

A Hybrid Monte Carlo algorithm for sampling rare events in space-time histories of stochastic fields

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We introduce a variant of the Hybrid Monte Carlo (HMC) algorithm to address large deviation statistics in stochastic hydrodynamics. Based on the path integral approach to stochastic (partial) differential equations, our HMC algorithm samples space-time histories of the dynamical degrees of freedom under the influence of random noise. First, we validate and benchmark the HMC algorithm by reproducing multi-scale properties of the one-dimensional Burgers equation driven by Gaussian and white-in-time noise. Second, we show how to implement an importance sampling protocol to significantly enhance, by order-of-magnitudes, the probability to sample extreme and rare events, making it possible for the first time to estimate moments of field variables of extremely high order (up to 30 and more). By employing reweighting techniques, we map the biased configurations back to the original probability measure in order to probe their statistical importance. Finally, we show that by biasing the system towards very intense negative gradients, the HMC algorithm is able to explore the statistical fluctuations around instanton configurations. Our results will also be interesting and relevant in lattice gauge theory since they provide a new insight on reweighting techniques.

I. INTRODUCTION

Intermittency and anomalous scaling are two key features of turbulent flows important for both fundamental questions of out-of-equilibrium systems and applied flow configurations [1, 2]. Although these phenomena have been subject of research for decades it is fair to say that we are still far from understanding their origin and controlling their statistical properties from first principles. Intermittency is connected to the strong non-Gaussian nature of turbulent energy dissipation, which is dominated by localized, quasi-singular structures. Anomalous scaling is connected to intermittency via the inertial-range turbulent energy cascade, which proceeds from large to small scales, breaking self-similarity, with power-law correlation functions that do not follow dimensional scaling. The two phenomena are correlated, with the small-scale energy dissipation being the result of the inertial-range energy transfer [2]. The problem is therefore how to characterize the statistical properties of intense, but rare hydrodynamical fluctuations, an issue that is difficult to attack with brute force forward-in-time-evolution of the underlying partial differential equations due to the unpredictability and sparsity of such events. This sobering state of affairs prompted repeated speculations whether techniques developed for quantum field theory (QFT) might eventually turn out to be useful to attack the existence of these (quasi-)singular struc-

tures in a nonperturbative way, free from any modeling assumptions [3–10].

The way to proceed is to use the Janssen-de Dominicis [11, 12] path integral approach based on the seminal work by Martin, Siggia, and Rose (MSR) [5, 13–17] to describe the space-time flow configuration when stirred by a random external forcing. This formalism is based on the introduction of an action that depends on the flow configuration and constructs the measure as a weighted sum of all possible flow-realizations. This opens up the possibility to address Navier-Stokes equations using Markov Chain Monte Carlo (MCMC) methods well-known from lattice QFT and/or statistical mechanics by sampling full *space-time* histories. Although computationally challenging, this provides a unique perspective on the problem of turbulence in the sense that it allows to consider systematic improvements of the importance sampling in regions of the phase space where standard (forward-in-time) numerical integration faces difficulties, e.g., due to insufficient statistics. In particular, it allows us to address questions regarding the probability of rare events associated with exceptionally large fluctuations, which are at the focus of turbulence research and often attacked by semi-analytical tools based on instanton calculus and large deviations theory.

Instantons were introduced in turbulence theory in [18] where the probability densities of positive velocity gradients and increments (smooth ramps) were calculated analytically. The calculation of the probability densities of negative velocity gradients and increments (shocks) were performed in [19] where the asymptotic behavior

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could be determined utilizing the Cole-Hopf transformation [20, 21]. Using instantons in the calculation of rare, irregular transitions between different attractors in fluid flows is presented in [22, 23]. Other important methods not related to instantons are, e.g., adaptive multilevel splitting techniques (see [24–26] and references therein). Comparison of these methods with our path integral based approach is envisaged for future studies.

The objective of this work is to implement, test, and employ a Hybrid Monte Carlo algorithm [27, 28] for hydrodynamic turbulence. The HMC algorithm was developed to tackle outstanding problems in the theory of strong interactions [29] and is advantageous for problems where the classical action involves nonlocal terms. We address the case of the one-dimensional random-noise-driven Burgers equation [30], which is widely considered the perfect testbed for new ideas in turbulence [31]. A previous attempt based on the path integral for hydrodynamical systems was explored in [32–34], based on a local successive over-relaxation algorithm [35, 36].

From a methodological point of view, our first important result is the validation of the HMC against pseudo-spectral (PS) forward-time-integration techniques that are widely used in simulations of the random-noise-driven Burgers equation. We clearly stress that while the HMC is certainly not competitive with standard PS methods whenever the interest is confined to low order flow moments, e.g., the total mean energy and total mean energy dissipation, it becomes unavoidable if the focus is on very large fluctuations, e.g., either high order moments of velocity increments or extreme events for the space-time distribution of the energy dissipation. Indeed, the main quantitative new result about the properties of Burgers' equation is the implementation of an importance sampling technique to steer the HMC algorithm to explore the phase-space region where rare and extreme fluctuations happen. We show later that thanks to several technical improvements of the basic HMC algorithm we are able to probe fluctuations 30 (and more) standard deviations away from the mean for the velocity gradient probability distribution function (PDF), something that would be simply impossible to achieve with standard time-advancing algorithms.

The outline of this article is as follows: In Sec. II we briefly discuss the phenomenology of the random-noise-driven Burgers equation and in Sec. III we introduce the path integral for stochastic dynamics. Sec. IV introduces the HMC algorithm and details the individual steps of our implementation. Then, in Sec. V we show that the HMC algorithm successfully reproduces the results of a standard PS forward-time-integration method (hereafter also referred to as direct numerical simulation, or DNS) at the example of the stochastic Burgers equation. In the following section, Sec. VI, we investigate different boundary conditions and constraints in space and time. First, in Sec. VIA we impose periodic boundary conditions in time, while in Sec. VIB we show how the HMC is capable to consistently enhance the sampling of extreme and

rare events by imposing field-force constraints to systematically support the occurrence of strong negative velocity gradients. Here, we will also discuss the significant performance improvements by the HMC compared to a standard DNS method in regards to the sampling of the tails of the probability distribution function of observables. Finally, in Sec. VII we emphasize the significance of instantons for the theory of turbulence and derive the instanton configuration for Burgers' equation. We also show numerical results associated with the methods developed in Sec. VIB to support the relevance of instantons in extreme events.

II. STOCHASTIC BURGERS' EQUATION: A SIMPLE MODEL FOR HYDRODYNAMIC TURBULENCE

In this work we are concerned with the one-dimensional, random-noise-driven Burgers equation [30], which can be seen as a prototype system for compressible hydrodynamic turbulence and is given by

$$\partial_t v + v \partial_x v - \nu \partial_x^2 v = \eta. \quad (1)$$

Specifically, we consider the time evolution of the scalar velocity field v in a periodic spatial domain $x \in [-L/2, L/2]$ on a given time interval $t \in [t_0, t_f]$ of length $T = t_f - t_0$; ν is the kinematic viscosity and the random noise $\eta = \eta(x, t)$ is assumed to be centered and Gaussian-distributed. Thus, the random noise can be fully characterized in terms of two-point correlations

$$\langle \eta(x, t) \eta(x', t') \rangle \equiv \int \mathcal{D}\eta \mathcal{P}_\eta \eta(x, t) \eta(x', t'), \quad (2)$$

where $\mathcal{P}_\eta \equiv \mathcal{P}[\eta]$ is the random-noise probability distribution functional and the integration $\int \mathcal{D}\eta \dots$ is taken over all field configurations $\eta = \eta(x, t)$.

Generally, in the following, $\mathcal{D}\phi$ will denote a functional measure associated to the field ϕ . Path integrals $\int \mathcal{D}\phi \dots$ will always be supplied with “boundary conditions” in field space. Furthermore, where appropriate, ensemble averages will be denoted by angular brackets, $\langle \dots \rangle$. E.g., for an observable $\mathcal{O}_\phi \equiv \mathcal{O}[\phi]$, we have $\langle \mathcal{O}_\phi \rangle = \int \mathcal{D}\phi \mathcal{P}_\phi \mathcal{O}_\phi$, and $\int \mathcal{D}\phi \mathcal{P}_\phi = 1$. Depending on context we might drop the index indicating the field degrees of freedom to be averaged over.

In this paper, we restrict our attention to the case where the random noise is self-similar in space and delta-correlated in time; the corresponding two-point Fourier correlation given by

$$\langle \eta(k, t) \eta(k', t') \rangle = \Gamma(k) \delta_{k+k', 0} \delta(t - t'), \quad (3)$$

where $k, k' \in \mathbb{Z}$ and $\Gamma(k) = \Gamma_0 |k|^\beta$ with negative power-law exponent β that controls the scale-by-scale energy

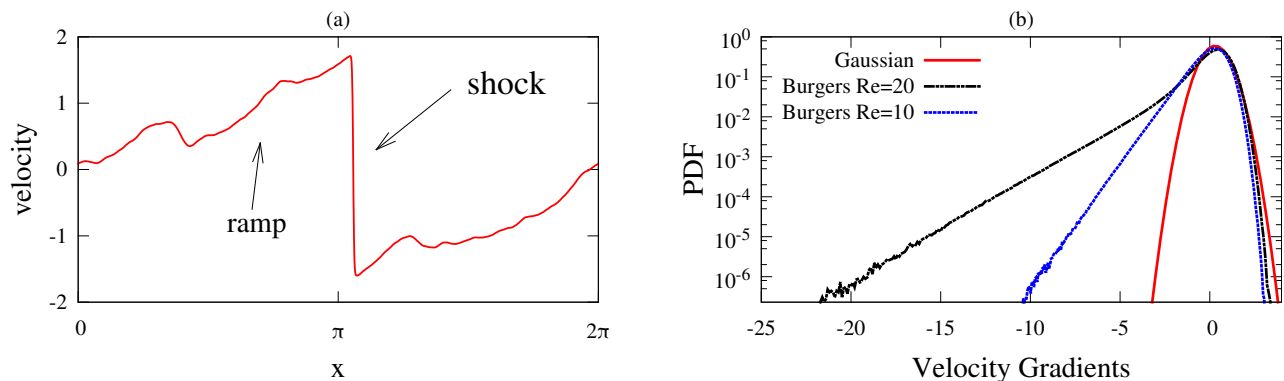


FIG. 1. (a) Shock wave as a particular realization of Burgers' equation. Its two main features are the ramps and jumps of finite width. (b) PDF of velocity gradients of Burgers' equation for two different Reynolds numbers compared with a Gaussian distribution. The finite jumps in the shock wave profile are responsible for the heavy left tail, while the right tail is due to the ramps.

injection.¹

From Eq. (1) it is easy to derive the evolution equation for the energy spectrum, $E(k, t) = |v(k, t)|^2$:

$$\partial_t E(k, t) = T(k, t) - 2\nu k^2 E(k, t) + 2\Re\{v(k, t)^* \eta(k, t)\}, \quad (4)$$

where $T(k, t) = (k/L) \sum_{k'} \Im\{v(k, t)^* v(k', t) v(k - k', t)\}$ is the energy transfer [2]. Eq. (4) can be further simplified if we average over noise realizations and assume stationarity:

$$\langle T(k) \rangle - 2\nu k^2 \langle E(k) \rangle + 2\Gamma(k) = 0. \quad (5)$$

The ensemble-averaged cumulative energy injection due to the stochastic forcing η is given by $\langle \varepsilon_{\text{in}}(k) \rangle = (2/L) \sum_{|k'| \leq k} \Gamma(k')$ and is dominated by the infrared regime only if $\beta < -1$. Thus, in order to mimic the standard large-scale injection we will always keep $\beta = -3$ in this paper (see [37–40] for a detailed investigation of the statistical properties at changing the forcing slope).

It is well known that the evolution to Burgers' equation is characterized by the formation of quasi-singular shocks, i.e., localized events with a steep negative velocity gradient where all the dissipation is concentrated. In the small-viscosity limit the typical width of the shock becomes smaller, but the ensemble-averaged mean energy dissipation $\langle \varepsilon_{\text{diss}} \rangle = (2\nu/L) \sum_k k^2 \langle E(k) \rangle$ remains nonvanishing. Since $T(k)$ only transfers the energy between different modes, but does not contribute to the total energy, the total energy injection matches the energy dissipation:

$$\lim_{k \rightarrow \infty} \langle \varepsilon_{\text{in}}(k) \rangle = \langle \varepsilon_{\text{diss}} \rangle. \quad (6)$$

Writing Eq. (1) in a dimensionless way, reveals that the problem has only one control parameter, the Reynolds

number, Re . This is made manifest by introducing characteristic scales of length L_0 , and velocity V_0 , and a time scale $T_0 = L_0/V_0$. We change x, t, v , and η according to

$$\begin{aligned} x &\mapsto x L_0, & v &\mapsto v V_0, & t &\mapsto t T_0 = t L_0/V_0, \\ \eta &\mapsto \eta V_0/T_0 = \eta V_0^2/L_0, \end{aligned} \quad (7)$$

to obtain the dimensionless stochastic Burgers equation

$$\partial_t v + v \partial_x v - \frac{1}{\text{Re}} \partial_x^2 v = \eta, \quad (8)$$

with $\text{Re} \equiv L_0 V_0/\nu$. Consequently, in the remainder of this paper we will speak about the large Reynolds number and the small-viscosity limits interchangeably.

