

Instanton based importance sampling for rare events in stochastic PDEs

Lasse Ebener,¹ Georgios Margazoglou,^{2,3} Jan Friedrich,^{1,4} Luca Biferale,² and Rainer Grauer¹

¹*Institut für Theoretische Physik I, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany*

²*Dept. Physics and INFN, University of Rome “Tor Vergata”, Via della Ricerca Scientifica 1, I-00133 Roma, Italy*

³*Computation-based Science and Technology Research Center, Cyprus Institute, 20 Kavafi Str., 2121 Nicosia, Cyprus*

⁴*Laboratoire de Physique, Ecole Normale Supérieure de Lyon, CNRS, Université de Lyon, F-69007, Lyon, France*

(Dated: 11 December 2018)

We present a new method for sampling rare and large fluctuations in a non-equilibrium system governed by a stochastic partial differential equation (SPDE) with additive forcing. To this end, we deploy the so-called instanton formalism that corresponds to a saddle-point approximation of the action in the path integral formulation of the underlying SPDE. The crucial step in our approach is the formulation of an alternative SPDE that incorporates knowledge of the instanton solution such that we are able to constrain the dynamical evolutions around extreme flow configurations only. Finally, a reweighting procedure based on the Girsanov theorem is applied to recover the full distribution function of the original system. The entire procedure is demonstrated on the example of the one-dimensional Burgers equation. Furthermore, we compare our method to conventional direct numerical simulations as well as to Hybrid Monte Carlo methods. It will be shown that the instanton-based sampling method outperforms both approaches and allows for an accurate quantification of the whole probability density function of velocity gradients from the core to the very far tails.

PACS numbers: 05.10.Gg, 05.40.-a, 47.52.+j, 05.45.Jn, 05.45.Pq, 47.27.E-

Keywords: Rare events sampling, large deviations, instanton, stochastic PDEs, turbulence

I. INTRODUCTION

Non-equilibrium systems that possess a large number of interacting degrees of freedom typically exhibit strongly anomalous statistical properties which can be attributed to rare large fluctuations. Typical examples include the occurrence rate of earthquakes¹, the existence of rogue waves²⁻⁴, crashes in the stock market⁵⁻⁷, the occurrence of epileptic seizures⁸, or perhaps the most enigmatic case, the distribution of velocity increments in hydrodynamic turbulence⁹. In turbulence theory, a central notion is the energy cascade which implies a non-linear and chaotic transfer between different scales¹⁰. Although well-established descriptions by Richardson, Kolmogorov, Onsager, Heisenberg, and others (see the reviews^{9,11}) can capture the mean field features of the cascade process in a phenomenological way, the nature of small-scale turbulent energy dissipation is far less understood and is usually attributed to nearly singular localized vortical structures^{12,13}. Empirically, the energy transfer from large to small scales is accompanied by a breaking of self-similarity of the probability density function (PDF) of velocity increments, a phenomenon called *intermittency*. Intermittency is intimately connected to non-Gaussian statistics and extreme events and is often described in a statistical sense, using random multiplicative cascades leading to multifractal measures^{9,14}. On the other hand, it manifests itself by the presence of singular or quasi-singular structures, highly concentrated in a few spatial locations. From a mathematical point of view, large fluctuations of the fluid variables are controlled by

the theory of large deviations¹⁵⁻¹⁸, which is concerned with the exponential decay of the PDF for large field values, see, e.g., the paper¹⁹ for a numerical application based on the Onsager-Machlup functional in the context of geophysical flows.

Besides numerical large deviation methods, cloning and selection strategies (that favor the desired event) have evolved into mature simulation techniques, too^{20,21}. Recently, such methods have been deployed in order to investigate return times in Ornstein-Uhlenbeck processes, in the drag forces acting on an object in turbulent flows²², as well as for extreme heat waves in weather dynamics²³. Other numerical methods include direct importance sampling in configuration space²⁴, a modification of transition path methods¹⁷ in form of the so-called string method²⁵ and the geometric minimum action method²⁶.

In this paper we are interested to apply saddle point techniques to estimate extreme events (also called instantons or optimal fluctuations) as originally introduced in the context of solid state disordered systems²⁷⁻³¹ (see also³² for an overview). Especially, we refer to the works of Zittartz and Langer²⁹⁻³¹ which contain nearly all the recipes we are using today. Single- and multi-instantons dynamics have often been advocated as some of the possible mechanisms of anomalous fluctuations in hydrodynamical systems and models thereof³³⁻³⁷. We will use the so-called Janssen-de Dominicis^{38,39} path integral formulation of the Martin-Siggia-Rose (MSR) operator technique⁴⁰ for classical stochastic systems. In particular, we will apply it to the important case of the one-dimensional

stochastically forced Burgers equation:

$$u_t(x, t) + u(x, t)u_x(x, t) = \nu u_{xx}(x, t) + \eta(x, t), \quad (1)$$

where the nonlinearity tends to form shock fronts that are ultimately smeared out by viscosity and lead to the appearance of large negative velocity gradients (see below for further details on the equations). The Burgers equation constitutes a high-dimensional and highly non-trivial example of a complex system with fluctuations far away from Gaussianity. The Burgers equation can be also considered as a simplified one-dimensional compressible version of the Navier-Stokes equation and has been extensively studied in the past decades^{33,34,41–52} (see also the review⁵³) using numerical simulations^{41–43}, the replica method⁴⁴, operator product expansion^{47,48,52,54}, asymptotic methods^{49–51} as well as instanton methods^{32–34,45,46}. Similarly, the Kardar-Parisi-Zhang equation, which is strictly connected to (1), has also recently been studied using instantons^{55,56}.

The main problem when dealing with instanton approximations of the whole probability distribution is to evaluate the fluctuations around them, which is, in turn, connected to the most important problem of quantifying the influence of the saddle-point solution to all field values, including the ones that are not extremal.

