HPC Summit Week – PRACEdays18

A Hybrid Monte Carlo importance sampling of rare events in Turbulence and in Turbulent Models

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Ljubljana, Slovenia, May 2018

The research leading to these results has received funding from the EU Horizon 2020 research and innovation programme under grant agreement No.642069, and from the EU Seventh Framework Programme (FP7/2007-2013) under ERC grant agreement No. 339032.

Our interest: A systematic study of extreme and rare events

Figure : Extreme rogue wave

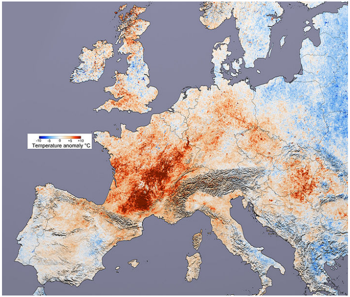


Figure : Europe: 2003 heat wave

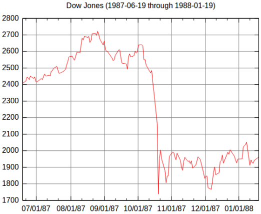


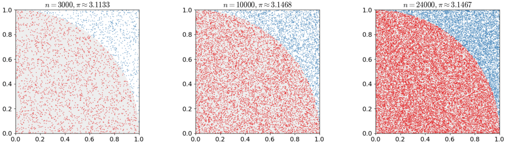
Figure : 1987 Stock market crash

Figure : 2006 hurricane Katrina

Outline

- We introduce a variant of the well-known Hybrid Monte Carlo (HMC) algorithm to address the statistics of large fluctuations in stochastic dynamics.
- Based on the path integral approach to stochastic (partial) differential equations the HMC algorithm samples (space-)time histories of the dynamical degrees of freedom under the influence of random noise.
- **Why?**: Extreme and rare events are a defining feature of stochastic systems but present a severe challenge to standard computational approaches that struggle to systematically sample these events.
- **Idea**: Here, we present a Monte Carlo importance sampling method that is capable of selectively exploring those remote areas of phase space associated to extreme and rare events.
- **How**: By systematically modifying the action – i.e applying sampling constraints – allowing to highlight rare configurations.
- **Current model**: stochastic 1D Burgers' equation – a simple 1D model of turbulence.

What is Monte Carlo?



- A broad class of computational algorithms that rely on repeated random sampling to obtain numerical results.
- In physics-related problems, Monte Carlo methods are useful for simulating systems with many coupled degrees of freedom, such as fluids, disordered materials, strongly coupled solids, and cellular structures.
- The general motivation to use the Monte Carlo method in statistical physics is to evaluate a multivariable integral.

An estimation, under Monte Carlo integration, of an integral defined as:

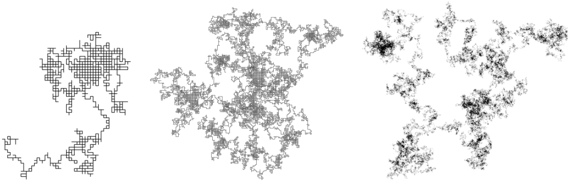
$$\langle \mathcal{O} \rangle = \mathcal{Z}^{-1} \int \mathcal{D}\phi \, \mathcal{O}[\phi] \, e^{-\beta E[\phi]} \qquad (1) \qquad \text{is} \qquad \langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}_i^*, \qquad (2)$$

provided that:

1. We sample states that are more relevant to the integral $\rightarrow$ importance sampling.
2. Let the Boltzmann distribution be the one to identify those states.

Monte Carlo and random walks

Markov chain Monte Carlo (MCMC) methods are based on constructing a Markov chain that has the desired distribution as its equilibrium distribution. The more steps there are, the more closely the distribution of the ensemble matches the actual desired distribution.



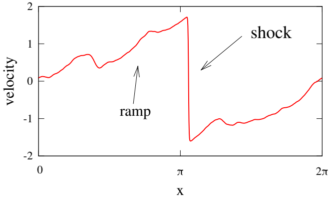
- When a Markov chain Monte Carlo method is used for approximating a multi-dimensional integral, an ensemble of "walkers" move around randomly in the phase space of states.
- Metropolis algorithm: generates a random walk using a proposal mechanism and a method for rejecting some of the proposed moves.
- Random walk Monte Carlo methods generate autocorrelated ensembles especially close to critical points.
- NON-random walk MCMC $\rightarrow$ Hybrid Monte Carlo (HMC)
  - Implements Hamiltonian dynamics, so the potential energy function is the target density.
  - Proposals move across the configuration space in larger steps.
  - Less correlated ensemble, faster convergence to the target distribution.

