12th European Fluid Mechanics Conference

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

G. Margazoglou[1,2]

in collaboration with:

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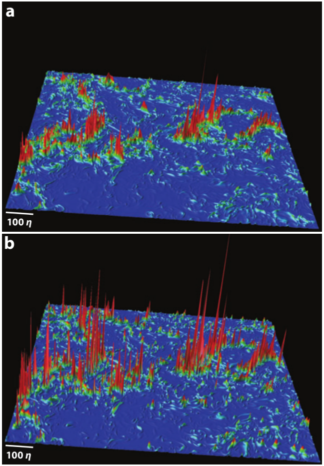
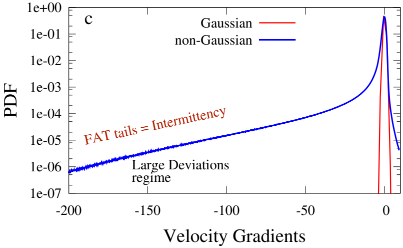
Large Deviations



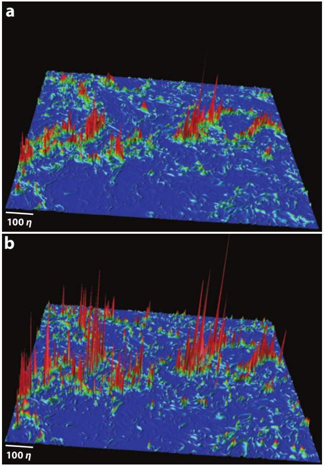


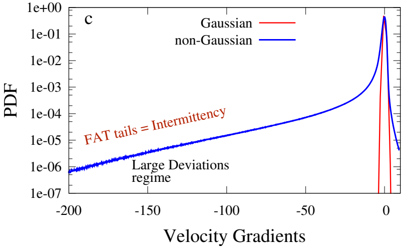
a) intensity distribution of energy dissipation rate
b) intensity distribution of enstrophy
c) PDF of velocity gradients of 1d stochastic Burgers equation.

- a and b from Ishihara *et.al*, 2009.

Large Deviations

- Sampling extreme events in time-advancing numerical schemes is a matter of chance.
- Introduction of a novel – path integral based – computational approach to systematically sample in areas of the configuration space related to extreme events.
- **Idea**: Use the Hybrid Monte Carlo (HMC) – standard algorithm in Lattice QCD community.
- **Current model**: stochastic 1D Burgers' equation





a) intensity distribution of energy dissipation rate
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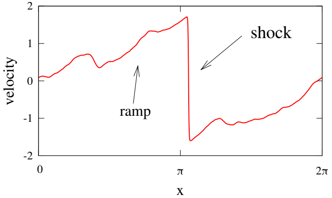
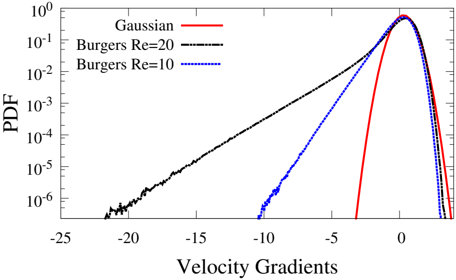
Stochastic 1D Burgers' equation

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

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

$$\langle f(k,t)f(k',t')\rangle = 2D_0|k|^\beta \delta(k+k')\delta(t-t') = \Gamma(k,t;k',t').$$





The Hybrid Monte Carlo

A few words

1. A highly efficient Markov Chain Monte Carlo method – NOT a random walk in the configuration space.

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2. Requires an action functional which describes exactly the physical system under consideration.

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

Action: $S_{\text{Burgers}} = \frac{1}{2}\int dk\, dt\, \Gamma^{-1}\, \hat{\chi}(u)^2$ and $\hat{\chi}(u) \equiv FT\{\partial_t u + u\partial_x u - \nu\partial_x^2 u\}$.

The Hybrid Monte Carlo

A few words

1. A highly efficient Markov Chain Monte Carlo method – NOT a random walk in the configuration space.
2. Requires an action functional which describes exactly the physical system under consideration.
3. The HMC creates a Markov Chain and moves inside the configuration space considering the whole $1+1$ spatio-temporal evolution of the system.