In this paper, we propose a new method to study the shape of the PDF of the Burgers velocity gradients u_x , in those parameter regions where it is dominated by instantons, considering also the fluctuations around the saddle point configurations. To do that, we will decompose the velocity field in the MSR action into a contribution that stems from the instanton as well as a fluctuation around this object. We then proceed and derive an evolution equation for the fluctuation in the *background* of the instanton solution for a given gradient. A subsequent reweighting procedure allows us to calculate the full PDF with a much more accurate description of the tails in comparison to ordinary direct numerical simulations (DNS) of Burgers turbulence. We also show that our method is computationally less substantially challenging than other approaches based on Markov Chain Monte Carlo methods to generate extreme and rare flow configurations⁵⁷. Hence, the method can be considered as an optimal application of rare events importance sampling and we call it the *Instanton based Importance Sampling* (IbIS), see also the work⁵⁸ for a similar idea. In our formulation, the method is general enough to be applied to many different SPDEs.

The paper is organized as follows: In section II we review the path integral formulation of stochastic systems. Section III constitutes the core of the paper, where we present our reweighting procedure. In section IV we describe in detail the numerical protocol and we compare the results obtained with IbIS against those obtained using DNS and a Hybrid Monte Carlo approach⁵⁷. We close with a summary and an outlook on further applications.

II. PATH INTEGRAL FORMULATION AND INSTANTONS

To make our exposition self-consistent, here we describe the path integral formulation of stochastic systems, the subsequent derivation of the instanton equations, and the calculation of fluctuations around the instanton using an appropriate reweighting procedure. The presentation follows closely the seminal work of Balkovsky *et al.*³³.

A. Path integral formulation of stochastic systems

The Martin-Siggia-Rose-Janssen-de Dominicis formalism (hereinafter referred to as MSRJD formalism)^{38–40} was developed in the early 1970's to calculate statistical properties of classical systems using a path integral formulation. Following the same notation as in^{32,59}, we consider a stochastic differential equation

$$\dot{u} + N[u, x] = \eta(x, t), \quad (2)$$

where η is an additive Gaussian noise with correlation

$$\langle \eta(x, t)\eta(x+r, t+s) \rangle = \chi(r)\delta(s). \quad (3)$$

Here, the δ -correlation implies that the forcing η is white in time, while $\chi(r)$ is some arbitrary spatial correlation. Considering that from Eq. (2) the field u is a functional $u[\eta]$ of the forcing η , we introduce the MSRJD formalism as follows. The expectation value of an observable $\langle \mathcal{O}[u] \rangle$, as the average over all possible noise realizations, can be defined as

$$\langle \mathcal{O}[u] \rangle = \int \mathcal{D}\eta \mathcal{O}[u[\eta]] e^{-\int dt \langle \eta, \chi^{-1}\eta \rangle / 2}, \quad (4)$$

where the integral in the exponent derives from η being normally distributed, with $\langle \cdot, \cdot \rangle$ being the L^2 inner product. Changing the integration from η to u , given Eq. (2), modifies the measure in Eq. (4) as $\mathcal{D}\eta = J[u] \mathcal{D}u$, where $J[u] = \det \left(\frac{\delta \eta}{\delta u} \right) = \det \left(\partial_t + \frac{\delta N}{\delta u} \right)$ is the Jacobian associated to the map $\eta \mapsto u$. This results into what is called the Onsager-Machlup functional⁶⁰

$$\langle \mathcal{O}[u] \rangle = \int \mathcal{D}u \mathcal{O}[u] J[u] e^{-\int dt \langle \dot{u} + N[u], \chi^{-1}(\dot{u} + N[u]) \rangle / 2}. \quad (5)$$

It is the starting point for direct minimization of the Lagrangian action

$$S_{\mathcal{L}}[u, \dot{u}] = \frac{1}{2} \int dt \langle \dot{u} + N[u], \chi^{-1}(\dot{u} + N[u]) \rangle. \quad (6)$$

Most of the time, it is more convenient to work with the original correlation function χ instead of its inverse. We therefore perform a Hubbard-Stratonovich transformation, which introduces an auxiliary field \tilde{p} and by virtue

of a Fourier transform and completing the square eliminates the inverse of the correlation function χ^{-1} and in addition the noise appears only linearly in the action:

$$\langle \mathcal{O}[u] \rangle = \int \mathcal{D}\eta \mathcal{D}\tilde{p} \mathcal{O}[u[\eta]] e^{-\int dt [\langle \tilde{p}, \chi \tilde{p} \rangle / 2 - i \langle \tilde{p}, \eta \rangle]} . \quad (7)$$

We then execute the coordinate transformation from η to u

$$\langle \mathcal{O}[u] \rangle = \int \mathcal{D}u \mathcal{D}\tilde{p} \mathcal{O}[u] J[u] e^{-S[u, \tilde{p}]}, \quad (8)$$

with the action function $S[u, \tilde{p}]$ given by

$$S[u, \tilde{p}] = \int dt \left[-i \langle \tilde{p}, \dot{u} + N[u] \rangle + \frac{1}{2} \langle \tilde{p}, \chi \tilde{p} \rangle \right] .$$

For the purpose of convenience to obtain an Euclidian path integral we now substitute \tilde{p} with p , by use of the relation $\tilde{p} = i p$ and obtain the Hamiltonian action

$$S_{\mathcal{H}}[u, p] = \int dt \left[\langle p, \dot{u} + N[u] \rangle - \frac{1}{2} \langle p, \chi p \rangle \right] . \quad (9)$$

The next step is to minimize this action functional to obtain the instanton solutions.