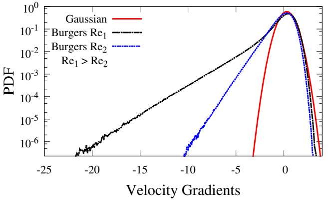
Stochastic 1D Burgers' equation

$$\partial_t u + u\partial_x u - \nu\partial_x^2 u = f(x,t),$$

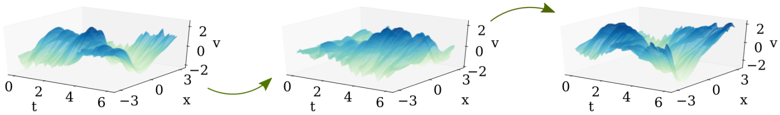
where f is a white noise power-law correlated Gaussian forcing, for which the two-point correlation function in Fourier space is given by:

$$\begin{aligned}\langle f(k,t)f(k',t')\rangle &= 2D_0|k|^{\beta}\delta(k+k')\delta(t-t')\\ &= \Gamma(k,t;k',t').\end{aligned}$$





The HMC generates space-time velocity field configurations and efficiently moves inside the sample space.



The Hybrid Monte Carlo – How it works

What we need:

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Path integral approach: $\partial_t u + u\partial_x u - \nu\partial_x^2 u = f(x,t) \xrightarrow[\text{formalism}]{\text{Martin-Siggia-Rose}} S_{\text{Burgers}}\,,$

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- Noise 2-point: $\langle f(k,t) f(k',t')\rangle = 2D_0 |k|^\beta \delta(k+k')\delta(t-t') = \Gamma(k,t;k',t')$.
- Path integral over the Gaussian noise: $\mathcal{Z} = \int \mathcal{D}f\, e^{-\frac{1}{2}(f,\,\Gamma^{-1} f)}$,
- where $(\cdot\,,\cdot) \equiv \int \cdot\, dt\, dt'\, dx\, dx'$. is an appropriate inner product.
- change of variables: $f \to u \longrightarrow$ Jacobian: $J[u] = det(\frac{\delta f}{\delta u}) \longrightarrow \mathcal{D}f = \mathcal{D}u\, J[u]$
- $\mathcal{Z} = \int \mathcal{D}u\, J[u]\, exp(-S_{Burgers}) = \int \mathcal{D}u\, J[u]\, e^{-\frac{1}{2}(\chi(u),\Gamma^{-1}\chi(u))}$
- Action: $S_{\text{Burgers}} = \frac{1}{2}(\chi(u), \Gamma^{-1}\chi(u))$ and $\chi(u) \equiv \partial_t u + u\partial_x u - \nu\partial_x^2 u$
- in detail:
  $S_{\text{Burgers}} = \frac{1}{2}\int dt \int dx\, \left(\partial_t v + v\partial_x v - \nu\partial_x^2 v\right) \int dy\, \Gamma^{-1}(x-y)\left(\partial_t v + v\partial_y v - \nu\partial_y^2 v\right)$

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Partition Function: $\mathcal{Z} = \int \mathcal{D}u\, exp(-S_{Burgers})$

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The HMC requires a Hamiltonian: $H(\pi(x,t), u(x,t)) = \frac{1}{2}\sum_{x,t}(\pi_{x,t}, \Omega * \pi_{x,t}) + S_{\text{Burgers}}$

Introducing momenta π = auxiliary Gaussian distributed fields, which are completely unrelated to u, and Ω which acts as a mass term. It may have a space-time dependency.

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What we need:

1. An Action functional which describes exactly the physical system under consideration.
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3. A methodology to efficiently update the velocity field.

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The system now obeys the Hamilton's equations of motion (**Molecular Dynamics**|):

$$\frac{\partial u}{\partial \tau} = \frac{\partial H}{\partial \pi} \text{ and } \frac{\partial \pi}{\partial \tau} = -\frac{\partial H}{\partial u}$$

where a "Monte Carlo" time τ is introduced.