In Fig. 1 two of the most characteristic elements of “Burgers turbulence” are shown. Fig. 1(a) depicts the shock formation as a solution of Burgers' equation, which is described by the finite width jumps and approximately linear ramps. The localized jumps at the shock are the source of intermittency in this model, and they are responsible for the heavy left tail in the PDF of negative velocity gradients (see Fig. 1(b)), while the ramps are related to the right tail (we refer to [31] for an in-depth review of Burgers turbulence). From the previous discussion the question we ultimately want to address becomes clear: Is it possible to develop new algorithms which are able to focus specifically on phenomenon of shock formation by exploring only the far left tail of the PDF shown in Fig. 1(b)? This will be the aim of the novel HMC approach we propose.

III. PATH INTEGRAL FOR STOCHASTIC DYNAMICS

The path integral for stochastic dynamics was first introduced in Refs. [41–43]. To make our exposition self-consistent, however, we briefly repeat the main steps of its derivation. While we employ the same notation as in

¹ In practice, when $\beta < -1$, the correlator will be regularized by an infrared cutoff $k_{\text{IR}} \sim 1/L$, $k_{\text{IR}} > 0$.

Eq. (1) we emphasize that the following reasoning is in principle applicable to any stochastic (partial) differential equation (SPDE) driven by Gaussian random noise, delta-correlated in time. We will denote these SPDEs by the following short-hand notation:

$$F(x, t, v, \partial_x^m v, \partial_t^n v) = \eta, \quad (9)$$

with $m, n \in \mathbb{N}_0$. $F \equiv F(x, t, v, \partial_x^m v, \partial_t^n v)$ should be interpreted as a (nonlinear) differential operator, which acts on the dynamical field $v = v(x, t)$. We will only make some minimal assumptions regarding its form, namely that it should yield a well-posed initial value problem. By well-posed we mean that for any given random noise realization η , there exists one and only one solution v to Eq. (9) in the domain $-L/2 \leq x \leq L/2$ and for finite times $0 \leq t \leq T$.

To derive the path integral associated to Eq. (9) we define the partition sum \mathcal{Z} by integrating \mathcal{P}_η over all noise realizations. Since η is Gaussian and white in time, we have

$$\mathcal{P}_\eta \propto e^{-\frac{1}{2} \int dt \int dx \eta(x, t) \int dx' \Gamma^{-1}(x-x') \eta(x', t)}, \quad (10)$$

where Γ^{-1} is the inverse of the correlation function of the noise defined in Eq. (3). Accordingly, we define the partition sum as

$$\mathcal{Z} = \int \mathcal{D}\eta e^{-\frac{1}{2} \int dt (\eta, \Gamma^{-1} * \eta)}, \quad (11)$$

where the binary operator $*$ denotes the convolution, i.e., $(f * g)(x) = \int dx' f(x') g(x - x')$ and by (\cdot, \cdot) we designate the integral over the (bounded) spatial domain $[-L/2, L/2]$, i.e., $(f, g) \equiv \int dx f(x) g(x)$, with $\|f\|^2 \equiv (f, f)$. Changing the integration in Eq. (11) from η to v modifies the functional measure as

$$\mathcal{D}\eta = \mathcal{D}v |\det(\delta F / \delta v)|, \quad (12)$$

where $\mathcal{J} = |\det(\delta F / \delta v)|$ is the Jacobian associated to the map $v \mapsto \eta$. The latter is assumed to be nonsingular and therefore $\mathcal{J} > 0$.

Putting everything together, we may write the partition sum in the form of a path integral over v

$$\mathcal{Z} = \int \mathcal{D}v \mathcal{J} e^{-\frac{1}{2} \int dt (F, \Gamma^{-1} * F)} \equiv \int \mathcal{D}v e^{-\mathcal{S}}, \quad (13)$$

with action

$$\mathcal{S} = \frac{1}{2} \int dt (F, \Gamma^{-1} * F) - \ln \mathcal{J}, \quad (14)$$

associated to the stochastic PDE (9). Note that the action bares resemblance to the well-known Onsager-Machlup functional [44].² The probability distribution

² More generally, one arrives at the following action:

$$\mathcal{S} = -\ln\{\mathcal{Z} \mathcal{P}_\eta[\eta = F]\} - \ln \mathcal{J}, \quad (15)$$

functional \mathcal{P}_v for the dynamical field v is given by $\mathcal{P}_v = \mathcal{Z}^{-1} e^{-\mathcal{S}}$ and satisfies the normalization condition $\int \mathcal{D}v \mathcal{P}_v = 1$.

Specifically, for Burgers' equation, $F = \partial_t v + v \partial_x v - \nu \partial_x^2 v$ and $\mathcal{J} = \text{const.}$ (which holds for causal, forward-time propagation, see, e.g., [45] and Sec. V of this paper), the action Eq. (14) takes the following form:

$$\begin{aligned} \mathcal{S} = & \frac{1}{2} \int dt \int dx (\partial_t v + v \partial_x v - \nu \partial_x^2 v) \\ & \times \int dx' \Gamma^{-1}(x - x') (\partial_t v + v \partial_{x'} v - \nu \partial_{x'}^2 v), \end{aligned} \quad (16)$$

where we dropped the constant contribution from the Jacobian.

IV. HYBRID MONTE CARLO ALGORITHM

The Hybrid Monte Carlo algorithm, originally introduced in [27], has become a standard computational tool to tackle demanding numerical simulations of quantum field theories in the path integral formulation (see [46, 47] for reviews). It belongs to the broad class of Markov Chain Monte Carlo methods, and uses artificial Hamiltonian dynamics to advance the dynamical degrees of freedom in Monte Carlo time to generate unbiased field samples. A main feature of the HMC is that dynamical fields and their conjugate momenta can be evolved in parallel in a given time step of the evolution, if, e.g., a leap-frog type integrator is used. This makes the HMC most suitable for problems where the classical action of the theory features strong, nonlocal interactions (as is the case in Burgers' equation).

In this work, for the first time, we apply the HMC algorithm for a stochastically driven PDE at the example of Burgers' equation. In order to be self-contained, we will first briefly review its basic elements. Then, we proceed to discuss important improvements to the HMC algorithm, which allow for a significant enhancement of performance to sample various statistical estimators in a stable and consistent way.

In the HMC algorithm a set of momenta is introduced which are conjugate to the, in our case, velocity fields. Adding these momenta to the partition sum of Eq. (13) leads to an (artificial) Hamiltonian, which governs the dynamics in Monte Carlo time s via Hamilton's equations of motion. In practice, the numerical solution of Hamilton's equations starting from some initial Monte Carlo time, say $s = 0$ to a final time, $s = \tau$, has to be performed in discrete steps, which leads to the fact that the energy of the artificial Hamiltonian system is not conserved. This can be repaired by adding a global reject/accept step which makes the algorithm exact and guarantees the convergence to the desired probability distribution. See [48] for a general review on the HMC algorithm.

To be more concrete, the HMC algorithm starts by generating a set of Gaussian-distributed momenta $\pi =$

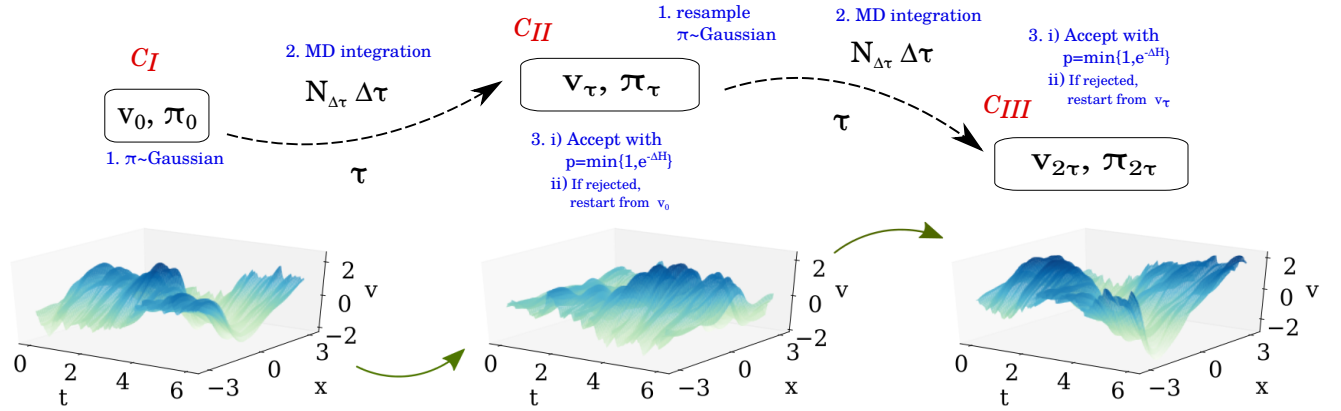


FIG. 2. *Top*: HMC evolution steps (1-3) as described in Sec. IV A. The dashed arrows represent the $N_{\Delta\tau}$ number of intermediate steps of size $\Delta\tau$. *Bottom*: Example of three successive velocity field configurations generated by the HMC algorithm (note, the conjugate momentum fields are not shown).

$\pi(x, t)$ such that the partition sum is modified as

$$\mathcal{Z} \propto \int \mathcal{D}\pi e^{-\frac{1}{2} \int dt \|\pi(t)\|^2} \int \mathcal{D}v e^{-\mathcal{S}}. \quad (17)$$

Identifying $\mathcal{K} = \frac{1}{2} \int dt \|\pi(t)\|^2$ as the “kinetic term” and \mathcal{S} as the “potential” we may interpret $\mathcal{H} = \mathcal{K} + \mathcal{S}$ as the Hamiltonian of the system, with probability distribution functional: $\mathcal{P}_{v, \pi} \propto e^{-\mathcal{H}}$. Since $\int \mathcal{D}\pi \mathcal{P}_{(v, \pi)} = \mathcal{P}_v$, the ensemble average of any velocity-dependent observable \mathcal{O}_v remains unaltered. The so constructed Hamiltonian system can now be evolved using Hamilton’s equations of motion. In this evolution, the role of “time” is played by s . In order to make the dependence on s explicit, we will introduce $v_s(x, t)$ and $\pi_s(x, t)$ where the subscript indicates the Monte Carlo time. Hamilton’s equations for the Hamiltonian \mathcal{H} , with the action as in Eq. (16), are then given by

$$\frac{dv_s}{ds} = \frac{\delta \mathcal{H}}{\delta \pi_s(x, t)} = \pi_s(x, t), \quad (18a)$$

$$\frac{d\pi_s}{ds} = -\frac{\delta \mathcal{H}}{\delta v_s(x, t)} = -\frac{\delta \mathcal{S}}{\delta v_s(x, t)}. \quad (18b)$$

In the case of the one-dimensional Burgers equation, the forces $f_\pi \equiv -\frac{\delta \mathcal{S}}{\delta v_s(x, t)}$ acting on the conjugate momenta are given by:

$$f_\pi = (\partial_t + v\partial_x + \nu\partial_x^2) \times \int dx' \Gamma^{-1}(x - x') (\partial_t v + v\partial_{x'} v - \nu\partial_{x'}^2 v). \quad (19)$$

A. HMC implementation

The equations of motion (18) are solved for (v_s, π_s) , $0 \leq s \leq \tau$, starting at Monte Carlo time $s = 0$ and integrating up to $s = \tau$; τ defines the trajectory length. We apply a symmetric symplectic integrator (leapfrog

scheme) with stepsize $\Delta\tau = \tau/N_{\Delta\tau}$, with $N_{\Delta\tau}$ a parameter that gives the number of steps to complete the trajectory of length τ .

Due to the finite integration step size error the Hamiltonian reached at $s = \tau$ will be different from the initial Hamiltonian. To correct for this deficiency, we apply a global Metropolis accept/reject step of the proposed new momentum and velocity field configuration: the new field configuration is accepted with probability $p = \min(1, e^{-\Delta\mathcal{H}})$, where $\Delta\mathcal{H} = \mathcal{H}[v_\tau, \pi_\tau] - \mathcal{H}[v_0, \pi_0]$, i.e., the difference of the Hamiltonian at the beginning and the end of the trajectory. If the proposal is rejected, we resample the conjugate momenta and restart from the old set $v = v_0$. The resampling of the momenta is necessary to satisfy ergodicity. Other important requirements for the HMC algorithm to be exact is preservation of the phase space volume and the reversibility in the fictitious time s . In particular the latter requirement needs to be monitored in the actual simulation and indeed, we constantly checked that reversibility violations are negligible in our simulations.

Let us finally briefly summarize the three basic steps of the HMC algorithm:

1. *Momentum heat-bath*: Sample π according to the Gaussian distribution

$$\mathcal{P}_\pi \propto e^{-\frac{1}{2} \int dt \|\pi(t)\|^2}. \quad (20)$$

2. *Hamiltonian evolution*: Use a symplectic integrator to numerically solve the system of Eqs. 18 starting from (v_0, π_0) and propose (v_τ, π_τ) .

3. *Metropolis step*: Accept the proposed field configuration (v_τ, π_τ) with probability

$$p = \min(1, e^{-\Delta\mathcal{H}}), \quad (21)$$

where $\Delta\mathcal{H} = \mathcal{H}[v_\tau, \pi_\tau] - \mathcal{H}[v_0, \pi_0]$.