B. Instantons

We are interested in rare and large fluctuations of velocity gradients $u_x(x, t)$ in the Burgers equation (1). Since this chaotic and turbulent system is invariant under time translations and Galilean transformations, the probability function of velocity gradients can be cast into the following form as a path integral

$$\begin{aligned} \mathcal{P}(a) &= \langle \delta(u_x(0, 0) - a) \rangle \\ &= \int \mathcal{D}u \mathcal{D}p \int_{-i\infty}^{i\infty} d\mathcal{F} \exp\{-S_{\mathcal{H}} + \mathcal{F}[u_x(0, 0) - a]\} . \end{aligned} \quad (10)$$

Here \mathcal{F} stems from the Fourier transform of the δ -function and serves as a Lagrange multiplier. Hence, from Eq. (9) we have

$$\begin{aligned} S_{\mathcal{H}}[u, p] &= \int_{-\infty}^0 dt \int dx p(x, t) (u_t + uu_x - \nu u_{xx}) \\ &\quad - \frac{1}{2} \int_{-\infty}^0 dt \int dx dx' p(x, t) \chi(x - x') p(x', t) . \end{aligned} \quad (11)$$

Now \mathcal{F} is treated as a large parameter so that the saddle point approximation can be used in order to derive instanton configurations, i.e. ‘‘classical’’ solutions that minimize the action and therefore dominate the path integral of Eq. (10). The instanton equations are obtained from the conditions

$$\frac{\delta S}{\delta u} = 0 \quad \text{and} \quad \frac{\delta S}{\delta p} = 0 . \quad (12)$$

When carried out, the functional derivatives above yield the so called instanton equations:

$$u_t + uu_x - \nu u_{xx} = \chi * p, \quad (13)$$

$$p_t + up_x + \nu p_{xx} = \mathcal{F} \delta(t) \delta'(x), \quad (14)$$

where $u(x, t)$ and $p(x, t)$ have the following boundary conditions:

$$\begin{aligned} \lim_{t \rightarrow -\infty} u(x, t) &= 0 & \lim_{t \rightarrow -\infty} p(x, t) &= 0 \\ \lim_{|x| \rightarrow +\infty} u(x, t) &= 0 & \lim_{|x| \rightarrow +\infty} p(x, t) &= 0 \end{aligned}$$

and $\chi * p$ is the convolution

$$(\chi * p)(x) = \int dx' \chi(x - x') p(x', t) . \quad (15)$$

Because of the δ -function, the RHS of Eq. (14) is an initial condition for p . Furthermore, the RHS of Eq. (13) will often be abbreviated:

$$\chi * p = P . \quad (16)$$

Making use of Eqs. (11) and (13) we may calculate the instanton action

$$S^{I(a)} = \frac{1}{2} \int_{-\infty}^0 dt \int dx dx' p(x, t) \chi(x - x') p(x', t) , \quad (17)$$

where $I(a)$ denotes that the instanton has a gradient of $u_x = a$. We denote all other instanton related quantities in a similar way.

III. INSTANTON BASED REWEIGHTING

The process of reweighting allows us to assemble the PDF related to the stochastic Burgers equation by solving the stochastic PDE for the fluctuations around the instanton. In order to derive the instanton equations, we considered the minimum of the Janssen-de Dominicis action $S_{\mathcal{H}}[u, p]$. However, to derive this stochastic PDE, we will work again with the original Onsager-Machlup action (see Eq. (6)):

$$\begin{aligned} S_{\mathcal{L}}[u, \dot{u}] &= \frac{1}{2} \int dt \langle \dot{u} + N[u], \chi^{-1}(\dot{u} + N[u]) \rangle \\ &= \frac{1}{2} \int dt dx dx' [u_t + uu_x - \nu u_{xx}] \\ &\quad \times \chi^{-1}(x - x') [u_t + uu_{x'} + \nu u_{x'x'}] . \end{aligned} \quad (18)$$

We then decompose the field into instanton and fluctuation

$$u = u^{I(a)} + \delta u . \quad (19)$$

This results in

$$\begin{aligned} S_{\mathcal{L}} &= \frac{1}{2} \int dt dx dx' \left[P^{I(a)} + \delta u_t + \delta u \delta u_x - \nu \delta u_{xx} \right. \\ &\quad \left. + (u^{I(a)} \delta u)_x \right] \chi^{-1}(x - x') [\dots] \\ &= S^{I(a)} + \tilde{S}^a - \frac{1}{2} \int dt dx p_x^{I(a)} (\delta u)^2 , \end{aligned} \quad (20)$$

with

$$\tilde{S}^a = \frac{1}{2} \int dt dx dx' [\delta u_t + \delta u \delta u_x - \nu \delta u_{xx} + (u^{I(a)} \delta u)_x] \times \chi^{-1}(x - x') [\dots]. \quad (21)$$

Here [...] denotes the appropriate expression evaluated at the position x' . Note that all linear variations vanish by definition of the instanton. Thus we define

$$\Delta S^a = S_{\mathcal{L}} - \tilde{S}^a = S^{I(a)} - \frac{1}{2} \int dt dx p_x^{I(a)} (\delta u)^2. \quad (22)$$

Now to derive the stochastic equation corresponding to the action \tilde{S}^a , we reverse the derivation of the path integral formulation and obtain

$$\delta u_t + \delta u \delta u_x - \nu \delta u_{xx} = \eta - (u^{I(a)} \delta u)_x. \quad (23)$$

Next, we have to change the path measure for this process in order to connect the statistics to the original one. To do that, we first consider the identity

$$\begin{aligned} P_{S_{\mathcal{L}}}(s) &:= \delta(u_x(0,0) - s) e^{-S_{\mathcal{L}}} \\ &= \delta(u_x(0,0) - s) e^{-(\tilde{S}^a + \Delta S^a)} \\ &= \delta(\delta u_x(0,0) + a - s) e^{-\tilde{S}^a} e^{-\Delta S^a}, \end{aligned} \quad (24)$$

where $P_{S_{\mathcal{L}}}(s)$ denotes the path measure of the distribution of gradients, $s = u_x(x,t)$ at $(x,t) = (0,0)$ in the original Burgers equation as one would obtain it by performing numerical simulations of (1). On the other hand, if we sample events for the gradient of the fluctuations, δu , around the instanton $I^{(a)}$, i.e. when $u_x = a$ through the new stochastic equation (23) we would get a PDF generated by the measure $e^{-\tilde{S}^a}$. The last equality in (24) tell us that in order to get the unbiased original PDF we need to reweight with a factor $e^{-\Delta S^a}$. A similar approach was formulated in a simpler setting by Bühler⁵⁸.

