Functional Integral for SPDEs

The what, why, and how

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“Two hundred thousand dollars is a lot of money.
We’re gonna have to earn it.”

– Blondie
The Good, the Bad and the Ugly

The statistical dynamics of nonlinear systems with a large number of degrees of freedom **far from equilibrium** poses a severe challenge to theory.

Perhaps one of the most pressing problems in this domain concerns the phenomenon of **intermittency** and the experimental observation of **universal scaling of small-scale fluctuations** in turbulent fluid motion.

[. . .] *“the most important unsolved problem of classical physics.”*

– Richard Feynman

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– Richard Feynman

"I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic."

– Horace Lamb

So, what are we talking about?

We will be concerned with the statistical properties of the **random-noise-driven one-dimensional Burgers' equation**

$$\partial_t u = -u\partial_x u + \nu\partial_x^2 u + f, \quad x \in [0, 2\pi],\ t \geq 0,$$

where ν is the kinematic viscosity, the real-valued velocity field $u(t, \cdot)$ takes values in the function space $L^2([0, 2\pi], \mathbb{R})$, and f denotes a noise term, which is a centered, distribution-valued Gaussian random field, i.e.,

$$\overline{f(x, s)f(y, t)} = \kappa(x - y)\delta(s - t).$$

The overbar denotes the random noise ensemble average, and we employ the following boundary and initial conditions

$$\begin{cases} u(t, x = 2\pi) = u(t, x = 0), & t \geq 0, \\ u(t = 0, x) = u_0(x), & x \in [0, 2\pi]. \end{cases}$$

Originally, the one-dimensional Burgers' equation was proposed as a simple model for **hydrodynamic turbulence**, which is widely *believed* to be governed by the **incompressible Navier-Stokes equations**

$$\begin{aligned} \partial_t u &= -(u \cdot \nabla_x)u + \nu \Delta_x u - \nabla_x p, \\ \nabla_x u &= 0, \quad t \geq 0. \end{aligned}$$

The vector field $u(t, \cdot)$ denotes the velocity of the fluid and takes values in $L^2([0, 2\pi]^d, \mathbb{R}^d)$, while the scalar field p denotes the pressure. Note that within the class of 2π-periodic functions the latter can easily be eliminated by solving the Poisson equation

$$\nabla_x \cdot ((u \cdot \nabla_x)u) = -\Delta_x p.$$

The presence of the same type of advective nonlinearity and dissipation as encountered in Navier-Stokes equations makes **Burgers' equation a unique testbed for new numerical and theoretical approaches** to the "problem of turbulence", even if it lacks some important features as, e.g., vorticity stretching or incompressibility.

Essentially, it describes the dynamics of excitations in a compressible medium without pressure (i.e., acoustic flow).

However, Burgers' equation has also found **manifold applications beyond its original conception in hydrodynamics**, e.g., in regards to

- structure formation in the early universe
  [Shandarin *et al.* 1989, Gurbatov *et al.* 1989 & Vergassola *et al.* 1994]
- the dynamics of vortex lines in high-temperature superconductors
  [Blatter *et al.* 1994]
- charge-density waves in an impurity potential
  [Feigelman 1980]
- dynamics of traffic congestion
  [Helbig 2001]

. . .

Most notably, in the potential form $u = -\partial_x h$, Burgers' equation is equivalent to the **Kardar-Parisi-Zhang (KPZ) equation**

$$\partial_t h = \frac{\lambda}{2}(\partial_x h)^2 + \nu \partial_x^2 h + \eta,$$

with $\lambda = 1$ and $\eta = -\partial_x f$, which (apart from other things) describes the kinetic roughening of growing interfaces.

[Kardar *et al.* 1986]

