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Efficient Computation of Instantons for Multi-Dimensional Turbulent Flows with Large Scale Forcing

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Abstract. Extreme events play a crucial role in fluid turbulence. Inspired by methods from field theory, these extreme events, their evolution and probability can be computed with help of the instanton formalism as minimizers of a suitable action functional. Due to the high number of degrees of freedom in multi-dimensional fluid flows, traditional global minimization techniques quickly become prohibitive in their memory requirements. We outline a novel method for finding the minimizing trajectory in a wide class of problems that typically occurs in turbulence setups, where the underlying dynamical system is a non-gradient, non-linear partial differential equation, and the forcing is restricted to a limited length scale. We demonstrate the efficiency of the algorithm in terms of performance and memory by computing high resolution instanton field configurations corresponding to viscous shocks for 1D and 2D compressible flows.

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1 Introduction

Systems in nature are almost always subject to noise. Even though these random perturbations often are small in amplitude, they nevertheless have drastic consequences on the behavior of the system as a whole by facilitating rare but extreme excursions of the dynamics. Many processes in biology, chemistry, physics and economics, including phase

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transitions [12], ocean dynamics [27], rates of chemical reactions [23], genetic switches [2] and option pricing in finance [3,5] are caused by rare extreme events.

In the small noise limit, these extreme events are in fact very predictable. The arising most probable transition trajectory of the rare event in turn allows for predictions regarding both the evolution of the rare event and its probability. In the context of the Martin-Siggia-Rose/Jansen/de Dominicis formalism [8,22,25] these field configurations are termed *instantons*. They correspond to the minimizers of the rate function in the Freidlin-Wentzell theory of large deviations [9,14].

A number of numerical algorithms have been devised to compute these field configurations. Some of them, like the nudged elastic band method [19] or the string method [11], are only applicable to the important sub-class of gradient systems, while others, most notably the minimum action method [10] and variants thereof [21, 30], are able to find the instanton configuration for more general cases. All have in common that they solve the problem *globally*, by discretizing the trajectory along the physical time and applying global operations on its entirety. For PDE systems with an infinite number of degrees of freedom, in particular in higher dimensions, such as arising in turbulent fluids, the memory requirements of these algorithms quickly become prohibitive.

Many questions in fluid dynamics, such as shock formation in compressible flows [15] or the generation of rogue waves [26], allow an alternative to the global formulation due to the nature of their mixed initial/final boundary conditions. Here, it is feasible to iteratively solve the equations of motion (the *instanton equations*) of the underlying Hamiltonian system instead [7]. The boundary conditions are propagated throughout the domain, which opens up possibilities to avoid saving the field configuration at every instance in time. In particular, a drastic reduction in memory is possible by combining a number of techniques: (a) considering the "geometric" reparametrization of the trajectory instead of parametrization by physical time, (b) recursive storage of transition states, inspired by multigrid techniques, (c) exploiting the compactness of the support of the force correlation in turbulence setups, and (d) further memory reductions through wavelet compression. The detailed presentation of the resulting algorithm constitutes the core of this work. We illustrate its effectiveness by applying it to 1D and 2D compressible turbulence. In fact we demonstrate that the combined optimizations reduce the memory footprint enough to fit optimization problems with $N=10^{10}$ degrees of freedom on a single graphics card. It therefore becomes feasible to solve the numerical problem on graphics processing units (GPUs) instead of their host machines at a considerable gain in runtime performance. In consequence, all algorithms presented in this paper are implemented on GPUs using the CUDA framework [1]. Furthermore, due to its memory efficiency, the scheme in principle allows attacking the important problem of the computation of instanton configurations for the 3D incompressible Navier-Stokes equation, which would yield scaling predictions for turbulent statistics.

This paper is organized as follows: We first establish the instanton formalism and the associated minimization problem in Section 2. We introduce the Martin-Siggia-Rose/Janssen/de Dominicis formalism and present a beneficial modification of the action func-