If we would proceed in choosing one value $u_x = a$ to calculate the instanton with $u_x^{I(a)}(x=0, t=0) = a$, we will be able to sample the statistics near this value very efficiently. However, values $u_x = s$ far away from a will be sampled with poor performance. Thus a major step is to choose $s = a$, which means that for every point $u_x = a$ in the PDF we first calculate the instanton and then using Eq. (22) obtain the PDF at $u_x = a$. This procedure is further motivated in Fig. 1. This figure shows the PDFs for the gradient of the fluctuations $\delta u_x(0,0)$ around the instanton $u^{I(a)}$, measured at $(0,0)$ and shifted by a (for comparison) using six different values of $u_x = a$, obtained from simulations of Eq. (23). Thus the actual form of the Girsanov transformation used in our instanton reweighting approach reads

$$\begin{aligned} P_{S_{\mathcal{L}}}(s) &:= \delta(u_x(0,0) - s) e^{-S_{\mathcal{L}}} \\ &= \delta(\delta u_x(0,0)) e^{-(\tilde{S}^a + \Delta S^a)} \end{aligned} \quad (25)$$

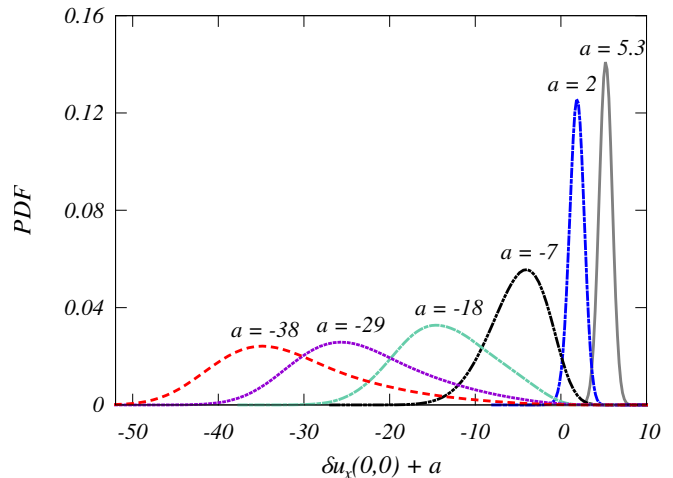


FIG. 1: Shape of the PDFs for the gradient of the fluctuations δu_x (shifted by a) around the instanton $u^{I(a)}$ for six different values of $u_x = a$.

IV. NUMERICAL SIMULATIONS OF RARE EVENTS

In this section we describe the numerical procedure to calculate the full PDF of velocity gradients step by step. The numerical integration of the stochastic PDE given in Eq. (23)

$$\delta u_t + \delta u \delta u_x - \nu \delta u_{xx} = \eta - (u^{I(a)} \delta u)_x$$

is achieved using the Euler-Maruyama method⁶¹ in combination with an integrating factor⁶² for the dissipative term. The spatial correlation function of the forcing (3) follows a power law proportional to k^{-3} in Fourier space and has a cutoff at $k_F = N_x/3$, where N_x is the spatial number of grid points. The nonlinear term is evaluated with the pseudospectral method. The instanton equations (13)-(14) are solved using an iterative method as described in Chernykh and Stepanov^{32,59}.

Results of an instanton configuration for a certain gradient $u_x^{I(a)}(x=0, t=0) = a$, and a snapshot of a typical realization of Eq. (23) δu added with $u^{I(a)}$ are displayed in Fig. 2.

A. Generating the PDF

In order to generate the PDF of velocity gradients, we define a set of Lagrange multipliers \mathcal{F} that implicitly define the set of gradients a . For each of these Lagrange multipliers we complete the following iteration scheme:

1. Solve the instanton equations Eqs. (13)-(14) and save both the velocity field $u^{I(a)}$ and the auxiliary field $p^{I(a)}$ as well as the convolution $P^{I(a)}$ in space and time.
2. Calculate the instanton action $S^{I(a)}$ according to Eq. (17).

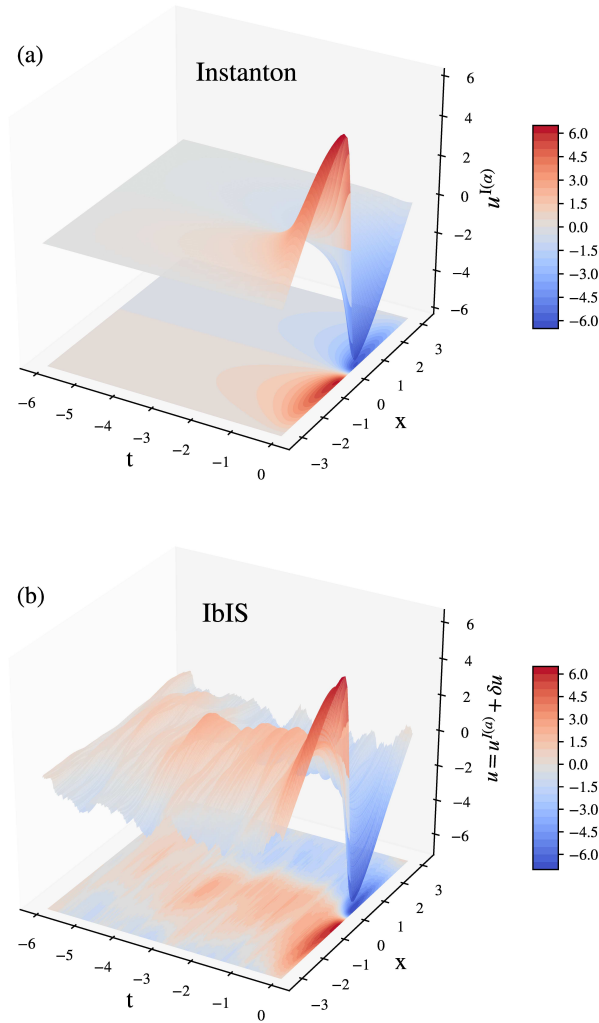


FIG. 2: (a) Instanton solution $u^{I(a)}$ for $N_x = 64$, $N_t = 576$, $\nu = 0.5$, $u_x^{I(a)}(0, 0) = a = -31.8$. (b) A realization $u(x, t) = u^{I(a)}(x, t) + \delta u(x, t)$, using the above instanton after solving Eq. (23)

3. For a chosen number of realizations N :

- (a) Calculate the fluctuations around the instanton as stated in section (III), whilst calculating the space integral

$$\frac{1}{2} \int dx p_x^{I(a)} (\delta u)^2 \quad (26)$$

at every time step, such that the sum over all time steps gives the space time integral from Eq. (22) that is required in order to calculate the reweighting factor

$$\Delta S^a = S^{I(a)} - \frac{1}{2} \int dt dx p_x^{I(a)} (\delta u)^2. \quad (27)$$

- (b) Add the instanton and the fluctuation

$$u = u^{I(a)} + \delta u \quad (28)$$

and subsequently calculate the gradient u_x at the space-time point $(x, t) = (0, 0)$.