Steps (1-3) are repeated multiple times to generate a statistically significant sample of velocity configurations on which physical observables of interest can be computed. In the simulation the number of integration steps are tuned such that acceptance rate originating from step (3) is close to 90%. This ensures that the autocorrelation time does not become too large and also avoids too many rejected velocity configurations. Steps (1-3) are also illustrated at the top of Fig. 2, where we show how the HMC moves inside the configuration space of (1+1)-dimensional velocity fields.

B. Fourier acceleration

We observe that the application of the standard HMC, based on Eq. (17), leads to very large autocorrelation times. The problem with the large autocorrelation time is essentially due to the multi-scale nature of the stochastic forcing, which in turn means that different Fourier modes are forced with different intensity. In order to deal with this problem, we made use of a well-known approach from the area of lattice field theory, i.e., the method of Fourier acceleration [49–52]. The latter assigns different effective trajectory lengths to the evolution of the Fourier modes. Indeed, this technique proved highly effective in our approach and it improved the performance of the HMC algorithm by considerably decreasing autocorrelation effects.

In practice, we apply the Fourier acceleration by introducing the space-time dependent kernel $\Omega(x, t)$ to multiply the momenta $\pi_s(x, t)$. This gives rise to the following ‘‘Hamiltonian’’:

$$\mathcal{H}^{\text{eff}} = \frac{1}{2} \int dt (\pi_s, \Omega * \pi_s) + \mathcal{S}. \quad (22)$$

It is important to note that $\Omega(x, t)$ does not depend on the Monte Carlo time s . The introduction of the kernel $\Omega(x, t)$ and the redefinition of the Hamiltonian does not affect the physical results, as the redefined kinematic term is still independent of the velocity field, and can be factored out of the path integral (17).

V. BENCHMARKING THE HMC AGAINST A FIRST-ORDER EULER-MARUYAMA EXPLICIT SOLVER

A. Fixed/open boundary conditions in time

As this is a novel approach for the sampling of stochastic PDEs, we took considerable care to benchmark the HMC with standard numerical methods that are employed in computational fluid dynamics. In the following we will demonstrate that our simulations match results obtained via a first-order Euler-Maruyama explicit solver (referred in short by DNS, i.e., direct numerical simulation) for a wide range of viscosities [53, 54].

In both implementations, Burgers’ equation is expressed in Fourier space, and the nonlinear term is written in a flux-conservative form, i.e., $v\partial_x v = \frac{1}{2}\partial_x(v^2)$. We apply the pseudospectral method, i.e., first v^2 is measured in real space and afterwards transformed to Fourier space so that the partial derivative can be conveniently treated as $\partial_x \mapsto ik$. Therefore, the nonlinear term is calculated as $\frac{ik}{2}\text{FT}(v^2)$, where by FT we denote the (forward) Fourier transform. To further ensure stability we apply two further steps in the numerics: First, we transform $v(k, t) \rightarrow \exp(-\nu k^2 \Delta t)v(k, t)$, which corresponds to an exact integration of the viscous term in the limit $\Delta t \rightarrow 0$. It relaxes the restriction on the time step Δt by the diffusive term and significantly improves the convergence for large wave numbers. Second, we effectively remove the aliasing error by setting $v(k \geq N_x/3, t) = 0$.

Here, we present three different runs, with parameters summarized in Tab. I. Both the DNS and the HMC, share the same setup, i.e., the same forcing correlation function, same discretization, and same periodic boundary conditions in space. As for the HMC, we choose fixed/open boundary conditions in time, corresponding to a standard initial-value problem. Note, that this choice yields a Jacobian \mathcal{J} that is field-independent [45], which therefore can be neglected for the purposes of importance sampling.

In Fig. 3(a) we compare the HMC and DNS temporal evolution of the mean kinetic energy, $\bar{\epsilon}_{\text{kin}}(t) = \|v(t)\|^2/L$, for configurations corresponding to three different viscosities. As one can see the overall intensity of fluctuations are very similar. More quantitatively, in Fig. 4(a) we show the temporal evolution of the ensemble average of the mean kinetic energy, i.e., $\langle \bar{\epsilon}_{\text{kin}}(t) \rangle$, starting from $v(x, t_0) = 0$. Around time $t_s \approx 3$ the system reaches stationarity, meaning that the dissipa-

| ν | Re | v_{rms} | ℓ_d | ℓ | $\langle \bar{\epsilon}_{\text{diss}} \rangle$ | T_ℓ | τ_{int} |
|-------|----|------------------|----------|--------|--|----------|---------------------|
| 0.08 | 90 | 1.14 | 0.15 | 1.5 | 1 | 1.31 | 7 |
| 0.1 | 70 | 1.12 | 0.18 | 1.4 | 1 | 1.24 | 4 |
| 0.2 | 30 | 1.03 | 0.3 | 1.1 | 1 | 1.03 | 1 |

TABLE I. Parameters and observables of the numerical simulations for fixed/open boundary conditions. Here, we employ the following parameters: $N_t = 1056$ number of grid points in time, $N_x = 128$ number of grid points in space, $T = 6$ and $L = 2\pi$. The Reynolds number is defined as $\text{Re} = \frac{v_{\text{rms}} L}{\nu}$ with root-mean-square velocity $v_{\text{rms}} = \langle \sqrt{\|v\|^2/L} \rangle$. $\ell_d = (\nu^3 / \langle \bar{\epsilon}_{\text{diss}} \rangle)^{1/4}$ defines the Kolmogorov dissipation length scale and $\ell = \frac{\bar{\epsilon}_{\text{kin}}^{3/2}}{\langle \bar{\epsilon}_{\text{diss}} \rangle}$ is the integral length scale with $\bar{\epsilon}_{\text{kin}} = v_{\text{rms}}^2$. $\langle \bar{\epsilon}_{\text{diss}} \rangle$ denotes the ensemble-averaged mean energy dissipation, i.e., $\langle \bar{\epsilon}_{\text{diss}} \rangle = 2\nu \langle \|\partial_x v\|^2 \rangle / L$ and $T_\ell = \ell / v_{\text{rms}}$ is the large-eddy turnover time. The last column contains τ_{int} , the integrated autocorrelation time of the kinetic energy, when we measure every 10 MD trajectories. τ_{int} is an HMC-related observable and is averaged in the stationary regime. For the HMC we fix the trajectory length $\tau = 1024$, and number of steps of the MD integrator $N_{\Delta\tau} = 20480$.

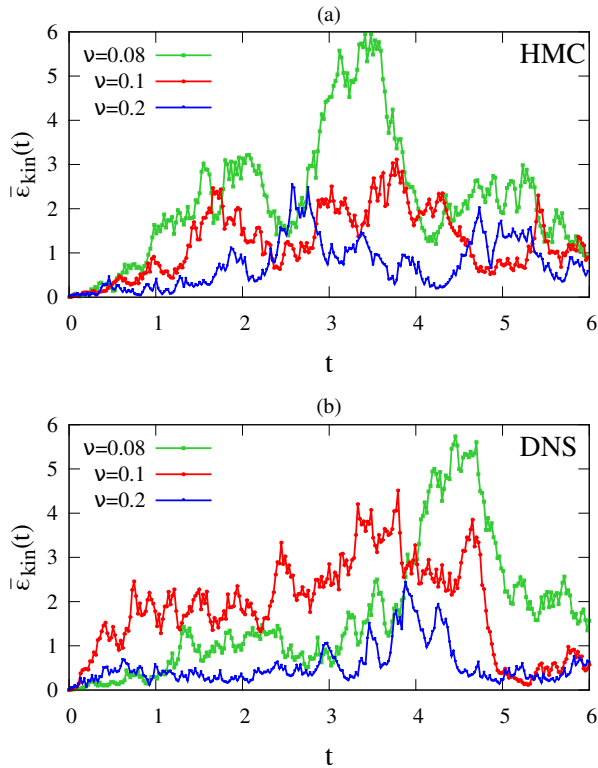


FIG. 3. Kinetic energy as a function of time for three samples corresponding to three different viscosities, (a) HMC and (b) DNS.

tive and injection forces are balanced and the system is driven to a nonequilibrium steady state – beyond t_s , the $\langle \bar{\varepsilon}_{\text{kin}}(t) \rangle$ is constant in time. Fig. 4(b) shows the temporal evolution of the ensemble-averaged mean energy dissipation $\langle \bar{\varepsilon}_{\text{diss}}(t) \rangle$, where $\bar{\varepsilon}_{\text{diss}}(t) = 2\nu \|\partial_x v(t)\|^2/L$, while in Fig. 5(a) we consider the ensemble average of the energy spectrum $\langle \bar{E}(k) \rangle$, which is averaged in time t , i.e., $\bar{E}(k) = \frac{1}{T'} \int_{t_s}^{t_f} dt E(k, t)$, $T' = t_f - t_s$.

In Fig. 5(b) we show the probability distribution function of the velocity gradients, defined as

$$P(w) = \langle \delta(\partial_x v(x, t) - w) \rangle. \quad (23)$$

In practice, the PDF is approximated by determining the counts of a fixed number of bins (w_{\min}, w_{\max}) with equal width δw . The velocity gradients measured on the generated ensemble are counted only if $t > t_s$. The resulting histogram is normalized by dividing with the total number of counts, in other words

$$\sum_i \int_{w_i - \delta w/2}^{w_i + \delta w/2} dw P(w) = 1. \quad (24)$$

From Figs. 3, 4, and 5, we conclude that the HMC produces the same results as the DNS. Furthermore, we identify the same discretization effects in both implementations, which can be removed by taking the continuum

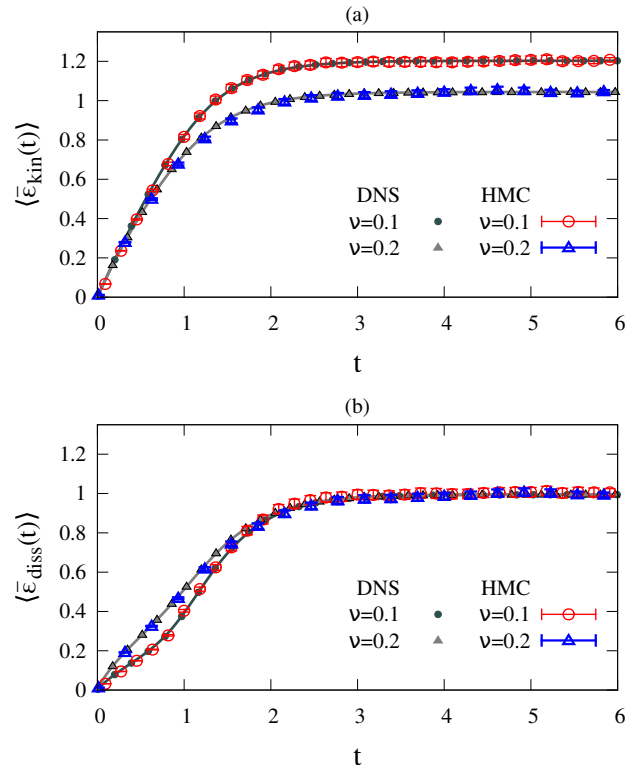


FIG. 4. (a) Temporal evolution of the ensemble-averaged mean kinetic energy, $\langle \bar{\varepsilon}_{\text{kin}}(t) \rangle$. (b) Temporal evolution of the ensemble-averaged mean energy dissipation $\langle \bar{\varepsilon}_{\text{diss}}(t) \rangle$. Note, that $\langle \bar{\varepsilon}_{\text{diss}}(t > t_s) \rangle = 1$ because the energy injection is fixed to $\lim_{k \rightarrow \infty} \langle \bar{\varepsilon}_{\text{in}}(k) \rangle = 1$; filled, gray points correspond to DNS results (lines denotes their interpolation) and colored open points HMC results.

limit. This has been thoroughly checked but we skip this discussion here.

There are two interesting remarks regarding the behavior of the HMC and in connection with Tab. I. First, we notice that for fixed resolution and trajectory length τ , the integrated autocorrelation times τ_{int} increase with decreasing viscosity. Second, we manage to perform highly efficient simulations simply by increasing the trajectory length τ , while keeping $\Delta\tau$ fixed. Contrary to common practice in Lattice QCD, where τ is kept of order $O(1)$, to avoid energy and reversibility violations [55], in our case it proved a safe and beneficial choice to set τ of order $\tau \approx 10^2$ or $\tau \approx 10^3$ without introducing significant effects of reversibility violations or loss of acceptance rate. This allowed to significantly decrease autocorrelation times, and avoided the disposal of many generated configurations between measurements. In principle we can increase the trajectory length to higher values that will allow to generate statistically independent configurations at each MD trajectory, as it is done for the runs in Sec. VI, but we did not check this systematically for the present section.