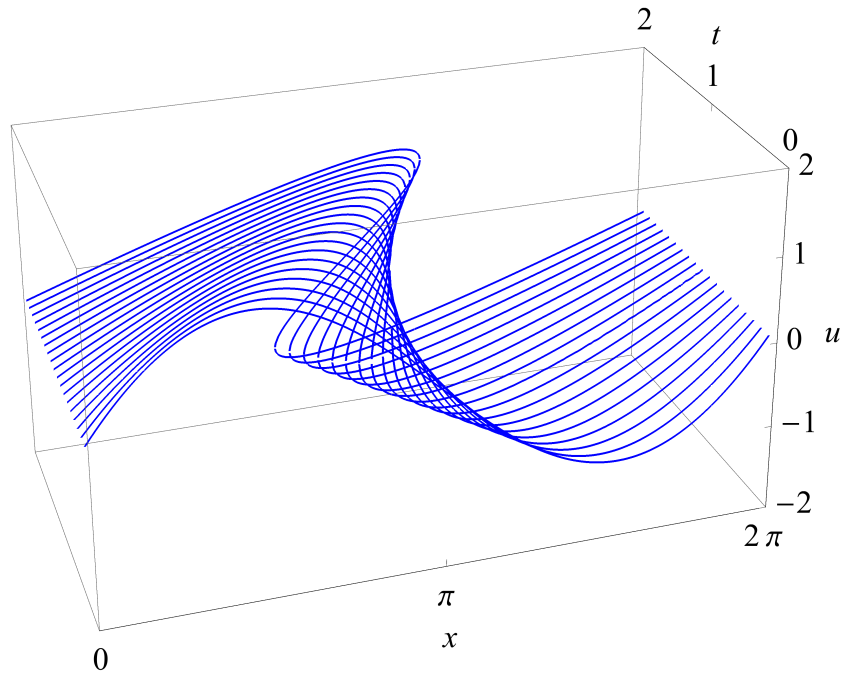
In the absence of random noise, the **inviscid Burgers' equation** ($\nu = 0$) can be written in the form of a conservation equation, i.e.,

$$\partial_t u + \frac{1}{2}\partial_x u^2 = 0.$$

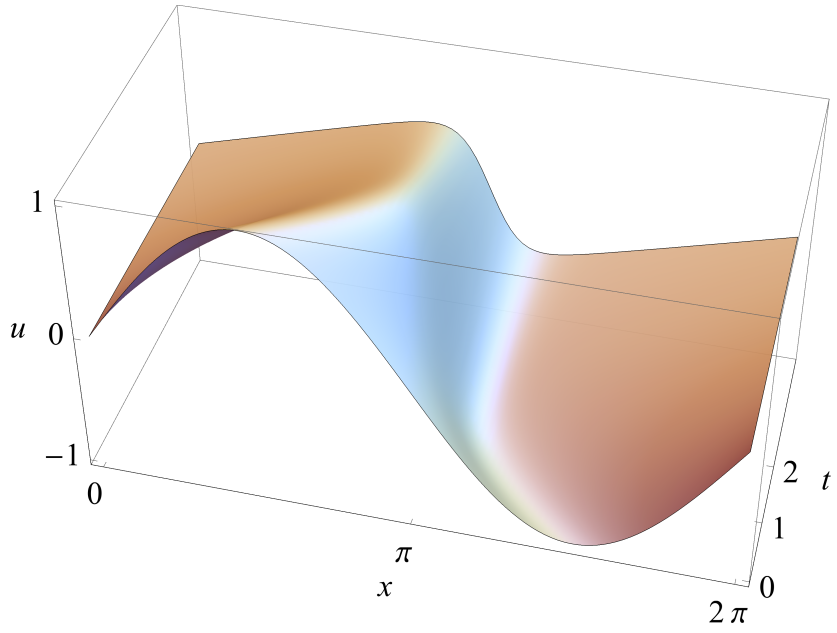
It admits solutions only in the weak sense, which are not unique – an additional entropy criterion needs to be invoked to resolve this ambiguity.

[Lax 1954]

Nevertheless, the nature of these solutions are well-known and are simply characterized. They correspond to **traveling shock waves** with a finite jump discontinuity.



On the other hand, in the presence of viscosity any shock wave discontinuity is smeared out over a finite (nonzero) dissipative width and it can be shown that a unique solution always exists.



The statistical properties of these shock wave solutions (with random initial conditions), e.g., their strength and spatial distribution, as well as the associated energy spectrum, are known exactly in the limit of large Reynolds numbers (Re $\propto \nu^{-1} \to \infty$).

[Tatsumi *et al.* 1972, Kida 1979, She *et al.* 1992,
Gotoh *et al.* 1993, Gotoh 1994& Avellanda *et al.* 1995]

With **spatially correlated noise** Burgers' equation displays a **complex interplay of coherent structures and random fluctuations** (*stationary state when energy input and dissipation are balanced*).