- (c) Create the histogram of u_x around a , where the bin size corresponds to the spacing of the gradients a , and the current realization of $u_x(0, 0)$ is weighted by the factor $e^{-\Delta S^a}$.

4. Take the mean value of all the histograms to obtain the value of the PDF at $u_x = a$.

This structure allows it to run the process in parallel, because each of the levels in the iteration scheme is independent. First the iteration for each of the Lagrange multipliers can be done in parallel as well as the subroutine for each of the realizations of the fluctuations.

B. Results

We performed two sets of simulations for two different Reynolds numbers determined by the prescribed viscosities $\nu = 0.5$ and $\nu = 0.2$. A set consists of i) direct numerical simulations (DNS) of the Burgers equation, ii) a hybrid Monte Carlo⁵⁷ (HMC) sampling of the path integral and iii) our instanton based importance sampling (IbIS).

The hybrid Monte Carlo approach utilizes the action S_L (6) that depends on the flow configuration and constructs the measure as a weighted sum of all possible flow-realizations. Then S_L together with an additional gradient maximization constraint

$$S' = S_L + c_1 u_x(0, 0) \quad (29)$$

is sampled via the HMC algorithm⁶³, where the prefactor c_1 defines the strength of the constraint. The choice of the additional functional can, in principle, be arbitrary, here it is specifically designed to systematically generate a large (positive, if $c_1 < 0$ or negative, if $c_1 > 0$) velocity gradient at a specified space-time point, here at $(x, t) = (0, 0)$. Hence, the system favors the sampling of extreme and rare events in a similar spirit as an a posteriori filtering of strong gradient events generated by a standard DNS⁶⁴.

To test its validity and capabilities, the IbIS method is put in comparison to the HMC and the DNS by measuring the PDF of the velocity gradients. Both the IbIS and the HMC consider the reweighted statistics of the velocity gradient measured only at $(x, t) = (0, 0)$ (as explained in Sec. IV A and in⁵⁷), while for the DNS we consider any site that belongs to the stationary regime. In Figs. 3(a,b) we compare the cases of $\nu = 0.5$ and $\nu = 0.2$, respectively. The inset plot is an enlargement of the central region of the PDF, to strain that both reweighted PDFs of IbIS and HMC, successfully reproduce it. On the other hand,

ν	# meshpoints	# timesteps	time interval	# realizations	method	computing time (cpu hrs)
0.5	64	576	6	1×10^9	DNS	1×10^3
0.5	64	576	6	6×10^5	HMC	1×10^3
0.5	64	576	6	170×10^5	IbIS	24
0.2	256	1152	4	2×10^8	DNS	2.7×10^3
0.2	256	1152	4	4×10^5	HMC	1.2×10^4
0.2	256	1152	4	180×10^5	IbIS	250

TABLE I: The parameters used for the numerical simulations. ν is the viscosity, # meshpoints is the number of grid points N_x in space, # timesteps is the number of points N_t in time, while time interval denotes the physical temporal length. By # realizations we denote the number of produced space-time configurations. In the case of the IbIS method the notation 170×10^5 implies that we produced 10^5 space-time configurations for each of the 170 instantons with a given $u_x(0,0) = a$.

Accordingly for the HMC we produced 10^5 configurations for each of the six values of c_1 : (1.9, 1.6, 1.2, -1, -10, -20) for $\nu = 0.5$, and of the four c_1 : (0.9, 0.8, 0.6, 0.5) for $\nu = 0.2$, which were finally combined. The computing time in cpu hours is the total budget required to produce the corresponding # realizations, that were used in Fig. 3. Notice that the IbIS method is substantially cheaper than the HMC in providing similar quality of extreme events.

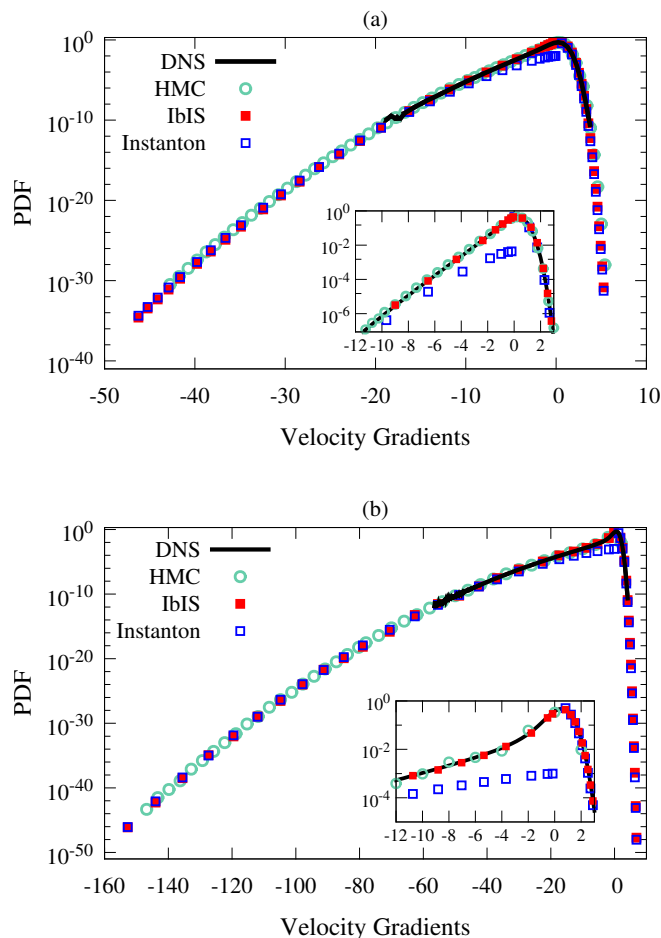


FIG. 3: Velocity gradients PDF. Reweighted IbIS (red filled squares) and HMC (green open circles) versus the DNS (black line) and the instanton (open blue squares)