Finally, a key element of a Monte Carlo based approach

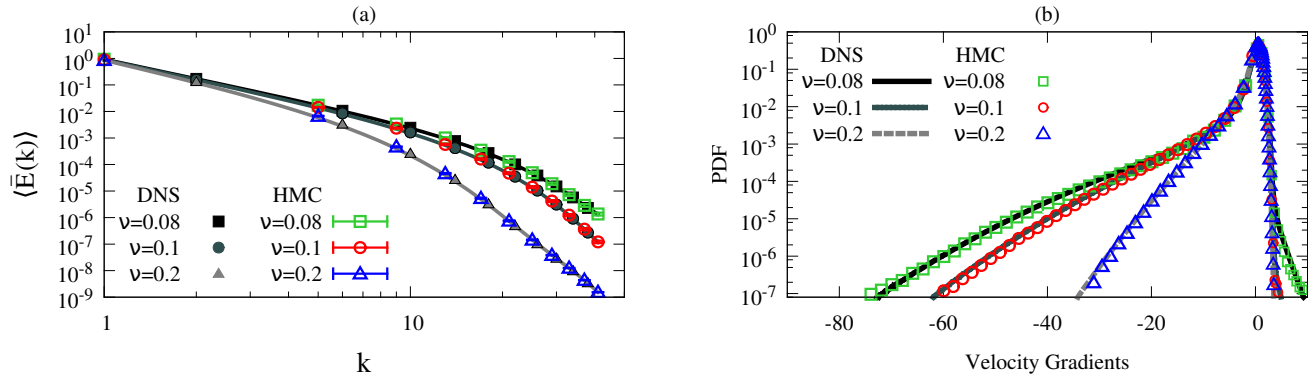


FIG. 5. (a) Ensemble-averaged energy spectra, $\langle \bar{E}(k) \rangle$; filled gray points correspond to DNS results (lines denote their interpolation) and colored open points correspond to HMC results. (b) Probability distribution functions of velocity gradients; gray, dashed lines correspond to DNS results, while colored open points to HMC.

is a rigorous error analysis, for which there are well established methodologies [56–58]. Since Markov chain Monte Carlo simulations, are known to be prone to autocorrelation effects, we had to go through a thorough investigation of the integrated autocorrelation times τ_{int} for each observable. Therefore, as a post-production step, we used the data analysis package provided in [59], as a tool to estimate the errors of the observables, which takes into account the corresponding autocorrelation effects. This recipe for the error calculation will be followed throughout this article.

VI. CONSTRAINED SPACE-TIME EVOLUTION USING HMC

Now that we have benchmarked the HMC against a standard DNS algorithm, we will present the new features and advantages that this novel path integral based approach can bring to the numerical studies of turbulent models, and stochastic PDEs in general. First, since the HMC considers the full temporal evolution of the field, this provides an additional flexibility towards the choice of boundary conditions in time. Therefore, in Sec. VIA we show, for instance, that one can apply periodic boundary conditions in time, i.e., $v(x, t) \equiv v(x, t + T)$. Then in Sec. VIB we turn towards the motivation for this article. That is to introduce field constraints, which will affect the Monte Carlo sampling in a controlled way, in order to favor the generation of specific configurations, that will comply with the imposed constraint. More specifically, as a first application, we apply a protocol to systematically generate configurations where a large negative velocity gradient is produced at a prescribed space-time point. This also provides with some insight on the underlying dynamics of how the system evolved in time t to reach this extreme condition.

A. Time-periodic boundary conditions

As a first application, we discuss the use of periodic boundary conditions in time. Under this scenario, we observe that after the system has equilibrated (to the desired target distribution), the ensemble consists of configurations that have reached stationarity at any time $t \in [t_0, t_f]$. This can be better understood by looking at Fig. 6, where the ensemble average of the mean kinetic energy (a) and the mean energy dissipation (b) are constant in time in the example of the HMC (colored points). We also show the results of the DNS (lines and points in gray color) using zero initial conditions as a further comparison. The parameters used for the three different runs are summarized in Tab. II.

The use of periodic boundary conditions in time leads to a field-dependent Jacobian \mathcal{J} [45] and therefore we must expect it to affect the importance sampling. Nevertheless, in this work, we have consistently neglected the evaluation of the Jacobian (which, in the lattice field theory literature, is often referred to the quenched limit). To get a better impression of the systematic error associated with this approximation, we have chosen to compare our results with periodic boundary conditions to the case of fixed/open boundary conditions. As can be seen from Fig. 6 our results overlap with the stationary

| ν | Re | v_{rms} | ℓ_d | ℓ | $\langle \bar{\epsilon}_{\text{diss}} \rangle$ | T_ℓ | τ_{int} |
|-------|----|------------------|----------|--------|--|----------|---------------------|
| 0.3 | 20 | 0.93 | 0.40 | 0.81 | 1 | 0.87 | 5 |
| 0.6 | 7 | 0.64 | 0.68 | 0.26 | 0.99 | 0.41 | 1.3 |
| 1.4 | 1 | 0.31 | 1.29 | 0.03 | 0.97 | 0.09 | 0.5 |

TABLE II. Parameters and observables of the numerical simulations for periodic boundary conditions of the HMC. Here the fixed parameters for both implementations are $N_t = 1056$, $N_x = 128$, $T = 6$, and $L = 2\pi$. Also for the HMC $\tau = 128$, and $N_{\Delta\tau} = 2560$, while τ_{int} is derived from the kinetic energy, when we measure after every MD trajectory. See also Tab. I for definitions.

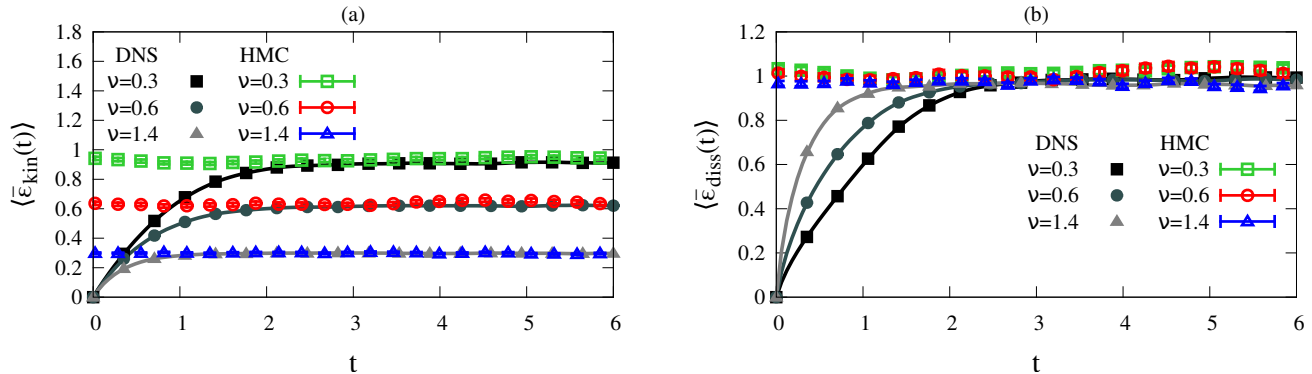


FIG. 6. Results for the HMC using periodic boundary conditions in time. (a) Temporal evolution of the ensemble-averaged mean kinetic energy $\langle \bar{\epsilon}_{\text{kin}}(t) \rangle$. (b) Temporal evolution of the ensemble-averaged mean energy dissipation $\langle \bar{\epsilon}_{\text{diss}}(t) \rangle$; filled gray points denote DNS results (lines correspond to their interpolation) and colored open points denote HMC results.

regime attained by using fixed/open boundary conditions with reasonable accuracy. In fact, it is possible to show that the error by neglecting the Jacobian vanishes in the limit $T \rightarrow \infty$. Thus, for those cases considered here, the systematic error is likely negligible. We delegate the evaluation of the Jacobian determinant to future work.

B. Enhanced sampling of extreme and rare events

We will now describe the important steps towards constraining the sampling of the HMC to generate a large negative velocity gradient at a specified space-time point. Also, we will explain how to directly compare the observables obtained from the constrained ensemble with the ones related to an unconstrained ensemble, by using reweighting techniques, and therefore estimate their relative importance with respect to the typical statistics of the system. We note two important points. First, that we will use the same boundary conditions as in Sec. V, i.e., periodic in space and fixed/open in time. Second, the statistics of the DNS will be referred to as the ones related to the unconstrained system. We could use the corresponding ones from the HMC with unconstrained sampling, but another purpose of ours is to demonstrate the benefits of employing this method for the purpose of systematically sampling extreme and rare events, compared to a standard DNS implementation, where such instances are a matter of chance.

a. Reweighting Reweighting is a standard technique introduced in [60] that proved very helpful in the study of phase transitions and critical phenomena. In short, it allows one to exploit the information of a generated ensemble of a single Monte Carlo simulation performed at a certain parameter (e.g., at fixed inverse temperature β) and obtain results for a range of nearby parameters (e.g., β_i). Reweighting can also provide a way to modify the sampling in a Monte Carlo simulation, which is how we use it here by constraining the sampling of the HMC to enhance the generation of strong negative gra-

dients. What is common in both cases is that we include a reweighting factor in the ensemble averages to obtain the desired ensemble (see [61] for a review on the topic).

In our application, reweighting is employed at the post-production stage as a means to relate the observable $\langle \mathcal{O} \rangle'$, measured using the ensemble which is generated by sampling with respect to the action \mathcal{S}' , to $\langle \mathcal{O} \rangle$, measured on the ensemble sampled with the action \mathcal{S} . We briefly revisit here the standard steps of the derivation. Note that any probability density functional $\mathcal{P}'_v = e^{-\mathcal{S}'}/\mathcal{Z}'$ can be related to another \mathcal{P}_v for the same field configuration $v = v(x, t)$, via

$$\mathcal{P}_v = \frac{1}{\mathcal{Z}} e^{-\mathcal{S}} = \frac{\mathcal{Z}'}{\mathcal{Z}} e^{-(\mathcal{S}-\mathcal{S}')} \mathcal{P}'_v, \quad (25)$$

The expectation value of an observable $\langle \mathcal{O} \rangle$ using \mathcal{S} is given by:

$$\begin{aligned} \langle \mathcal{O} \rangle &= \int \mathcal{D}v \mathcal{P}_v \mathcal{O} \\ &= \frac{\mathcal{Z}'}{\mathcal{Z}} \int \mathcal{D}v \mathcal{P}'_v e^{-(\mathcal{S}-\mathcal{S}')} \mathcal{O} \\ &= \frac{\mathcal{Z}'}{\mathcal{Z}} \langle e^{-(\mathcal{S}-\mathcal{S}')} \mathcal{O} \rangle', \end{aligned} \quad (26)$$

where the notation $\langle \dots \rangle'$ implies that the expectation value is evaluated with the action \mathcal{S}' . From the identity $\langle 1 \rangle = 1$ we may derive the following relation $\mathcal{Z}/\mathcal{Z}' = \langle e^{\Delta\mathcal{S}} \rangle'$ with $\Delta\mathcal{S} = \mathcal{S}' - \mathcal{S}$, whereby

$$\langle \mathcal{O} \rangle = \frac{\langle e^{\Delta\mathcal{S}} \mathcal{O} \rangle'}{\langle e^{\Delta\mathcal{S}} \rangle'}. \quad (27)$$

As a next step we determine the error of the estimator $\langle \mathcal{O} \rangle$. Notice that in Eq. (27) both the numerator and denominator have fluctuations. Furthermore, as they are calculated from the same ensemble we expect that both errors are correlated. As explained in [62] to estimate the error $\delta\langle \mathcal{O} \rangle$ of $\langle \mathcal{O} \rangle$ we employ the propagation of error of two dependent variables including the covariance and the

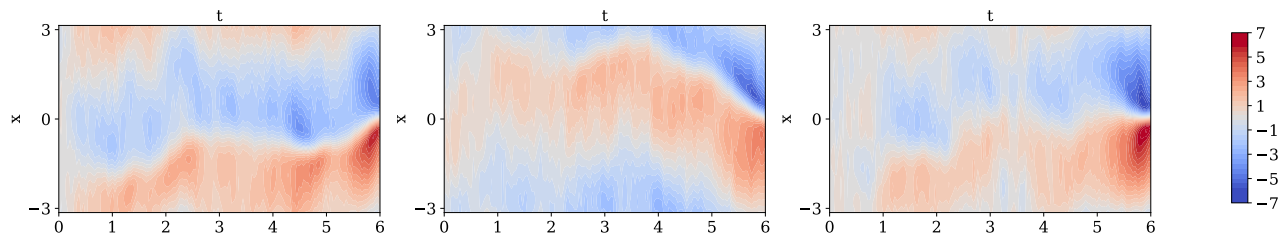


FIG. 7. Sample configurations from HMC simulation using the constraint $\Delta\mathcal{S}_1$ with $c_1 = 1.9$, enforcing a negative velocity gradient maximization at $x = 0$, $t = t_f$. The color spectrum corresponds to the intensity of the velocity field.

cross-covariance of the nominator and the denominator. Simplifying Eq. (27) to $\langle\mathcal{O}\rangle = A/B$ the final expression is

$$\delta\langle\mathcal{O}\rangle = \langle\mathcal{O}\rangle\sqrt{\left(\frac{\delta A}{A}\right)^2 + \left(\frac{\delta B}{B}\right)^2 - 2\left(\frac{\delta(AB)}{AB}\right)^2}, \quad (28)$$

where $\delta(AB) = \langle AB \rangle - \langle A \rangle \langle B \rangle + 2\sum_{i,j>i}(A_i - \langle A \rangle)(B_j - \langle B \rangle)$.

b. Implementation of sampling constraints The idea is to define a different action \mathcal{S}' to sample via the HMC, which consists of the original \mathcal{S} (14) in addition to a constraint functional $\Delta\mathcal{S}$:

$$\mathcal{S}' = \mathcal{S} + \Delta\mathcal{S}. \quad (29)$$

The choice of $\Delta\mathcal{S}$ cannot be arbitrary. If there is no overlap of the distributions $e^{-\mathcal{S}}$ and $e^{-\mathcal{S}'}$ is small, the reweighting procedure will likely not work. Therefore, it is not clear from the beginning, for which parameter values a successful reweighting can be performed. We remark that in cases where reweighting fails, it could be attempted to insert intermediate reweighting steps as explained in [63]. We also need to stress that any constraint functional $\Delta\mathcal{S}$ will contribute to the MD forces through the functional derivative $\delta\mathcal{S}'/\delta v = \delta\mathcal{S}/\delta v + \delta\Delta\mathcal{S}/\delta v$ and this contribution needs to be evaluated exactly.