The Hybrid Monte Carlo – How it works

What we need:

1. An Action functional which describes exactly the physical system under consideration.
2. A Hamiltonian for the accept/reject step
3. A methodology to efficiently update the velocity field.
4. A procedure that is comparable with DNS.

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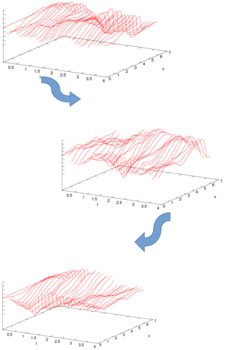
Hybrid Monte Carlo = Molecular Dynamics + Monte Carlo



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Hamiltonian:

$$H(\pi, u) = \frac{1}{2} \sum_{x,t} (\pi, \Omega * \pi) + S[u]$$

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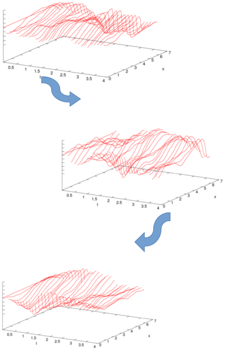
Hybrid Monte Carlo = Molecular Dynamics + Monte Carlo



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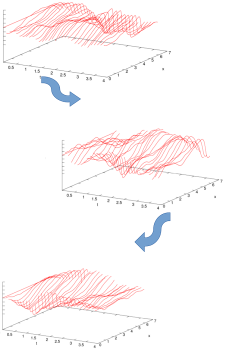

The fields are evolved along a trajectory on a hypersurface $H(\pi, u) = const$ defined by the effective hamiltonian H. We apply a symplectic integrator that is accurate to $O(\varepsilon^2)$:

$$u_{x,t}(\tau + \varepsilon/2) = u_{x,t}(\tau) + \Omega_{x,t} * \pi_{x,t}(\tau)\, \varepsilon/2$$

$$\pi_{x,t}(\tau + \varepsilon) = \pi_{x,t}(\tau) - \frac{\partial S}{\partial u}_{x,t}(\tau + \varepsilon/2)\, \varepsilon$$

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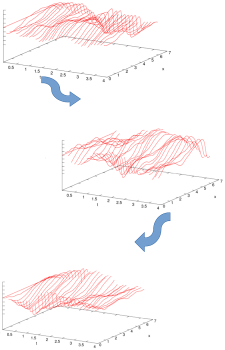

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Fourier Acceleration

- The use of a Gaussian power-law forcing requires specific handling.
- A naive implementation may cause severe slow-down of the dynamics.
- The Fourier Acceleration technique significantly improves the importance sampling by introducing different timescales for each of the modes in the MD part of the HMC

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by rescaling:

$$\pi \to \xi = (dt\Omega)^{\frac{1}{2}}\,\pi\ , \quad \varepsilon \to \tilde{\varepsilon} = \left(\frac{\Omega}{dt}\right)^{\frac{1}{2}} \varepsilon .$$

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MD integration:

$$u_{x,t}(\tau + \tilde{\varepsilon}/2) = u_{x,t}(\tau) + \xi_{x,t}(\tau)\,\tilde{\varepsilon}/2\ ,$$

$$\xi_{x,t}(\tau + \tilde{\varepsilon}) = \xi_{x,t}(\tau) - dt\,\frac{\partial S}{\partial u}_{x,t}(\tau + \tilde{\varepsilon}/2)\,\tilde{\varepsilon}\ ,$$

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where we rescaled:

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We require that the fields should satisfy $\xi \sim O(1)$, with $\Delta\xi \sim O(\varepsilon)$, *i.e.*,

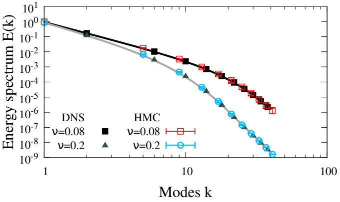
$$dt\,\frac{\partial S}{\partial u}\,\tilde{\varepsilon} = (dt\Omega)^{\frac{1}{2}}\,\frac{\partial S}{\partial u}\,\varepsilon \sim O(\varepsilon)\ .$$