We assume white-in-time random noise with spatial correlations $\kappa(x)$ that decay algebraically with a steep tail at large wavenumbers k, i.e.,

$$\kappa(k) = \int_{[0,2\pi]} \mathrm{d}x\, \kappa(x) e^{-ikx} = C_\alpha\, |k|^{-\alpha}, \quad \alpha > 0,$$

where C_α is a positive number, defined such that $\sum_{k\in\mathbb{Z}} \kappa(k) = \text{const}$. The choice of a nonanalytic power-law forcing allows us to compare different scenarios

$$\kappa(x) \propto \begin{cases} \delta(x), & \alpha \to 0^+, \quad \textit{UV dominated} \\ 1 + a_{\mathrm{II}}\, |x|^{\alpha-1}, & 0 < \alpha < 1, \\ 1 - a_{\mathrm{III}}\, \ln|x|, & \alpha = 1, \\ 1 - a_{\mathrm{IV}}\, |x|^{\alpha-1}, & 1 < \alpha < 3, \\ 1 - a_{\mathrm{V}}\, |x|^2, & \alpha \geq 3, \quad \textit{IR dominated} \end{cases}$$

where only the leading order contributions for small separations $|x| \ll 1$ are shown and the coefficients a_i are all real and positive.

When the stochastic forcing is IR dominated ($\alpha \geq 3$) and the viscosity is small $\nu \to 0$, we observe a **separation of scales**. In the intermediate region of wavenumbers (**inertial range**), one expects *universal* statistics of the velocity field (gradients, field differences etc.), similar to the phenomenology of Navier-Stokes turbulence.

Taming the zoo of hydrodynamic models:

I & II The kinetic energy spectrum is given by

$$\overline{|u(k)|^2} \propto |k|^{-(1+2/3\alpha)},$$

while moments of velocity differences for $\alpha = 1/2$ behave as

$$\overline{|u(x+r) - u(x)|^q} \propto |r|^{\zeta_q}, \quad r \ll 1,$$

with $\zeta_q \approx 0.87$ for $q = 6, 8$ and somewhat lower for $q = 4$ [Hayot *et al.* 1997]. Another study found $\zeta_{q=4} \approx 0.65$, $\zeta_{q=6} \approx 0.47$, $\zeta_{q=8} \approx 0.20$ [Verma 2000]. Theoretically it is predicted: $\zeta_q = \min\left(1, (\alpha/3)q\right)$.

III **Kolmogorov energy spectrum**

$$\overline{|u(k)|^2} \propto |k|^{-5/3}.$$

The moments of velocity differences were found to scale with exponents $\zeta_q \approx 0.9$ for $q = 4, 6, 8$ [Chekhlov *et al.* 1995 & Yakhot *et al.* 1996], which lie close to the theoretical prediction $\zeta_q = \min(1, q/3)$.

IV Studied by [Boldyrev 1996], though no conclusive results for moments of field differences.

V The scaling spectrum of moments of velocity differences is theoretically predicted to be $\zeta_q = \min(1, q)$, while **different predictions for probability distribution function** of velocity gradients and field differences [Polyakov 1995, E *et al.* 1997].

Functional integrals for SPDEs: Why should you care?

While theoretical predictions seem to be clear (with the exception of the velocity statistics in the case of the IR dominated forcing, with exponent $\alpha \geq 3$) numerics still yield conflicting results.

This is largely due to **poor statistics**, which is relevant in particular for **high-order moments**, e.g., $|u(x+r) - u(x)|^q$, with $q \gg 1$.

Furthermore, most intriguing theoretical results suggests the relevance of **instantons** (optimal fluctuations) for these observables.

[Polyakov 1995]

Computationally it seems prohibitive to test this result via direct simulations. *Alternatives?*

In the functional integral representation of classical statistical dynamics observables are expressed in terms of an **average over field space-time histories** of the velocity field.

But, in contrast to direct numerical simulations such an approach is, to put it mildly, challenging. Monte Carlo techniques – so far – have not found many applications beyond single- and few-particle stochastic Langevin dynamics.

Nevertheless, importance sampling strategies provide a significant advantage with respect to DNS, as they may **selectively sample space-time field configurations** in distant corners of the phase space that are **(practically) not accessible by other numerical methods**.

Apart from fundamental questions related to the appropriate lattice regularization of the underlying dynamics and the choice of boundary conditions, a crucial question one needs to address in this framework, is that of *practicability*, i.e., the computational cost to generate a statistically independent field configurations.

OK, fine. How do we proceed?

The real-valued field $u = \{u(X)\}_{X\in\Lambda}$ is defined on the sites of a **regular space-time lattice** Λ; $X = (x, t)$ denotes the space-time coordinates. The field u is subject to centered, Gaussian-distributed random noise $f = \{f(X)\}_{X\in\Lambda}$, which acts at lattice sites X.

We may *naively* **approximate the continuum equation of motion** by

$$D_t^{(\varepsilon,1)} u = -uD_x^{(a,1)} u + \nu D_x^{(a,2)} u + f,$$

where $D_t^{(\varepsilon,1)}$, $D_x^{(a,1)}$, and $D_x^{(a,2)}$ correspond to finite-difference approximations of the continuum temporal/spatial derivatives; ε and a are the lattice spacing in the temporal and spatial direction, respectively.