Nevertheless, the histograms of the HMC are not directly comparable with the DNS. In the following, we will explain how to directly compare the statistics of the HMC using the action \mathcal{S}' , with the typical unconstrained statistics using the action \mathcal{S} , by utilizing reweighting techniques.

As a demonstration of reweighting techniques Eq. (27), we first discuss the example of the ensemble-averaged mean kinetic energy before and after reweighting. This is also a sufficient step to further ensure the consistency with the unconstrained statistics, meaning that after reweighting the observable measured by the constrained ensemble should collapse, within error bars, with the corresponding unconstrained one. Following Eq. (27) the reweighted ensemble-averaged mean kinetic energy will be

$$\langle\bar{\epsilon}_{\text{kin}}(t)\rangle = \frac{\langle e^{\Delta\mathcal{S}}\bar{\epsilon}_{\text{kin}}(t)\rangle'}{\langle e^{\Delta\mathcal{S}}\rangle'}, \quad (30)$$

As a first attempt we tried a series of local constraint functionals, with a suitable shape, that enhance the probability to produce a large negative velocity gradient at a certain point in the middle of the spatial domain at the last timeslice (i.e., $x = 0$, $t = t_f$). The parameters that we used for the HMC are summarized in Table III. A general way to define the local functional $\Delta\mathcal{S}$ is

$$\Delta\mathcal{S}_i = c_i \int dt \int dx f_i(\partial_x v/w_i) \delta(x)\delta(t - t_f), \quad (31)$$

where c_i is a prefactor to characterize the strength of the functional and w_i is an imposed velocity gradient value around which we want the functionals $\Delta\mathcal{S}_i$ to sample. The index i we label the different choices of f_i , for which we have tested the following

$$f_1(z) = z, \quad (32a)$$

$$f_2(z) = (z + 1)^2, \quad (32b)$$

$$f_3(z) = (z^2 - 1)^2. \quad (32c)$$

The HMC will sample around the region where $e^{-\mathcal{S}'}$ is maximal, i.e., where \mathcal{S}' is minimal, and the constraint functionals $\Delta\mathcal{S}_i$ contribute towards this procedure. In particular, the constraints imposed by $\Delta\mathcal{S}_2$ and $\Delta\mathcal{S}_3$ are of a localization nature in the sense that the generated configurations comply with the constraint by sampling in a narrow region around the imposed gradient w_i , where $\Delta\mathcal{S}_2$ and $\Delta\mathcal{S}_3$ are minimal. In the same spirit, as $\Delta\mathcal{S}_1$ is a linear function of $\partial_x v$, then for any negative $\partial_x v$ it will have a negative contribution to the action, which will favor the sampling towards this direction. It therefore allows us to sample across a wider range of negative velocity gradients. Nevertheless, we can redefine $\Delta\mathcal{S}_1$, as in this case w_1 can be absorbed by c_1 . Thus, we set $w_1 = 1$ and show only values of c_1 .

As for the numerical stability, we note that the grid resolution should always be sufficient to “fit” the strong shock. Therefore, we cannot increase c_i and w_i unconditionally for a fixed resolution. In practice, for a particular discretization, there is a threshold beyond which the HMC is not reliable anymore.

To identify the impact of constraining the sampling of the HMC on the generated configurations, we show three independent samples in Fig. 7. A large negative velocity gradient at $(x = 0, t = t_f)$ is achieved in all cases.

| only HMC | | | | | | | | | | | | |
|----------|-------|------------------|-------------------|-------------|--------------|-----------|------------|---|--|---------|---------------------|--------------|
| c_1 | w_1 | Re_ℓ | Re'_ℓ | Re | Re' | v_{rms} | v'_{rms} | $\langle \bar{\epsilon}_{diss} \rangle$ | $\langle \bar{\epsilon}_{diss} \rangle'$ | ℓ | κ | τ_{int} |
| 1.2 | 1 | 1.02(3) | 3 | 10(2) | 20 | 0.8(1) | 1.6 | 0.96(3) | 5 | 0.61(2) | 1.12 | 5.2(2) |
| 1.6 | 1 | 1.0(2) | 5 | 10(4) | 30 | 0.8(3) | 2.4 | 0.9(1) | 13 | 0.6(1) | 1.21 | 4.1(2) |
| 1.9 | 1 | 0.7(4) | 7 | 9(5) | 37 | 0.7(4) | 3 | 0.7(2) | 22 | 0.5(2) | 1.93 | 3.8(2) |
| c_2 | w_2 | Re_ℓ | Re'_ℓ | Re | Re' | v_{rms} | v'_{rms} | $\langle \bar{\epsilon}_{diss} \rangle$ | $\langle \bar{\epsilon}_{diss} \rangle'$ | ℓ | κ | τ_{int} |
| 80 | 12 | 0.83(5) | 5 | 10(2) | 30 | 0.8(2) | 2.4 | 0.79(4) | 11 | 0.55(3) | 418 | 0.50(5) |
| 80 | 18 | 0.8(2) | 7 | 9(4) | 35 | 0.8(4) | 2.8 | 0.8(2) | 17 | 0.6(1) | $2.6 \cdot 10^5$ | 0.50(4) |
| 160 | 24 | 1.4(6) | 8 | 12(6) | 42 | 1.0(5) | 3.3 | 1.2(3) | 31 | 0.7(3) | $5 \cdot 10^9$ | 0.50(4) |
| 160 | 30 | 1.7(6) | 9 | 14(7) | 46 | 1.1(5) | 3.7 | 1.6(4) | 39 | 0.8(2) | $2.6 \cdot 10^{11}$ | 0.50(5) |
| c_3 | w_3 | Re_ℓ | Re'_ℓ | Re | Re' | v_{rms} | v'_{rms} | $\langle \bar{\epsilon}_{diss} \rangle$ | $\langle \bar{\epsilon}_{diss} \rangle'$ | ℓ | κ | τ_{int} |
| 80 | 12 | 1.5(4) | 5 | 12(6) | 29 | 1.0(5) | 2.3 | 1.3(3) | 10 | 0.8(2) | $3.9 \cdot 10^5$ | 0.50(4) |
| 80 | 18 | 1.0(3) | 7 | 11(5) | 35 | 0.8(4) | 2.8 | 1.0(2) | 17 | 0.6(1) | $5.4 \cdot 10^8$ | 0.50(5) |
| 80 | 24 | 1.2(4) | 7 | 11(5) | 38 | 0.9(4) | 3 | 1.1(3) | 24 | 0.7(2) | $5.2 \cdot 10^{11}$ | 0.50(5) |
| 120 | 30 | 1.2(3) | 9 | 11(5) | 45 | 0.9(4) | 3.6 | 1.0(2) | 37 | 0.7(2) | $4.5 \cdot 10^{16}$ | 0.50(5) |
| only DNS | | | | | | | | | | | | |
| - | - | 1.01 | - | 10.5 | - | 0.83 | - | 0.95 | - | 0.61 | - | - |

TABLE III. Parameters for HMC simulations with constrained sampling. The integral length scale Reynolds number is defined as $\text{Re}_\ell = \frac{v_{rms}\ell}{\nu}$, while the large scale Reynolds as $\text{Re} = \frac{v_{rms}L}{\nu}$. The results for the HMC have been reweighted, and the temporal interval for averaging corresponds to the stationary regime. The parenthesis gives the error of the last digit of the mean. The primed observables (e.g., Re') are calculated without reweighting and consider only the last timeslice $t = t_f$, since the system is not stationary in time (see Fig. 10(a)). Here the fixed parameters for both DNS and HMC are: $N_t = 144$, $N_x = 64$, $T = 6$, $L = 2\pi$, $\nu = 0.5$, and $\ell_d = 0.59$. κ is defined in Eq. (35). The integrated autocorrelation time τ_{int} is calculated considering the time series of the velocity gradient measured at the point that we constrain, namely $(x = 0, t = t_f)$, after every MD trajectory. Finally, specifically for the HMC, $\tau = 128$, and $N_{\Delta\tau} = 2560$.

The general idea here is that we provide the HMC with a certain constraint, local or global, by which the HMC will consider all the possible realizations in the configuration space to fulfill the corresponding condition on the velocity field. In the case of extreme and rare events, for instance, the HMC provides a systematic way to sample the fluctuations around a particular extreme event (e.g., the occurrence of a strong velocity gradient).

Focusing now on the constraint functionals of Eqs. (32), Fig. 8(a) shows the ensemble average of the velocity field for the final timeslice $\langle v(x, t = t_f) \rangle'$ at changing c_1 . It further indicates the functionality of c_1 and the effect it has on the sampled configurations, i.e., the larger the c_1 , the more negative the sampled gradient will be. This can also be justified from Fig. 8(b), which, for different c_1 , depicts the PDF of the velocity gradients measured only at the point that we constrain, i.e., at $(x = 0, t = t_f)$. It is defined as

$$P'(w) = \langle \delta(\partial_x v(0, t_f) - w) \rangle', \quad (33)$$

where w is the value of the bin which is incremented according to the value of the velocity gradient $\partial_x v(0, t_f)$, and is generated using the action \mathcal{S}' . In this plot we see that by increasing c_1 , the peak of the histogram moves to the left towards larger negative velocity gradients.

As for the prefactors c_2 and c_3 , they have a slightly different behavior with respect to c_1 . In fact, as we increase c_2 and c_3 , the HMC will sample more systematically around the prescribed velocity gradient w_i . In Fig. 9 we show $P'(w)$ at varying c_i , w_i , with $i = 2, 3$. In Fig. 9(a) the functional $\Delta\mathcal{S}_2$ has been used, and in

Fig. 9(b), the functional $\Delta\mathcal{S}_3$. For the same parameters, the quartic functional $\Delta\mathcal{S}_3$ has a slightly better performance towards sampling the prescribed velocity gradient w than the quadratic functional $\Delta\mathcal{S}_2$. Notice that in Fig. 8(b) and both plots of Fig. 9 we also include the PDF of the velocity gradients of the DNS (black line) to give a qualitative description of how the constrained sampling compares with the original statistics.

To be more specific, we first refer to Fig. 10(a), where we show the non-reweighted ensemble-averaged mean kinetic energy, defined as $\langle \bar{\epsilon}_{kin}(t) \rangle'$ at changing c_1 , using the functional $\Delta\mathcal{S}_1$, and we compare it with the ensemble-averaged kinetic energy of the DNS (black line – unconstrained statistics). The larger the value of c_1 , the more pronounced the kinetic energy will be closer to the final time $t = t_f$, where the constraint is applied. Fig. 10(b) depicts the corresponding reweighted data, i.e., $\langle \bar{\epsilon}_{kin}(t) \rangle$, by using (30), where both the DNS and the reweighted HMC collapse within error bars.

We remark two points. First, through Fig. 10(a), we can also get an estimate of how important the constraint is as a function of time. For instance, on average, at time $t \approx 3$ the effects of $\Delta\mathcal{S}_1$ seem to have decayed. Second, for the particular observable, by increasing here c_1 we get increased error bars after reweighting. For instance, in the case of $\langle \bar{\epsilon}_{kin}(t) \rangle$ for $c_1 = 1.2$ we notice small error bars and a very good agreement with the DNS, while for $c_1 = 1.9$ the $\langle \bar{\epsilon}_{kin}(t) \rangle$ has much more pronounced error bars. This is related to a previous comment on the applicability of reweighting, for which we stated that the distributions $e^{-\mathcal{S}}$ and $e^{-\mathcal{S}'}$ should have a sufficient overlap.

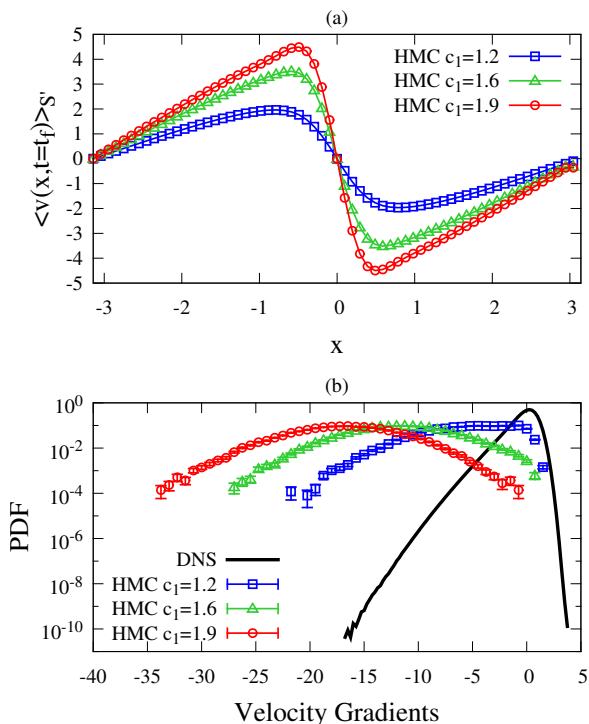


FIG. 8. (a) Ensemble average of the velocity field $v(t = t_f)$ using the HMC with action $S' = S + \Delta\mathcal{S}_1$ for different values of c_1 . (b) PDF of velocity gradients (DNS versus the HMC); for the HMC we measure $P'(w)$ only at the space-time point where we constrain the ensemble, i.e., at $x = 0, t = t_f$.