(a) $N_x = 64$, $N_t = 576$, $\nu = 0.5$, scanning for $a \in (-46, 5)$. (b) $N_x = 256$, $N_t = 1152$, $\nu = 0.2$, scanning for $a \in (-160, 10)$.

as expected, the instanton prediction for small negative velocity gradients is wrong and underestimates the real PDF, as in this region the instanton approach is invalid, while in the case of the right tails the instanton prediction is exact⁴⁵. Most importantly, the far left tail of the PDFs is reproduced identically both from the IbIS and the HMC simulations. In addition, the PDFs approach the instanton prediction for increasing $|u_x|$ as it is stated by large deviation theory. This also constitutes a proof of concept of the IbIS method, as both implementations are completely different and independent.

In Fig. 4 we plot the relative error of the bins in Fig. 3(a). We notice that in the case of the DNS, the errors quickly deviate for large velocity gradients due to the sparsity of the measurements. This result is expected and underlines the need for rare-event algorithms in turbulence. Contrary to the direct numerical simulations, both the IbIS and the HMC provide sufficient statistics, resulting to constant and controllable small relative errors over a substantially extended range of values of the PDF of velocity gradient fluctuations $\mathcal{P}(u_x)$. In this respect, both the HMC and IbIS strategy are of comparable quality to capture rare events in turbulence.

The difference between the HMC and the IbIS methods is captured in Table I. This table does not only show all parameters used in our simulations, but most importantly the run-time used for the different simulations. First, we note the run-time for the DNS is about the size (or even smaller) than the run-time used in the HMC simulations. However, we stress that the DNS is only capable to capture a tiny fraction of the PDF. The remarkable effectiveness of the IbIS compared to the HMC method can be deduced from the ratio of their computing times. Here for the parameters used in our test cases, the IbIS method turns out to be two orders of magnitudes faster than the HMC approach, a ratio that is even expected to increase for higher Reynolds numbers.

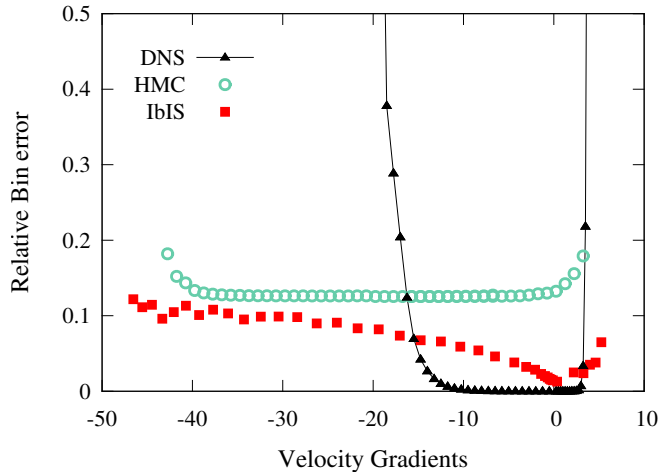


FIG. 4: Relative bin errors of the velocity gradient PDFs of Fig. 3(a). The errors of the DNS quickly deviate, while the errors of the IbIS and the HMC stay small and under control.

V. CONCLUSIONS AND OUTLOOK

In this paper we have presented a new method based on instanton importance sampling to calculate the probability distribution function of velocity gradients in Burgers equation for both typical and extremely intense events. By sampling fluctuations of the SPDE obtained on the background of one given instanton with a fixed (negative) intense velocity gradient in a certain (x, t) position, we explore the fluctuations around that specific flow configuration. At varying the reference gradient, and with a suitable reweighting protocol, we are able to reconstruct the whole PDF. The method is fully general and can – in principle – be applied to any SPDE. To be successful, a necessary condition is that a large deviation principle is applicable that guarantees the availability of unique instanton solutions. The IbIS method will work most efficiently when the PDF obtained solely from the instanton prediction is not too far from the true PDF. We also compared this new method with a Hybrid Monte Carlo approach⁵⁷ which does not rely on these assumptions and thus is applicable to a larger variety of physical problems. Concerning the Burgers case, IbIS is orders of magnitudes faster than the HMC. Both methods are much better than standard pseudo-spectral algorithms which are unable to focus on extreme-rare events. With the IbIS method it might be possible to calculate the scaling of the algebraic power law prefactors, which characterizes the inviscid limit of Burgers equations^{50,65} without using Lagrangian particle and shock tracking methods⁶⁶.

ACKNOWLEDGMENTS

J.F. acknowledges funding from the Humboldt foundation within a Feodor-Lynen fellowship. L.B. acknowledges funding from the European Research Council under the European Union’s Seventh Framework Programme, ERC Grant Agreement No. 339032. G.M. kindly acknowledges funding from the European Union’s Horizon 2020 research and innovation Programme under the Marie Skłodowska-Curie grant agreement No 642069 (European Joint Doctorate Programme ”HPC-LEAP”).