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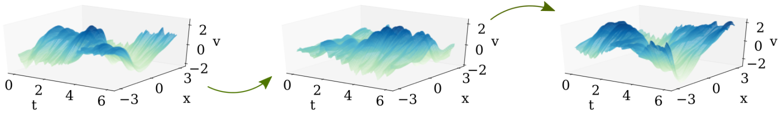
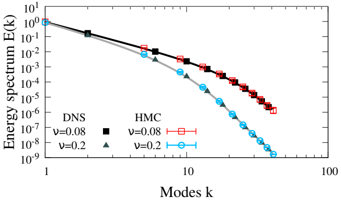
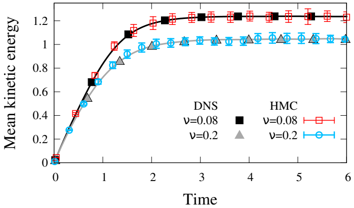


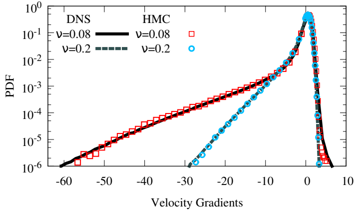
Benchmark/fine tune of the HMC

- 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.

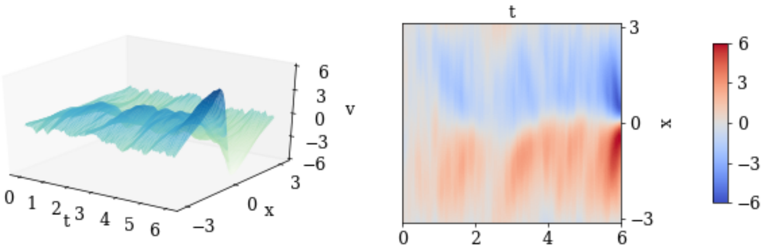


Implementation of sampling constraints

- **Goal**: Highlight specific field configurations by systematically modifying the action. We want to maximaze the velocity gradient at a particular space-time point.
- **Idea**: sample from a different action S':

$$\mathrm{S}' = \mathrm{S} + \Delta\mathrm{S}$$

- Bellow: local constraint acting only at $(x = 0, t = t_f)$.
- $\Delta\mathrm{S}_1 = c_1 \sum_{x,t} \partial_x u \, \delta(x)\delta(t - t_f) \rightarrow$ linear local constraint | unbounded.
- $\Delta\mathrm{S}_2 = c_2 \sum_{x,t} \left(\frac{\partial_x u}{s_2} + 1\right)^2 \delta(x)\delta(t - t_f) \rightarrow$ quadratic local constraint.
- $\Delta\mathrm{S}_3 = c_3 \sum_{x,t} \left[\left(\frac{\partial_x u}{s_3}\right)^2 - 1\right]^2 \delta(x)\delta(t - t_f) \rightarrow$ quartic local constraint.



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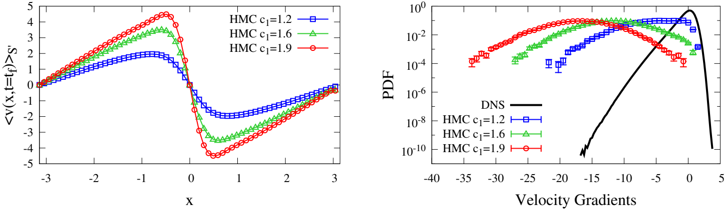

Figure : *Left plot:* Averaged HMC using S^1_A for different values of c_1. *Right plot:* Velocity gradients PDF $P(\mathrm{v}_x)$, with $\mathrm{v}_x = \partial_x v(x = 0, t = t_f)$, of HMC for different values of c_1 vs DNS.

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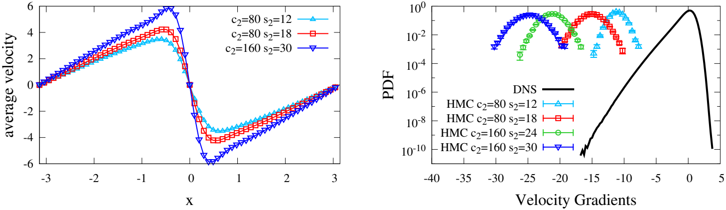

Figure : *Left plot:* Averaged HMC using S_A^2 for different values of c_2. *Right plot:* Velocity gradients PDF $P(\mathrm{v}_x)$, with $\mathrm{v}_x = \partial_x v(x = 0, t = t_f)$, of HMC for different values of c_2 vs DNS.