In this example, for $c_1 = 1.2$, the distribution of $\bar{\epsilon}_{\text{kin}}(t)$, for $t = t_f$, of the constrained ensemble, and the distribution of $\bar{\epsilon}_{\text{kin}}(t)$, for $t > t_s$, of the unconstrained system do overlap considerably, as seen in Fig. 10(c) (blue and black lines accordingly), which leads to the resulting collapse of the data (same colors in Fig. 10(b)). The difference with $c_1 = 1.9$ (red line in Fig. 10(a)) is that the corresponding overlap with the DNS is marginal. Also $c_1 = 1.9$ favors more the sampling of extreme velocity gradients $\partial_x v$, which, together with a (finite) characteristic dissipation scale ℓ_d , implies large values of $v_d \sim (\partial_x v)\ell_d$ (see Fig. 8(a)). The averaged kinetic energy is a global observable, which is mostly related to the bulk of the statistics of v , and consequently not sensitive to very strong and rare fluctuations. Therefore, if we did wanted to improve the behavior of $\langle \bar{\epsilon}_{\text{kin}}(t) \rangle$ for $c_1 = 1.9$, we should simply increase the statistics of the particular constrained ensemble to capture, by chance, events with smaller v that are more representative of the unconstrained ensemble. This translates to the fact that for the constrained ensemble, a rare event can be an event, which, for the unconstrained ensemble, is a typical one.

To sum up, reweighting of the ensemble-averaged kinetic energy is a sufficient but not a necessary condition to determine whether the particular constrained ensemble is representative of the original system. In fact, here it

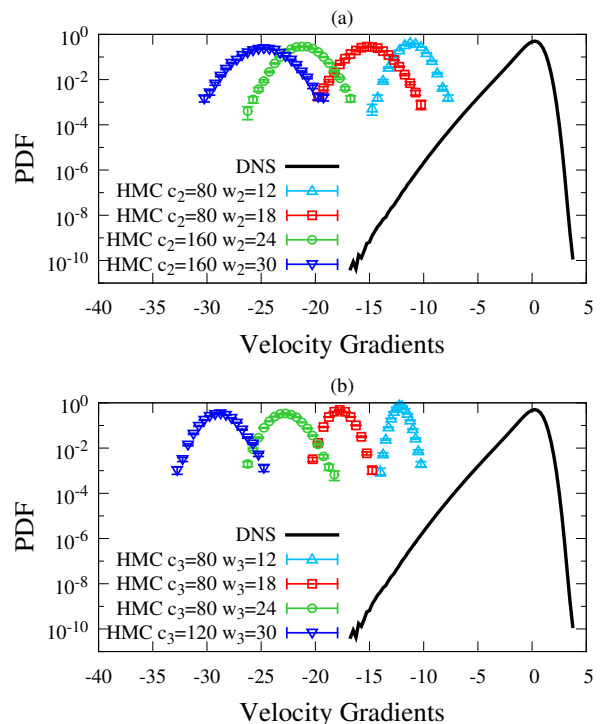


FIG. 9. PDF of velocity gradients (DNS versus the HMC), i.e., $P'(w)$, generated using the action S' , and measured only at the point that we constrain, i.e., at $(x = 0, t = t_f)$, for different values of c_i and w_i , $i = 2, 3$. (a) Using $\Delta\mathcal{S}_2$. (b) Using $\Delta\mathcal{S}_3$.

was a simple demonstration of the reweighting technique (27) in our application. As we shall see in the following, we can achieve a very well behaved reweighting for the PDF of the velocity gradients for any c_i, w_i , considering that the latter are appropriately chosen, as stated earlier, so that the HMC is numerically stable.

C. Velocity gradient statistics

To assess the performance of generating extreme and rare events, we compare the HMC, when using sampling constraints, with the DNS, by studying the statistics related to the velocity gradients, such as their PDF. We note that, in the following, the observables that we consider are measured only at the single point that we constrain, i.e., at $(x = 0, t = t_f)$. This is related to the introduction of the local constraint $\Delta\mathcal{S}$, which breaks the space-time symmetry of the system. In principle, after applying Eq. (27) we restore the symmetries of the system, in the limit of infinite statistics, but in practice this is not the case. However, for histogram reweighting, by considering only the site on which the local constraint acted, we restore homogeneity and we will show that it is sufficient to obtain a systematic comparison with the unconstrained statistics, regardless the mutual overlap of

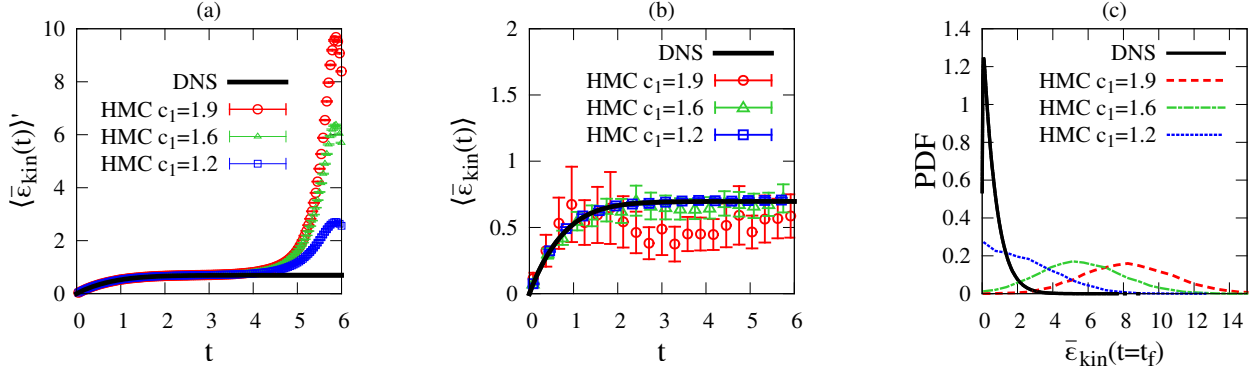


FIG. 10. (a-b): Ensemble-averaged mean kinetic energy of HMC vs DNS using $\Delta\mathcal{S}_1$ for different c_1 . (a): Before reweighting. (b): After reweighting. Notice that the error bars for the $c_1 = 1.9$ case after reweighting are pronounced as for this choice, the fluctuations introduced by the reweighting factor become significantly large. (c): PDF of the non-reweighted mean kinetic energy $\bar{\epsilon}_{\text{kin}}(t)$ measured only for the last timeslice $t = t_f$, in the case of the HMC, and using $\Delta\mathcal{S}_1$ for different c_1 .

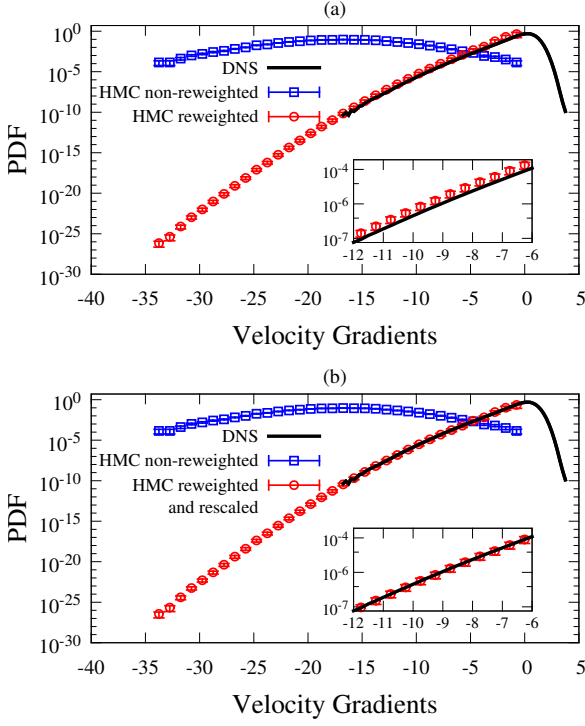


FIG. 11. PDF of velocity gradients for the HMC (blue/red points) versus DNS (black line). For HMC we use the constraint $\Delta\mathcal{S}_1$ with $c_1 = 1.9$, and $P'(w)$ is measured considering only the site ($x = 0$, $t = t_f$) on which the constraint is enforced. The inlet plot shows the chosen interval $[-12, -6]$. (a) Without rescaling, (b) rescaling the reweighted HMC histogram by dividing it with $\kappa = 1.93$.

the non-reweighted histogram and the unconstrained histogram (e.g., of the DNS). For instance, in Fig. 9(b) the case of the HMC with $c_3 = 120$, $w_3 = 30$ has no overlap with the DNS – even though there would be if we increased the statistics to infinite – yet in the following we will demonstrate that this particular PDF, together

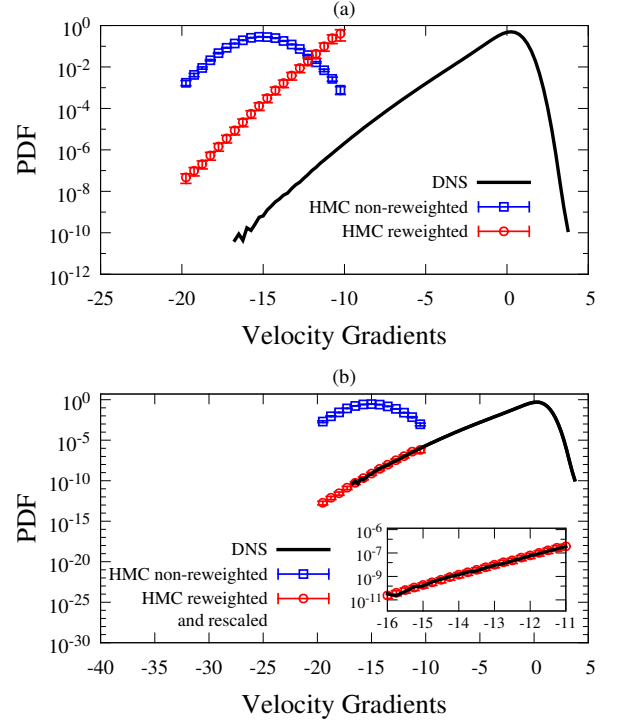


FIG. 12. PDF of velocity gradients for HMC (blue/red points) against DNS (black line). We consider only the extracted histogram from the lattice point on which the constraint $\Delta\mathcal{S}_2$ acted (i.e., $x = 0$, $t = t_f$) in the case of the HMC, with $c_2 = 80$ and $w_2 = 18$. The inlet plot shows the chosen interval $[-16, -11]$ for the rescaling. (a) Without rescaling, (b) rescaling the reweighted HMC histogram by dividing it with $\kappa = 2.63 \cdot 10^5$.

with other similar cases, will be successfully reweighted to the unconstrained statistics. Nevertheless, if we consider other sites, we encounter similar problems as the ones discussed already in the previous section, e.g., for the kinetic energy, where by increasing c_i , w_i we notice increasing error bars.