- ¹L. Knopoff and Y. Kagan, “Analysis of the theory of extremes as applied to earthquake problems,” *Journal of Geophysical Research* **82**, 5647–5657 (1977).
- ²M. Onorato, S. Residori, U. Bortolozzo, A. Montina, and F. Arecchi, “Rogue waves and their generating mechanisms in different physical contexts,” *Physics Reports* **528**, 47–89 (2013).
- ³G. Dematteis, T. Grafke, and E. Vanden-Eijnden, “Rogue waves and large deviations in deep sea,” *Proceedings of the National Academy of Sciences* **115**, 855–860 (2018).
- ⁴A. Hadjihosseini, M. Wächter, N. P. Hoffmann, and J. Peinke, “Capturing rogue waves by multi-point statistics,” *New Journal of Physics* **18**, 013017 (2016).
- ⁵S. Ghashghaie, W. Breyman, J. Peinke, P. Talkner, and Y. Dodge, “Turbulent cascades in foreign exchange markets,” *Nature* **381**, 767 (1996).
- ⁶F. Longin, *Extreme events in finance: A handbook of extreme value theory and its applications* (John Wiley & Sons, 2016).
- ⁷J. Bouchaud and M. Potters, *Theory of Financial Risk and Derivative Pricing: From Statistical Physics to Risk Management* (Cambridge University Press, 2009).
- ⁸K. Lehnertz, “Epilepsy: Extreme events in the human brain,” in *Extreme Events in Nature and Society*, edited by S. Albeverio, V. Jentsch, and H. Kantz (Springer Berlin Heidelberg, Berlin, Heidelberg, 2006) pp. 123–143.
- ⁹U. Frisch, *Turbulence: The legacy of A. N. Kolmogorov*. (Cambridge University Press, Cambridge, UK, 1995).
- ¹⁰A. Alexakis and L. Biferale, “Cascades and transitions in turbulent flows,” *Physics Reports* **767-769**, 1 – 101 (2018), cascades and transitions in turbulent flows.
- ¹¹A. S. Monin and A. M. Yaglom, *Statistical Fluid Mechanics: Mechanics of Turbulence* (Courier Dover Publications, 2007).
- ¹²P. Yeung, X. Zhai, and K. R. Sreenivasan, “Extreme events in computational turbulence,” *Proceedings of the National Academy of Sciences* **112**, 12633–12638 (2015).
- ¹³P. Debue, V. Shukla, D. Kuzzay, D. Faranda, E.-W. Saw, F. Daviaud, and B. Dubrulle, “Dissipation, intermittency, and singularities in incompressible turbulent flows,” *Phys. Rev. E* **97**, 053101 (2018).
- ¹⁴R. Benzi and L. Biferale, “Fully developed turbulence and the multifractal conjecture,” *Journal of Statistical Physics* **135**, 977–990 (2009).
- ¹⁵M. I. Freidlin and A. D. Wentzell, “Random perturbations,” in *Random perturbations of dynamical systems* (Springer, 1984) pp. 15–43.
- ¹⁶S. S. Varadhan, *Large deviations*, Vol. 27 (American Mathematical Soc., 2016).
- ¹⁷H. Touchette, “The large deviation approach to statistical mechanics,” *Physics Reports* **478**, 1–69 (2009).
- ¹⁸F. Cecconi, M. Cencini, A. Puglisi, D. Vergni, and A. Vulpiani, *Large Deviations in Physics: The Legacy of the Law of Large Numbers* (Springer, 2014).
- ¹⁹F. Bouchet, J. Laurie, and O. Zaboronski, “Langevin dynamics, large deviations and instantons for the quasi-geostrophic model and two-dimensional euler equations,” *Journal of Statistical Physics* **156**, 1066–1092 (2014).