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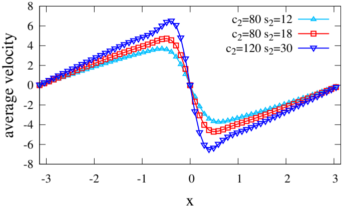

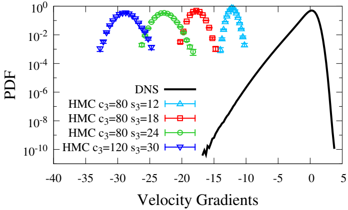

Figure : *Left plot:* Averaged HMC using S_A^3 for different values of c_3. *Right plot:* Velocity gradients PDF $P(\mathrm{v}_x)$, with $\mathrm{v}_x = \partial_x v(x = 0, t = t_f)$, of HMC for different values of c_3 vs DNS.

Reweighting

We need to probe the observable $\langle \mathcal{O} \rangle_{\mathrm{S}'}$ measured using the ensemble which is generated by sampling S', back to the original unbiased observable $\langle \mathcal{O} \rangle_{\mathrm{S}}$ generated using S.

$$\langle \mathcal{O} \rangle_{\mathrm{S}} = \frac{\langle \mathcal{O} e^{-(\mathrm{S}-\mathrm{S}')} \rangle_{\mathrm{S}'}}{\langle e^{-(\mathrm{S}-\mathrm{S}')} \rangle_{\mathrm{S}'}} = \frac{\langle \mathcal{O} e^{\Delta \mathrm{S}} \rangle_{\mathrm{S}'}}{\langle e^{\Delta \mathrm{S}} \rangle_{\mathrm{S}'}}, \qquad \text{where } \Delta \mathrm{S} = \mathrm{S}' - \mathrm{S}.$$

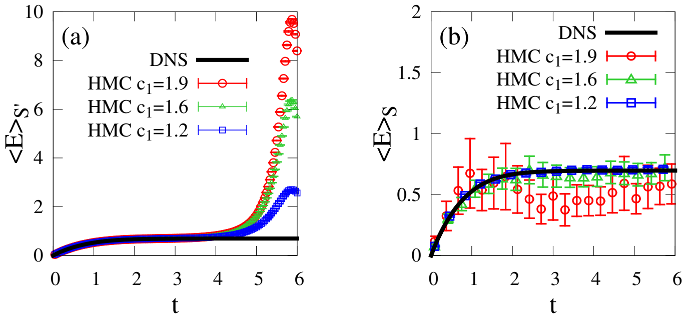

Figure : (*a*-*b*): Ensemble averaged kinetic energy of HMC vs DNS using $\Delta \mathrm{S}_1$ for different c_1. (*a*): Before reweighting. (*b*): After reweighting.

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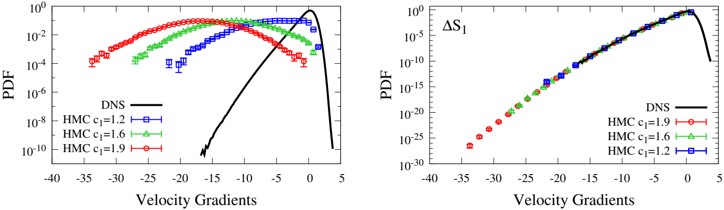

Figure : Velocity gradients PDF of HMC against DNS. We consider here only the lattice point on which the constraint $\Delta\mathrm{S}$ acted (i.e $x = 0$, $t = t_f$). The data of the HMC and the DNS were produced with the same computational cost.