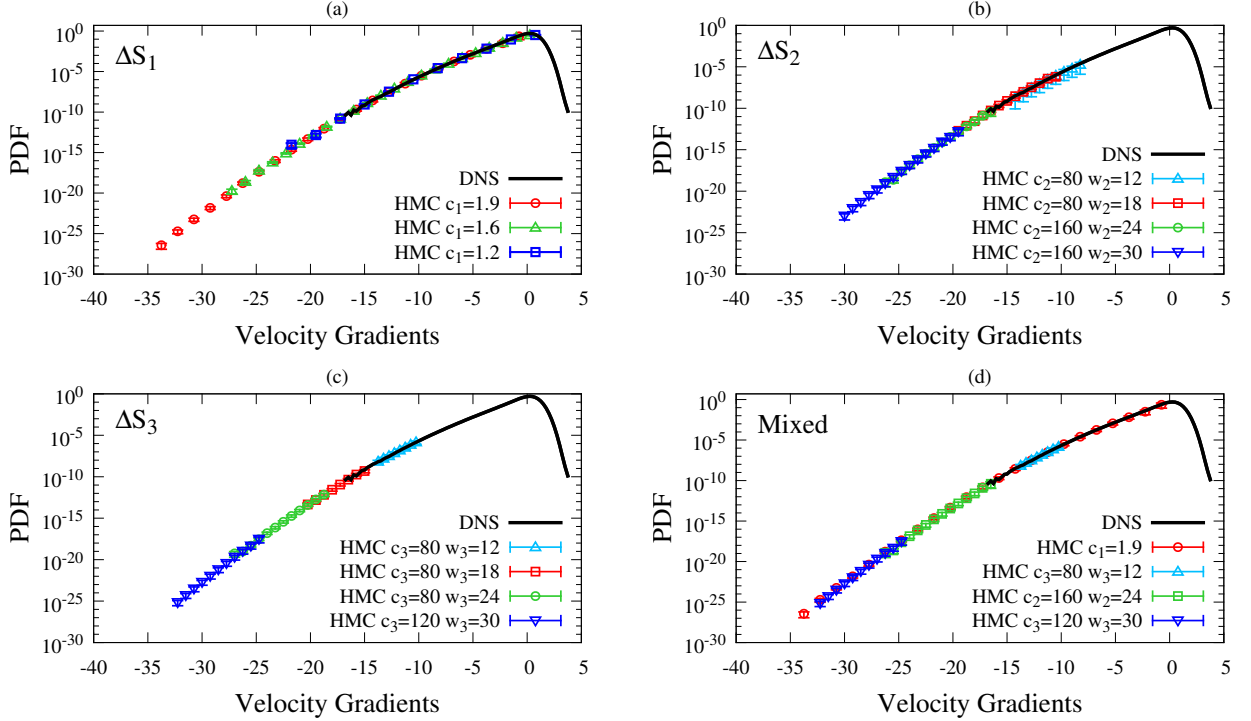


FIG. 13. PDF of velocity gradients $P(w)$ for HMC and DNS. We consider here only the extracted histogram from the lattice point on which the constraint $\Delta\mathcal{S}$ acted (i.e., $x = 0$, $t = t_f$) in the case of the HMC. We show the effect of reweighting for different parameters of the constraints. (a) Using $\Delta\mathcal{S}_1$. (b) Using $\Delta\mathcal{S}_2$. (c) Using $\Delta\mathcal{S}_3$. (d) A mixture of different $\Delta\mathcal{S}_i$. Regarding rescaling, for those $P(w)$ of which the overlap with the DNS was marginal or nonexistent, the rescaled $P(w)$ for $c_1 = 1.9$ was used.

To reweight the PDF of the velocity gradients $P'(w) = \langle \delta(\partial_x v(0, t_f) - w) \rangle'$, we use Eq. (27) to get

$$P(w) = \frac{\langle \delta(\partial_x v(0, t_f) - w) e^{\Delta\mathcal{S}} \rangle'}{\langle e^{\Delta\mathcal{S}} \rangle'}, \quad (34)$$

where in practice, for each measurement i of the ensemble, we increment the bin w by $e^{\Delta\mathcal{S}_i}$. In Fig. 11 we apply (34) on the ensemble that generated the non-reweighted PDF, $P'(w)$ (blue open squares), to produce the reweighted histogram $P(w)$ (red open circles), and compare it with the corresponding PDF of the DNS (black line). In Fig. 11(a) we identify a slight discrepancy between the $P(w)$ and the DNS (seen more clearly in the inset plot), while the trend is similar. This is related to the fact that the HMC is constrained to systematically sample large negative velocity gradients (far left tail), and therefore the support on the right tail is limited. As a result, by strictly applying (34), and since it normalizes the area under $P(w)$ to 1, the comparison between the HMC and the DNS is not straightforward, as $P(w)$ is actually an excerpt of the original PDF of velocity gradients, which is assumed to be the curve of the DNS here. For the same reason, $P(w)$ cannot be considered as a PDF. What is missing is to rescale $P(w)$ with an appropriate factor κ , so that both the DNS and the HMC calculate the same probability

$p(a, b)$ to sample in a particular interval (a, b) of velocity gradients. By definition, $p(a, b)_{\text{HMC}} = \sum_a^b P(w) \delta w$, and $p(a, b)_{\text{DNS}} = \sum_a^b P_{\text{DNS}}(w) \delta w$, with δw being the bin width, so κ is defined as the ratio of the two probabilities measured by the HMC and the DNS:

$$\kappa = \frac{p(a, b)_{\text{HMC}}}{p(a, b)_{\text{DNS}}}, \quad (35)$$

where we have tested that by increasing the statistics of the HMC, $\kappa \rightarrow 1$. We also assume that the DNS has enough support in both tails, to be claimed as a PDF, and therefore to be considered as a reliable benchmark for the rescaling of $P(w)$. In Fig. 11(b) we show the rescaled $P(w)/\kappa$, with $\kappa = 1.93$. Also here, κ is measured in the interval $[-12, -6]$ for the rescaling. In this way we achieve a collapse of the HMC and the DNS data. What is striking, in this example, is the unique ability of the HMC to systematically sample intense gradients that are up to $\sim 30\sigma$ and more, with $\sigma = 0.99$, far from the mean.

Another example, where the need to further treat the reweighted velocity gradients histogram $P(w)$, by rescaling it with an appropriate factor κ , becomes more evident, is when we consider one of $\Delta\mathcal{S}_2$ or $\Delta\mathcal{S}_3$. In Fig. 12 we show $P'(w)$ (blue open squares) and $P(w)$ (red open circles) using the functional $\Delta\mathcal{S}_2$, with $c_2 = 80$ and $w_2 = 18$ in the case of the HMC, against the DNS (black

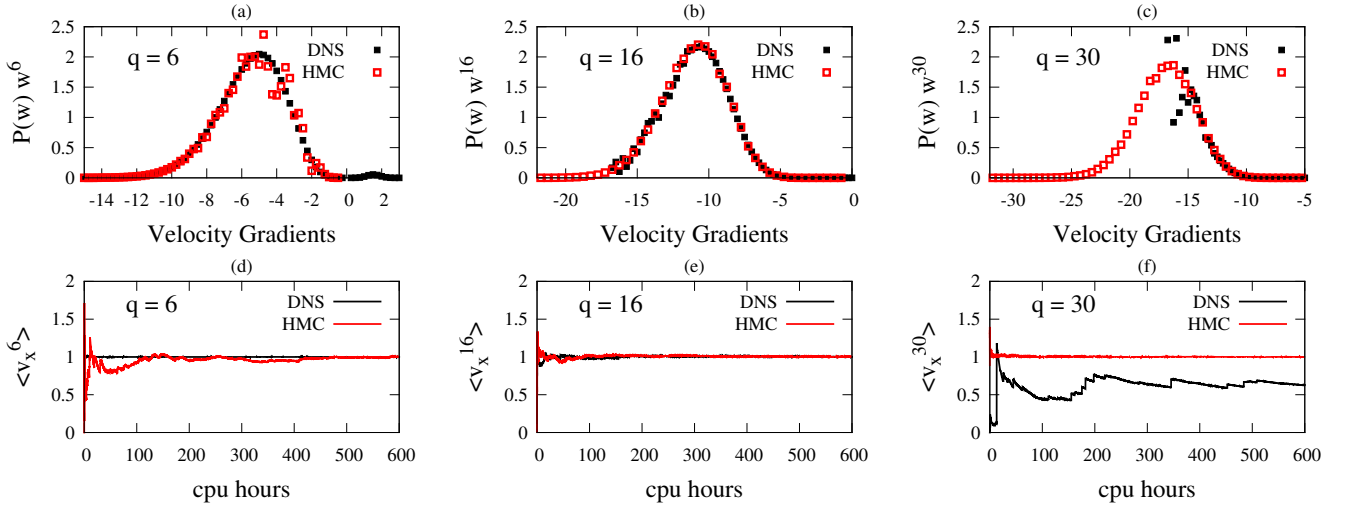


FIG. 14. (a-c) Velocity gradient PDF multiplied by a moment w^q . The $P(w)$ of the HMC is reweighted, rescaled with κ , and we consider only the lattice point that the constraint acts. Here, we used $\Delta\mathcal{S}_1$ for $c_1 = 1.9$. (d-f) Computational time to stabilized running average of velocity gradient moment $\langle (\partial_x v)^q \rangle$, divided with respect to the final stabilized value. Regarding DNS, any site belonging to the stationary regime is considered.

line). In Fig. 12(a), $P(w)$ (red points) is derived by applying (34) to the PDF of the HMC (blue points). As before, the area below $P(w)$ is equal to 1. However, by considering $P(w)$, the probability $p(a, b)_{\text{HMC}}$ to sample within an interval (a, b) of velocity gradients does not correspond to the one of the DNS, $p(a, b)_{\text{DNS}}$, so we employ again (35), to get $\kappa = 2.63 \cdot 10^5$. In Fig. 12(b) we plot $P(w)/\kappa$ (red points), instead, in order to achieve the collapse with the PDF of the DNS.

Now that we have clarified how to derive $P(w)^3$ and explained the need for a further rescaling with a constant, we can do the same procedure for all the different runs using the three different constraint functionals of Eqs. (32). This is done in Fig. 13, where we compare $P(w)$ for different combinations of $\Delta\mathcal{S}_i$, c_i , and w_i , with the velocity gradients PDF of the DNS (black line).

In Fig. 13(a) we show $P(w)$ for $\Delta\mathcal{S}_1$ and different c_1 , while in Fig. 13(b) the results correspond to $P(w)$ for $\Delta\mathcal{S}_2$ and different c_2 , w_2 . Then, Fig. 13(c) depicts the $P(w)$ for $\Delta\mathcal{S}_3$ and different c_3 , w_3 , while Fig. 13(d) shows a mixed selection of $P(w)$ for $\Delta\mathcal{S}_i$ and different c_i , w_i , to simply prove consistency among themselves. An important remark is that for those cases of the reweighted histogram $P(w)$, where the overlap with the DNS is marginal or absent, we used the rescaled $P(w)$ for $\Delta\mathcal{S}_1$, $c_1 = 1.9$, as a guide to rescale them. For instance, this was necessary for $w = 24, 30$. Furthermore, the different κ that were used for each case are shown in Table III.

Then we move towards quantifying the performance of the HMC for the purpose of systematically sampling very

intense velocity gradients. The top row of Fig. 14 shows $P(w)w^q$, i.e., the reweighted and rescaled histogram of the velocity gradients multiplied by a moment w^q . The idea is that the higher the power q , the more we focus towards larger negative gradients. If the statistics of $P(w)$ are sufficient in the corresponding “focused” region, then $P(w)w^q$ has a clear peak and shape. The bottom row of Fig. 14 depicts the computational cost that the ensemble running average of a moment of a velocity gradient $\langle (\partial_x v)^q \rangle$ requires in order to stabilize at a certain value and stop fluctuating. Here, for the HMC we used the functional $\Delta\mathcal{S}_1$, for $c_1 = 1.9$, and we consider only the velocity gradient at the point $(x = 0, t = t_f)$. The data here are the same as the red and black datasets of Fig. 11 for the HMC and the DNS, respectively. Also, the observable is reweighted according to Eq. (27) so that the comparison is equivalent. Finally, for visualization purposes, we normalize to one the observables by dividing them with the final value of the stabilized line (depending on q this might be either the line of HMC or DNS).

The plots in Fig. 14 are complementary, as a specific power q is chosen for each column. The plots in the left column (a and d) are for a small $q = 6$. In this region the DNS performs better as here the data of the HMC are only measured on the site on which the constraint acts, and therefore the appearance of relatively small negative gradients is suppressed. For $q = 16$ (middle column – b and e) we see that both the HMC and the DNS are equivalent in terms of the computational cost and quality of the statistics. Finally, for $q = 30$ (right column – c and f) the HMC significantly outperforms the DNS, as it immediately converges to the expectation value, while for the DNS we would have to remarkably increase the computational cost to achieve comparable statistics. Note that the data for both the HMC and the DNS in Figs. 13, 14

³ Note that for the rest of article, when referring to $P(w)$, it is implied that $P(w)$ is rescaled with an appropriate κ .

required the same computational cost to be produced, using the same processors.

Overall, Fig. 14 summarizes the ability of the HMC to consistently sample intense negative gradients that belong in the large deviations regime and furthermore gives a qualitative measure of the computational performance gained over a standard DNS method.

VII. THE RELEVANCE OF INSTANTONS IN EXTREME EVENTS

The application of instantons in turbulent flows was first proposed in [18] where the instanton contribution to the right tail of the velocity increment PDF was calculated for Burgers turbulence, while in a succeeding work [19], the left tail of the increment PDF was studied using the instanton approach. These works opened the door to other hydrodynamical models, such as the advection of a passive scalar by a turbulent velocity field [64, 65], shell models [66, 67], geophysical flows [22, 23, 68], and atmospheric and oceanic flows [69, 70] (see also [71] and citations therein).