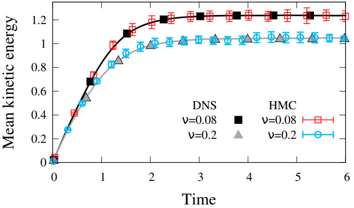
For the kernel Ω in Fourier space, we have

$$\Omega(k,t) \sim \frac{1}{dt\left\langle\left|\frac{\partial S}{\partial u}(k,t)\right|\right\rangle^2} \sim dt^3\Gamma(k)\ ,$$

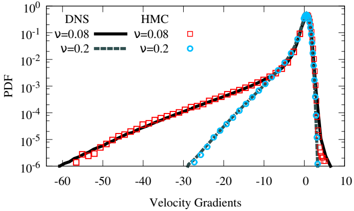
Benchmark/fine tune of the HMC

- Thorough validation tests of the HMC against a standard pseudo-spectral algorithm. Next follow results for fixed spatio-temporal resolution and different viscosities.



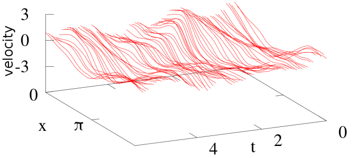


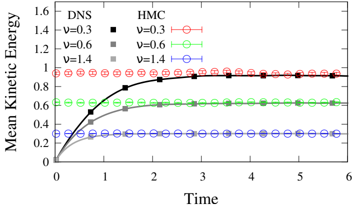
- DNS: greyscale ■, HMC: colored ○
- We measure the Fourier-space energy spectra
  $E(k) = \sum_{t_{stationary}}^{T} u^*(k,t)\, u(k,t)$
- The real-space kinetic energy:
  $K(t) = \frac{1}{L} \sum_{x=0}^{x=L} u(x,t)^2$
- And the velocity gradients PDF.

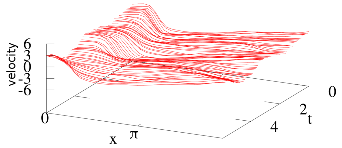


New feature – Periodic Boundary conditions in time!

- The HMC allows to properly define a full spatio-temporal periodic system. It is capable of reproducing the stationary regime of the system. After we reach Monte Carlo equilibrium we have:



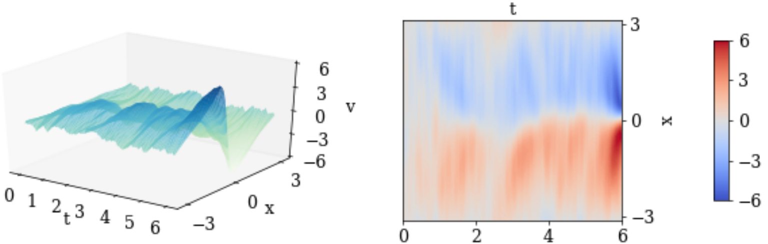




The HMC is agile to perform under a variety of boundary conditions, in both space and time. This allows us to rigorously introduce local or global constraints in space and/or time.

Implementation of sampling constraints

- **Goal**: Highlight specific field configurations by systematically modifying the action. This can be achieved by applying **reweighting techniques** and appropriate constraints on lattice configurations. We want to maximaze the velocity gradient at a particular space-time point.
- **Idea**: sample from a different action S' which consists of the original action S_0 in addition to a constraint functional S_A: $S' = S_0 + S_A$
- Bellow: local constraint acting only at $(x = 0, t = t_f)$.
- $S_A^1 = c_1 \sum_{x,t} \partial_x u \, \delta(x)\delta(t - t_f) \rightarrow$ linear local constraint | unbounded.
- $S_A^2 = c_2 \sum_{x,t} \left(\frac{\partial_x u}{s_2} + 1\right)^2 \delta(x)\delta(t - t_f) \rightarrow$ quadratic local constraint.
- $S_A^3 = c_3 \sum_{x,t} \left[\left(\frac{\partial_x u}{s_3}\right)^2 - 1\right]^2 \delta(x)\delta(t - t_f) \rightarrow$ quartic local constraint.



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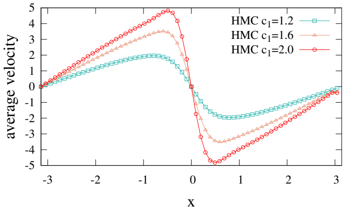

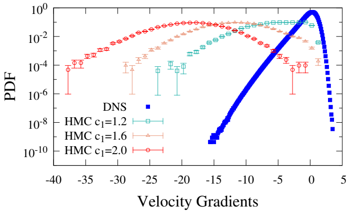

Figure : *Left plot:* Averaged HMC using S_A^1 for different values of c_1. *Right plot:* Velocity gradients PDF $P(v_x)$, with $v_x = \partial_x v(x = 0, t = t_f)$, of HMC for different values of c_1 vs DNS.

