas which can be subsequently applied to more computationally demanding problems [4]. As a lattice quantum field theory, it has many of the properties of more sophisticated models such as QCD, for example the numerical cost is still dominated by the fermion part of the action. The fact that this model, with far fewer degrees of freedom, does not require such large computational effort makes it the perfect choice for testing purposes.

We compare the behavior of numerical time integration schemes currently used for HMC [11] with the nested force-gradient integrator [3] and the adapted version introduced in [15]. We investigate the computational costs needed to perform numerical calculations, as well as the effort required to achieve a satisfactory acceptance rate during the HMC evolution. Our goal is to find a numerical scheme for the HMC algorithm which would provide a sufficiently high acceptance rate while not drastically increasing the simulation time.

The paper is organized as follows. In Section 2 we give a short overview of the HMC algorithm and numerical schemes for time integration, which are used in HMC. In Section 3 we present the 2-dimensional Schwinger model and introduce the idea of the force-gradient approach and the resulting novel class of numerical schemes. Section 4 is devoted to the results of a comparison between widely used algorithms and the new approach and Section 5 draws our conclusion.

2 Geometric integrators for HMC

In this section we provide a general overview of the HMC algorithm [5] to introduce our novel integrator. We also present some standard numerical time integrating methods