A. Derivation of the instanton configuration

In order to calculate ensemble averages of observables $\langle \mathcal{O}_v \rangle$ as, e.g., the probability distribution of the gradient $P(\partial_x v = w) = \langle \delta(\partial_x v(x=0, t=t_f) - w) \rangle$, we utilize the path integral formulation introduced in Sec. III:

$$\begin{aligned} P(w) &\propto \int \mathcal{D}v \delta(\partial_x v(x=0, t=t_f) - w) e^{-\mathcal{S}} \\ &= \int \mathcal{D}v \int_{-\infty}^{i\infty} d\lambda e^{-\mathcal{S}'(\lambda)}. \end{aligned} \quad (36)$$

Here, $\mathcal{S}' = \mathcal{S}'(\lambda)$ contains both the Onsager-Machlup action \mathcal{S} (cf. Eq. (14)) and the contribution of the observable $\delta(\partial_x v(x=0, t=t_f) - w)$:

$$\begin{aligned} \mathcal{S}' &= \mathcal{S} + \lambda(\partial_x v(0, t_f) - w) \\ &= \int_{t_0}^{t_f} dt \left\{ \frac{1}{2} (F, \Gamma^{-1} * F) \right. \\ &\quad \left. + \lambda(\partial_x v(x, t) - w, \delta(x)) \delta(t - t_f) \right\} - \ln \mathcal{J} \end{aligned} \quad (37)$$

Instanton configurations are “classical” solutions that extremize the action and therefore dominate the path integral of the stochastic Burgers equation (17). They can be computed by Laplace’s method or alternatively, as in many applications, instantons are found by numerically minimizing the action directly (see, e.g., [23]). Here, where the observable is evaluated only at final time $t = t_f$, it is advantageous to switch to another equivalent formulation by applying a Hubbard-Stratonovich transformation [72, 73] which leads to the following alternative

representation of the partition sum

$$\mathcal{Z} \propto \int \mathcal{D}v \mathcal{D}\mu e^{\int dt \{i(\mu, F) - \frac{1}{2}(\mu, \Gamma * \mu)\} + \ln \mathcal{J}}, \quad (38)$$

which prompts us to define

$$\mathcal{S}_{\text{MSRJD}} = - \int dt \left\{ i(\mu, F) - \frac{1}{2}(\mu, \Gamma * \mu) \right\} - \ln \mathcal{J}, \quad (39)$$

also known as Martin-Siggia-Rose/Janssen/de Dominicis (MSRJD) action [11, 12]. At the expense of an additional auxiliary field μ , we have “linearized” the action with respect to the noise $\eta (= F)$. Furthermore, the force correlator Γ now appears directly and not through its inverse Γ^{-1} . This allows for the implementation of more general types of forcing as the power-law forcing considered in this paper. Now, the corresponding expression for the PDF of velocity gradients reads

$$P(w) \propto \int \mathcal{D}v \mathcal{D}\mu \int_{-\infty}^{i\infty} d\lambda e^{-\mathcal{S}'_{\text{MSRJD}}}, \quad (40)$$

with

$$\mathcal{S}'_{\text{MSRJD}} = \mathcal{S}_{\text{MSRJD}} + \lambda(\partial_x v(0, t_f) - w). \quad (41)$$

Before we proceed, we note that attempting to compute path integrals of the form of Eq. (38) is not straightforward and might be impossible for most cases. For instance, perturbative approaches might be helpful, depending on the problem. In the context of fluid dynamics a diagrammatic approach (influenced by quantum field theory) was proposed by Wyld [6]. Using perturbation theory to expand the exponential in Eq. (38) in powers of the nonlinear term (see also Eq. (1)) proves insufficient in the turbulent limit $\nu \rightarrow 0$, since the path integral is dominated by the nonlinear term forming strong shocks. Therefore perturbative approaches must be abandoned, as a large parameter is required [18].

Nevertheless, the introduced Lagrange multiplier λ , in Eq. (37) can be used as a large parameter. This allows the use of the saddle-point approximation, by which the variation of the integrand in Eq. (40) is equal to zero. In the case of Burgers turbulence, we obtain the instanton equations (minimizer of the action $\mathcal{S}'_{\text{MSRJD}}$)

$$\partial_t v + v \partial_x v - \nu \partial_x^2 v = -i \Gamma * \mu, \quad (42a)$$

$$\partial_t \mu + v \partial_x \mu + \nu \partial_x^2 \mu = -i \lambda \delta'(x) \delta(t - t_f), \quad (42b)$$

where the term on the r.h.s. in Eq. (42b) implements the boundary condition for μ at t_f according which $\mu(x, t_f) = i \lambda \delta'(x)$. Recall that in the case of Burgers’ equation $\mathcal{J} = \text{const.}$ and therefore the Jacobian does not contribute to the saddle-point equations. In [74] an algorithm was proposed to numerically solve the above equations. In short, the sign in front of the viscous terms defines the temporal direction of the numerical integration, with v being integrated forward in time, and μ backwards. Using $\mu(x, t_f) = i \lambda \delta'(x)$ as an initial condition for

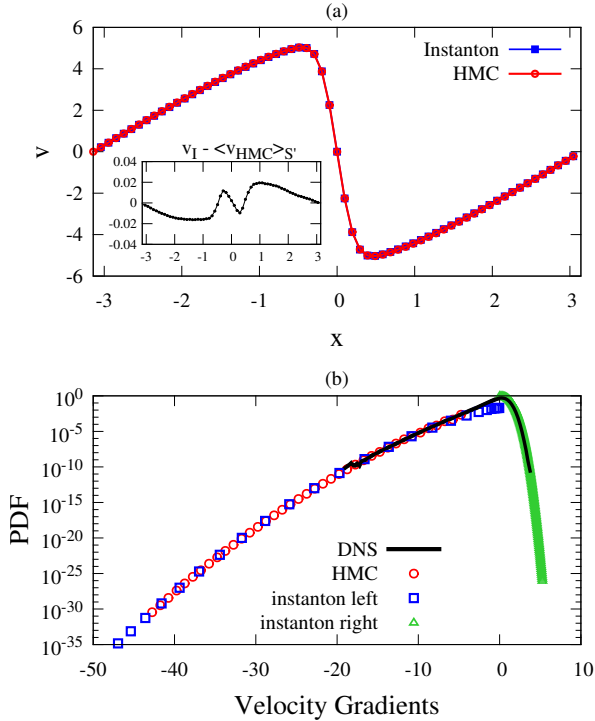


FIG. 15. (a) Ensemble average of velocity configurations generated by the HMC using $\Delta\mathcal{S}_1$ with $c_1 = 1.9$ compared to the classical instanton velocity-field profile generated for $\lambda = -1.148$ and $w = -24.23$. (b) PDF of velocity gradients for the classical instanton (for a range of values of λ and w), HMC simulation, and DNS.

some large value of t_f , and starting by setting $v(x, t) = 0$, Eq. (42b) is first integrated backwards until t_0 . Then the obtained $\mu(x, t)$ is used to integrate Eq. (42a) forward in time, with the whole procedure being iterated until convergence to the prescribed constraint $\partial_x v(0, t_f) = w$ is achieved. For more details see also [71, 75, 76] where the aforementioned methodology is revisited.

B. Numerical results

Instantons – strong field-force fluctuations and extremal points of the action $\mathcal{S}'_{\text{MSRJD}}$ – may be considered as particular examples of extreme and rare events. Constraining the HMC to sample at large negative gradients we observe that the generated configurations clearly resemble the “classical” instanton configurations determined via the saddle-point approximation. This will be checked directly via the averaged velocity field profile and through the probability distribution function of velocity gradients.

Fig. 15(a) compares the HMC ensemble average of the velocity field at the last time-slice ($t = t_f$) with the velocity field obtained by performing the numerical integration of the instanton equations (42). The profile of the classical instanton at time $t = t_f$ is reproduced to a remarkable

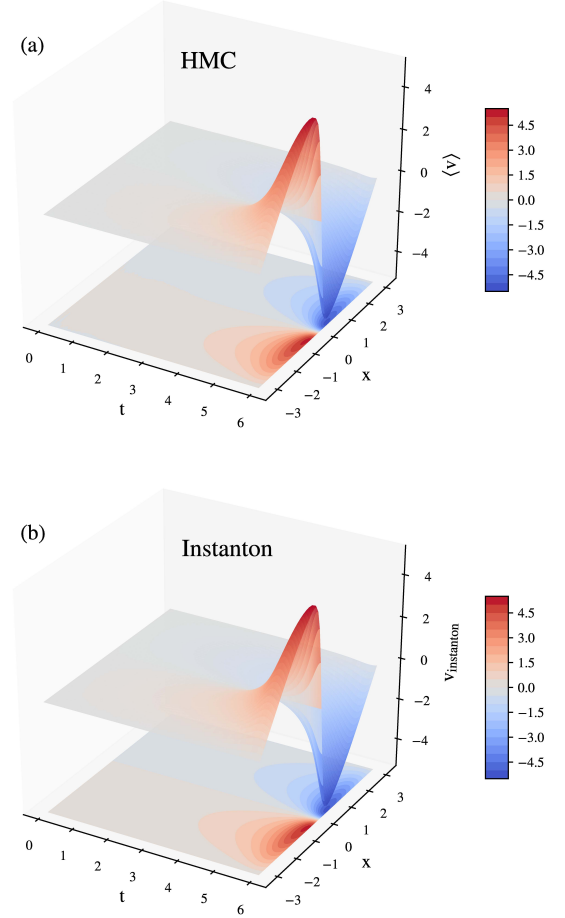


FIG. 16. (a) Ensemble average of velocity configurations generated by the HMC using $\Delta\mathcal{S}_1$ with $c_1 = 1.9$. (b) Instanton velocity field for $\lambda = -1.148$ and $w = -24.23$. By averaging over the HMC velocity field ensemble the spatio-temporal shape of the classical instanton is restored.

degree, implying that the ensemble average is equivalent to removing the fluctuations around the instanton. This confirms that instantons can be found in Burgers turbulence, as already shown in [75] using a post-production filtering protocol to consider only events with strong gradients generated using DNS. Furthermore, the inset plot depicts the difference of the two velocity fields, which are on the order of statistical error. Similarly, in Fig. 16 we compare the whole averaged spatio-temporal domain of the HMC with the instanton velocity field in space and time. For Figs. 15 and 16 a resolution of $N_t = 576$ points in time was used for the HMC, the DNS, and the instanton, while the rest of the parameters are the same as in Tab. III.

Fig. 15(b) compares the PDF of the velocity gradients of the DNS, the HMC with constrained sampling, and the instanton. In the case of the instanton we plot $e^{-\mathcal{S}_{\text{inst}}}$, with $\mathcal{S}_{\text{inst}} = \frac{1}{2} \int_{t_0}^{t_f} dt (\mu, \Gamma * \mu)$. We notice that the PDF predicted by the instanton follows the same trend as the

HMC and the DNS, and the agreement is extraordinary. However, in order to correctly interpret this result one should note the following: First, the PDF prediction for positive gradients is valid independently of the Reynolds number Re , and is actually valid for all positive values besides small corrections near $\partial_x v = 0$. This is a result already obtained by Feigel'man [77] in the context of charge density waves and also confirmed by the instanton formalism [18]. On the other hand, the PDF of negative gradients depends on the Reynolds number and for a given Reynolds number Re_ℓ the instanton prediction is only valid for $|\partial_x v| > |\partial_x v^*(Re_\ell)|$. A precise estimate for $\partial_x v^*$ is given in [76] [see Eq. (17) in the same reference]. For the Reynolds number $Re_\ell = 1$, used in our simulation and depicted in Fig. 15, this means that the instanton prediction is valid only for $\partial_x v < -10$.

VIII. CONCLUSIONS

In this work, we established how to apply Monte Carlo importance sampling for stochastic dynamics based on the Janssen-de Dominicis path integral, in order to address the statistics of large fluctuations in driven nonequilibrium systems. This approach allows us to access the phase-space of all possible field realizations of a stochastic system. Using reweighting techniques, we were able to systematically enhance the occurrence of extreme and rare events, by sampling in specific phase-space regions related to such events.

We have chosen to illustrate the HMC algorithm at the example of the random-noise driven one-dimensional Burgers equation, which often used model for benchmarking new numerical methods in computational fluid dynamics. However, the HMC approach is generally applicable to any stochastic PDE and generally free from any modeling assumptions. Also, while the random forcing was chosen to be Gaussian, self-similar, and white-in-time, this is by no means a necessary and other types of noises can be addressed within this approach. We thoroughly benchmarked our HMC implementation with a standard forward-time-integration pseudospectral method (see Figs. 4, 5). By constraining the sampling of the HMC to generate a strong negative velocity gradient at a specific site we increased the statistics of the left tail of the PDF of velocity gradients significantly, producing gradients as intense as 30 (and more) times the r.m.s. value (see Fig. 13). Although we restricted ourselves to the case of localized (in space and time) constraints, the technique can be easily extended to more general cases. Also, our constrained HMC sampling al-

lowed us to decrease of order-of-magnitudes the time-to-the-solution needed to collect sufficient statistics for high order moments (up to order 30) if compared with DNS (see Fig. 14). We expect that the types of local constraints considered in this work might have an impact on similar studies in lattice gauge theories, where they may lead to new observables.

We demonstrated that instanton configurations can be found in Burgers turbulence. We have recovered the full shape of the classical instanton by averaging the generated ensemble of the constrained configurations, with the agreement of the HMC and the instanton being remarkable (see Figs. 15(a) and 16). We further compared the PDF of the velocity gradients for a very large range of strong negative gradients and showed that, beyond a specific Reynolds number-dependent threshold of applicability of the instanton method, both the HMC and the instanton produce the same left tail, which further ensures the relevance of instantons in Burgers turbulence (see Fig. 15(b)). Thus, we established a one-to-one correspondence among the biased realizations of the HMC and the fluctuations around instantons. The present study focuses on low Reynolds number turbulence. However, the present method is not restricted to this case and actually opens the possibility to explore the role of fluctuations around instantons with unmatched precision. We are confident that the suggested novel approach can find suitable applications in the diverse field of stochastic PDEs and related studies on extreme and rare events.

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