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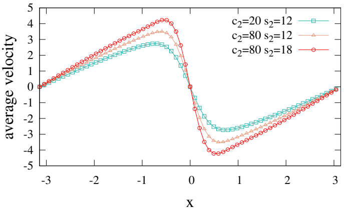

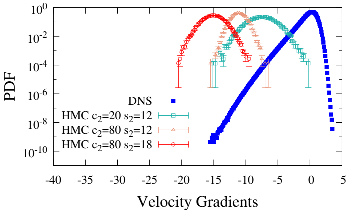

Figure : *Left plot:* Averaged HMC using S_A^2 for different values of c_2. *Right plot:* Velocity gradients PDF $P(\mathrm{v}_x)$, with $\mathrm{v}_x = \partial_x v(x = 0, t = t_f)$, of HMC for different values of c_2 vs DNS.

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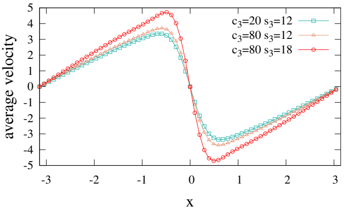

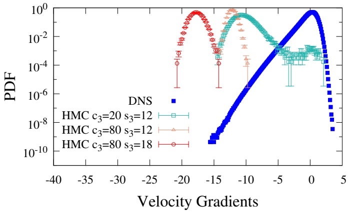

Figure : *Left plot:* Averaged HMC using S_A^3 for different values of c_3. *Right plot:* Velocity gradients PDF $P(v_x)$, with $v_x = \partial_x v(x = 0, t = t_f)$, of HMC for different values of c_3 vs DNS.

Reweighting

We need to compare the observable $\langle \mathcal{O} \rangle_{S'}$ measured using the ensemble which is generated by sampling S', with a regular observable $\langle \mathcal{O} \rangle_{S}$ using S.

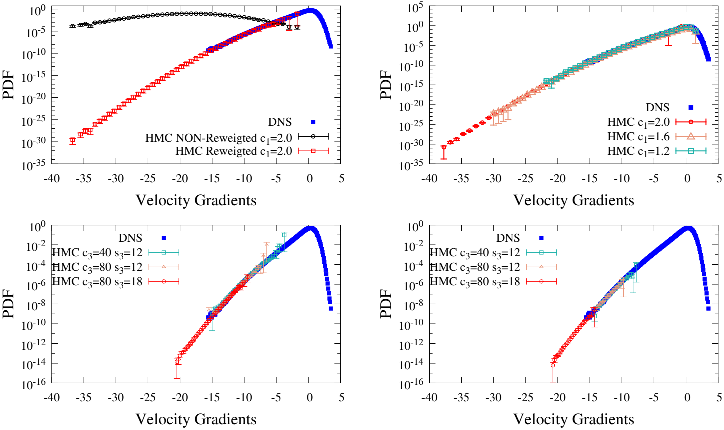

Figure : *Top left:* Velocity gradients PDF $P(v_x)$, with $v_x = \partial_x v(x = 0, t = t_f)$, of HMC vs DNS. We consider here only the extracted histogram from the lattice point on which the constraint S_a^1 for $c_1 = 2.0$ acted (i.e $x = 0$, $t = t_f$) in the case of the HMC. *Top right:* Using the constraint S_a^1 and showing the effect for different c_1 after reweighting. *Bottom left:* Using the constraint S_a^2 and showing the effect for different c_2 and s_2 after reweighting. *Bottom right:* Using the constraint S_a^2 and showing the effect for different c_3 and s_3 after reweighting.