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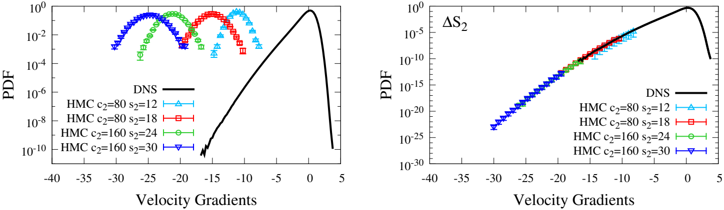

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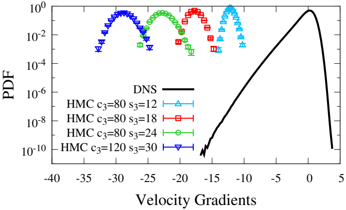

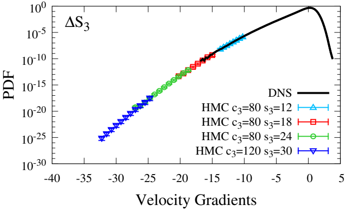

Figure : Velocity gradients PDF of HMC against DNS. We consider here only the lattice point on which the constraint $\Delta\mathrm{S}$ acted (i.e $x = 0$, $t = t_f$). The data of the HMC and the DNS were produced with the same computational cost.

Reweighting

We outstandingly increased the statistics of the left tail of the velocity gradients PDF, by systematically producing gradients as intense as 30-40 times the rms value

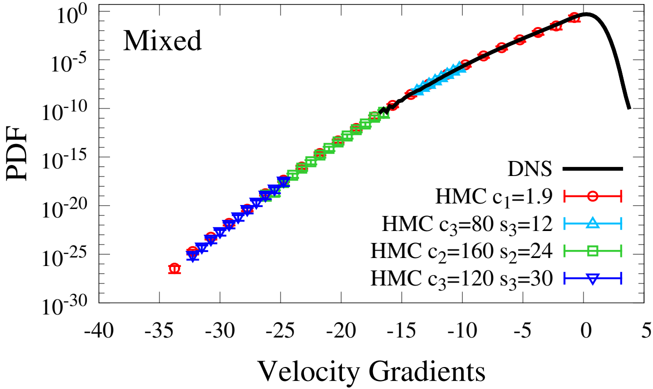

Figure : Velocity gradients PDF of HMC against DNS. We consider here only the lattice point on which the constraint ΔS acted (i.e $x = 0$, $t = t_f$). The data of the HMC and the DNS were produced with the same computational cost.

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:

$$u_t + uu_x - \nu u_{xx} = -i \int \Gamma(x - x')\, p(x', t) dx'$$

$$p_t + up_x + \nu p_{xx} = 4i\nu^2 \lambda \delta(t) \delta'(x)$$

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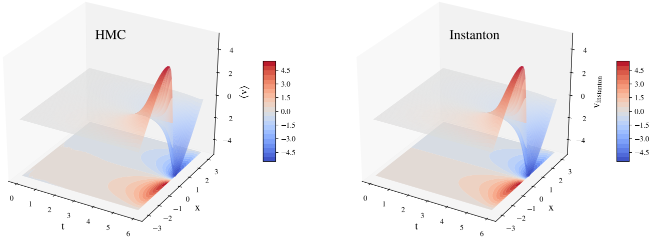

Figure : *Left plot:* Ensemble average of velocity configurations of the HMC using ΔS_1 with $c_1 = 1.9$. *Right plot:* Instanton velocity field profile for $\lambda = -1.148$ and $\alpha = -24.23$. It is clear that by averaging the ensemble of the HMC we remove the fluctuations around the instanton, restoring its spatio-temporal shape.

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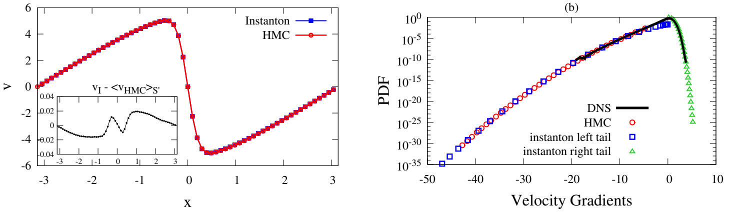

Figure : *Left plot:* Ensemble average of velocity configurations of the HMC using ΔS_1 with $c_1 = 1.9$. versus the instanton velocity field profile generated for $\lambda = -1.148$ and $\alpha = -24.23$. *Right plot:* Velocity gradients PDF of the instanton for a range of λ and α, against the HMC and the DNS.

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).

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!

12th European Fluid Mechanics Conference

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