- ²⁰P. Grassberger, “Go with the winners: a general monte carlo strategy,” *Computer Physics Communications* **147**, 64 – 70 (2002).
- ²¹C. Giardinà, J. Kurchan, V. Lecomte, and J. Tailleur, “Simulating rare events in dynamical processes,” *Journal of statistical physics* **145**, 787–811 (2011).
- ²²T. Lestang, F. Ragone, C.-E. Brhier, C. Herbert, and F. Bouchet, “Computing return times or return periods with rare event algorithms,” *Journal of Statistical Mechanics: Theory and Experiment* **2018**, 043213 (2018).
- ²³F. Ragone, J. Wouters, and F. Bouchet, “Computation of extreme heat waves in climate models using a large deviation algorithm,” *Proceedings of the National Academy of Sciences* **115**, 24–29 (2018).
- ²⁴C. Dellago, P. G. Bolhuis, F. S. Csajka, and D. Chandler, “Transition path sampling and the calculation of rate constants,” *The Journal of Chemical Physics* **108**, 1964–1977 (1998).
- ²⁵E. Weinan, W. Ren, and E. Vanden-Eijnden, “String method for the study of rare events,” *Physical Review B* **66**, 052301 (2002).
- ²⁶M. Heymann and E. Vanden-Eijnden, *Comm. Pure Appl. Math.* **61**, 1052–1117 (2008).
- ²⁷I. M. Lifshitz, “The energy spectrum of disordered systems,” *Adv. Phys.* **13**, 483–536 (1964).
- ²⁸B. I. Halperin and M. Lax, “Impurity-band tails in the high-density limit. i. minimum counting methods,” *Phys. Rev.* **148**, 722–740 (1966).
- ²⁹J. Zittartz and J. S. Langer, “Theory of bound states in a random potential,” *Phys. Rev.* **148**, 741–747 (1966).
- ³⁰J. Langer, “Theory of the condensation point,” *Annals of Physics* **41**, 108–157 (1967).
- ³¹J. Langer, “Statistical theory of the decay of metastable states,” *Annals of Physics* **54**, 258–275 (1969).
- ³²T. Grafke, R. Grauer, and T. Schäfer, “The instanton method and its numerical implementation in fluid mechanics,” *Journal of Physics A: Mathematical and Theoretical* **48**, 333001 (2015).
- ³³E. Balkovsky, G. Falkovich, I. Kolokolov, and V. Lebedev, “Viscous instanton for Burgers’ turbulence,” (1996), arXiv:chaodyn/9603015.
- ³⁴E. Balkovsky, G. Falkovich, I. Kolokolov, and V. Lebedev, “Intermittency of Burgers’ turbulence,” *Phys. Rev. Lett.* **78**, 1452 (1997), arXiv:chaodyn/9609005.
- ³⁵M. De Pietro, A. A. Mailybaev, and L. Biferale, “Chaotic and regular instantons in helical shell models of turbulence,” *Phys. Rev. Fluids* **2**, 034606 (2017).
- ³⁶A. A. Mailybaev, “Blowup as a driving mechanism of turbulence in shell models,” *Phys. Rev. E* **87**, 053011 (2013).
- ³⁷I. Daumont, T. Dombre, and J.-L. Gilson, “Instanton calculus in shell models of turbulence,” *Phys. Rev. E* **62**, 3592–3610 (2000).
- ³⁸H.-K. Janssen, “On a lagrangean for classical field dynamics and renormalization group calculations of dynamical critical properties,” *Zeitschrift für Physik B Condensed Matter* **23**, 377–380 (1976).
- ³⁹C. De Dominicis, “Techniques de renormalisation de la théorie des champs et dynamique des phénomènes critiques,” *J. Phys. Colloques* **37**, C1–247–C1–253 (1976).
- ⁴⁰P. C. Martin, E. D. Siggia, and H. A. Rose, “Statistical dynamics of classical systems,” *Phys. Rev. A* **8**, 423–437 (1973).
- ⁴¹T. Gotoh, “Inertial range statistics of Burgers turbulence,” *Phys. Fluids* **6**, 3985 (1994).
- ⁴²A. Chekhlov and V. Yakhot, “Kolmogorov turbulence in a random-force-driven Burgers equation,” *Phys. Rev. E* **51**, R2739 (1995).
- ⁴³A. Chekhlov and V. Yakhot, “Kolmogorov turbulence in a random-force-driven Burgers equation: Anomalous scaling and probability density functions,” *Phys. Rev. E* **52**, 5681 (1995).
- ⁴⁴J. P. Bouchaud, M. Mezard, and G. Parisi, “Scaling and intermittency in Burgers turbulence,” *Phys. Rev. E* **52**, 3656 (1995).
- ⁴⁵V. Gurarie and A. A. Migdal, “Instantons in Burgers equation,” *Phys. Rev. E* **54**, 4908 (1996), arXiv:hep-th/9512128.
- ⁴⁶G. Falkovich, I. Kolokolov, V. Lebedev, and A. A. Migdal, “Instantons and intermittency,” *Phys. Rev. A* **54**, 4896 (1996), arXiv:chaodyn/9512006.
- ⁴⁷A. M. Polyakov, “Turbulence without pressure,” *Phys. Rev. E* **52**, 6183 (1995), arXiv:hep-th/9506189.
- ⁴⁸S. Boldyrev, “A Note on Burgers’ turbulence,” *Phys. Rev. E* **55**, 6907 (1997), arXiv:hep-th/9610080.
- ⁴⁹W. E, K. M. Khanin, A. E. Mazel, and Y. G. Sinai, “Invariant measures for Burgers equation with stochastic forcing,” *Ann. Math.* **151**, 877 (2000), arXiv:math/0005306.
- ⁵⁰W. E and E. Vanden Eijnden, “Statistical theory for the stochastic burgers equation in the inviscid limit,” *Comm. Pure Appl. Math.* **53**, 852901 (2000).
- ⁵¹W. E and E. Vanden Eijnden, “Asymptotic theory for the probability density functions in burgers turbulence,” *Phys. Rev. Lett.* **83**, 25722575 (1999).
- ⁵²J. Friedrich, G. Margazoglou, L. Biferale, and R. Grauer, “Multiscale velocity correlations in turbulence and burgers turbulence: Fusion rules, markov processes in scale, and multifractal predictions,” *Phys. Rev. E* **98**, 023104 (2018).
- ⁵³J. Bec and K. M. Khanin, “Burgers turbulence,” *Phys. Rep.* **447**, 1 (2007), arXiv:0704.1611 [nlin.CD].
- ⁵⁴M. Lässig, “Dynamical anomalies and intermittency in Burgers turbulence,” *Phys. Rev. Lett.* **84**, 2618 (2000), arXiv:cond-mat/9811223.
- ⁵⁵M. Janas, A. Kamenev, and B. Meerson, “Dynamical phase transition in large-deviation statistics of the kardar-parisi-zhang equation,” *Phys. Rev. E* **94**, 032133 (2016).
- ⁵⁶N. R. Smith, A. Kamenev, and B. Meerson, “Landau theory of the short-time dynamical phase transitions of the kardar-parisi-zhang interface,” *Phys. Rev. E* **97**, 042130 (2018).
- ⁵⁷G. Margazoglou, L. Biferale, R. Grauer, K. Jansen, D. Mesterházy, T. Rosenow, and R. Tripiccone, “A Hybrid Monte Carlo algorithm for sampling rare events in space-time histories of stochastic fields,” *ArXiv e-prints* (2018), arXiv:1808.02020 [physics.comp-ph].
- ⁵⁸O. Bühler, “Large deviation theory and extreme waves,” in *Proc. 15th Aha Hulikoa Hawaiian Winter Workshop Proceedings* (2007) pp. 1–9.
- ⁵⁹A. I. Chernykh and M. G. Stepanov, “Large negative velocity gradients in burgers turbulence,” *Phys. Rev. E* **64**, 026306 (2001).
- ⁶⁰L. Onsager and S. Machlup, “Fluctuations and irreversible processes,” *Phys. Rev.* **91**, 1505–1512 (1953).
- ⁶¹D. Higham., “An algorithmic introduction to numerical simulation of stochastic differential equations,” *SIAM Review* **43**, 525–546 (2001), <https://doi.org/10.1137/S0036144500378302>.
- ⁶²C. Canuto, M. Hussaini, A. Quarteroni, and T. Zang, *Spectral Methods in Fluid Dynamics* (Springer-Verlag, New York, 1988).
- ⁶³S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, “Hybrid Monte Carlo,” *Phys. Lett. B* **195**, 216 (1987).
- ⁶⁴T. Grafke, R. Grauer, and T. Schäfer, “Instanton filtering for the stochastic Burgers equation,” *J. Phys. A* **46**, 062002 (2013).
- ⁶⁵E. W., K. Khanin, A. Mazel, and Y. Sinai, “Probability distribution functions for the random forced burgers equation,” *Phys. Rev. Lett.* **79**, 19041907 (1997).
- ⁶⁶J. Bec, “Universality of velocity gradients in forced burgers turbulence,” *Phys. Rev. Lett.* **87**, 104501 (2001).