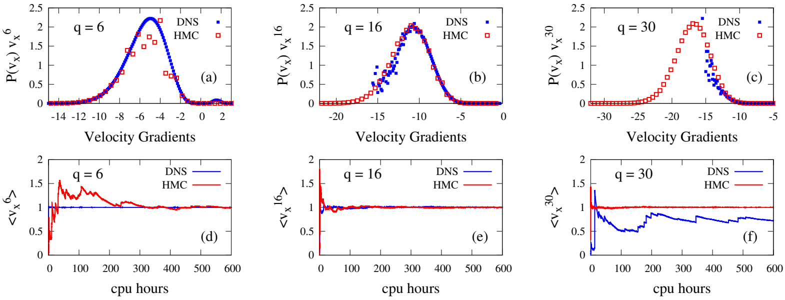

Figure : *Top row (a-c)*: Velocity gradient PDF $P(\mathrm{v}_x)$, with $\mathrm{v}_x = \partial_x v(x=0, t=t_f)$, i.e measured only at the lattice point that the constraint S^1_a acts, and multiplied by a moment of the velocity gradient v_x^q. *Bottom row (d-f)*: Computational time to stabilized running average of velocity gradient normalized moment $\langle(\partial_x \mathrm{v})^q\rangle$ with respect to the final stabilized value. Here, regarding DNS, any site belonging to the stationary regime is considered.

Instantons in Burgers equation

Idea: maximization of the velocity gradients $\xrightarrow[\text{formalism}]{\text{Martin-Siggia-Rose}}$ PDF of the velocity gradients can be written as:

$$\mathcal{P}(a) = \int \mathcal{D}u\mathcal{D}p\,\delta(\partial_x u|_{(t_0,x_0)} - \alpha)\ \exp(-\tilde{S}(u,p))$$

Instantons: saddle point configurations for the fields (u,p) that yield the largest contribution to the path integral for strong gradients.

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The instanton equations for the fields (u,p) are:

$$\begin{aligned} u_t + uu_x - \nu u_{xx} &= -i\int \Gamma(x-x')\, p(x',t)dx' \\ p_t + up_x + \nu p_{xx} &= 4i\nu^2\lambda\delta(t)\delta'(x) \end{aligned}$$

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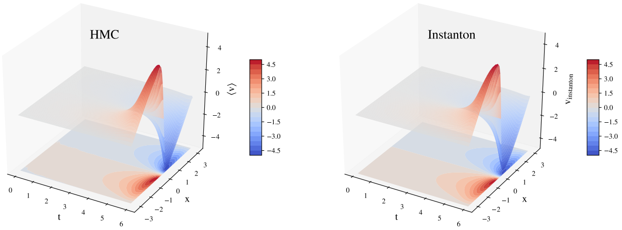

Figure : *Left plot:* Ensemble average of velocity configurations of the HMC using S_a^1 with $c_1 = 2$. *Right plot:* Instanton velocity field profile for $\lambda = -3.54$ and $\alpha = -24.75$. It is clear that by averaging the ensemble of the HMC we remove the fluctuations around the instanton, restoring its spatio-temporal shape.

Conclusion – Perspectives

To conclude

- Novel and generic path integral based method to study the properties of stochastic PDE's, which is ideal for imposing sampling constraints to the space/time domain.
- Successful benchmark of the stochastic 1D Burgers equation against DNS (pseudospectral code).
- Successful application of gradient maximization local constraints to enhance the occurrence of strong gradients. By averaging the generated velocity field ensemble we managed to reconstruct an instanton-alike spatio-temporal configuration (filtering off the fluctuations).
- The access to the configuration space, to which Monte Carlo sampling is related to, allows this method systematically sample extreme events in those remote areas of the configuration space associated to them.

Perspectives

- Give further insights into intermittency and anomalous scaling in hydrodynamical, out-of-equilibrium systems and quantify for the first time to what extent instantons –and fluctuations around them– are important for anomalous scaling exponents.
- Extension of the approach to other applications and stochastic models to specifically target the study of extreme and rare events.

Thank you for your attention!

HPC Summit Week – PRACEdays18

A Hybrid Monte Carlo importance sampling of rare events in Turbulence and in Turbulent Models

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in collaboration with:

L. Biferale[1], R. Grauer, K. Jansen, D. Mesterházy, T. Rosenow, and R. Tripiccione

[1]Department of Physics and INFN,
University of Rome, "Tor Vergata"

[2]Cyprus Institute

Ljubljana, Slovenia, May 2018

The research leading to these results has received funding from the EU Horizon 2020 research and innovation programme under grant agreement No.642069, and from the EU Seventh Framework Programme (FP7/2007-2013) under ERC grant agreement No. 339032.

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