Note that the chosen approximation is *not* guaranteed to converge to the right solution in the limit $a \to 0$. This is a rather subtle issue in the case of SPDEs ...

For the following considerations it is useful to introduce the short-hand notation

$$L(u) = D_t^{(\varepsilon,1)} u + uD_x^{(a,1)} u - \nu D_x^{(a,2)} u,$$

which defines a map $L : u \mapsto L(u)$ between vector spaces.

We assume that that the random field f has **nonvanishing support only on a subset of wavenumbers** (adapted to many problems of interest), which we will refer to collectively by the index A, i.e., $f = f_A$. We denote the complement set to A by $B = A^{\mathrm{c}}$, and therefore $f_B = 0$.

Similarly, it is useful to separate the dynamical field u into two distinct contributions

$$u = u_A + u_B.$$

The **derivation of the functional integral** starts from the the following identity

$$1 = \int [\mathrm{d}u]\, \overline{\delta[u - u_f]} = \prod_{X \in \Lambda} \int_{\mathbb{R}} \mathrm{d}u(X)\, \overline{\delta(u(X) - u_f(X))},$$

which is akin to the **BRS procedure** in QFT.

Here, u_f corresponds to a *particular solution* of the stochastic dynamics for a given realization f of the stochastic process and satisfies the following initial and boundary conditions:

$$u_f(x, t = 0) = 0, \quad u_f(x = 2\pi, t) = u_f(x = 0, t).$$

We *assume* that u_f exists and furthermore that it is unique.

We calculate ensemble averages of the observable $\mathcal{O}(u = u_f)$ by averaging over the random noise f:

$$\overline{\mathcal{O}(u_f)} = \int [\mathrm{d}u]\, \mathcal{O}(u)\, \overline{\delta[u - u_f]} = \int [\mathrm{d}u]\, \mathcal{O}(u)\, p[u],$$

where *formally*

$$p[u] = \overline{\delta[u - u_f]},$$

defines the **probability distribution functional (PDF)** for the velocity field.

While this provides a concise expression, it is actually of zero use in practice – it still involves the full solution u_f to the equation of motion.

We perform a change of variables $u \to L(u)$ and employ the relation

$$\delta[u - u_f] = \mathcal{J}(u)\delta\left[L(u) - f\right],$$

where $\mathcal{J}(u) = |\det(\delta L(u)/\delta u)|$ is the Jacobian associated with this change of variables.

The δ-functional admits a functional integral representation

$$\delta\left[L(u)-f\right] = \int [\mathrm{d}\lambda]\, e^{i\langle L(u)-f,\,\lambda\rangle},$$

where λ appears as a Lagrange multiplier field, which implements the SPDE "constraint" $L(u)-f=0$, and $\langle f, g\rangle \equiv \sum_{X\in\Lambda} f(X)g(X)$.

Performing a change of variables $\lambda \mapsto -i\lambda$, decomposing λ and $L(u)$ into orthogonal components (on the set of wavenumbers A and B), and putting all pieces together, arrive at the following representation of the velocity field PDF:

$$p[u] = \mathcal{J}(u) \int [\mathrm{d}\lambda_B]\, e^{\langle L_B(u),\lambda_B\rangle} \int [\mathrm{d}\lambda_A]\, \overline{e^{\langle L_A(u)-f_A,\lambda_A\rangle}} = \int [\mathrm{d}\lambda_B]\, e^{-S[u,\lambda_B]},$$

$$S[u,\lambda_B] = \frac{1}{2}\left\langle L_A(u), \left(\kappa_A^{-1}\circ L_A\right)(u)\right\rangle - \left\langle \lambda_B, L_B(u)\right\rangle - \ln \mathcal{J}(u).$$

For our purposes (power-law correlated random noise acting at all wavenumbers, i.e., $B = \emptyset$) the action reduces to the following form

$$S = \frac{1}{2}\left\langle L_A(u), \left(\kappa_A^{-1} \circ L_A\right)(u)\right\rangle - \cancel{\left\langle \lambda_B, L_B(u)\right\rangle} - \cancel{\ln \mathcal{J}(u)},$$

where in the following we assume that the stochastic forcing is power-law correlated with $\kappa_A(k) \propto |k|^{-3}$, with $\kappa_A(k=0) = 0$

The functional determinant is field independent (i.e., $\mathcal{J}(u) \propto 1$) if an explicit-time discretization is used (with a forward-time difference operator $D_t^{(\varepsilon,1)}$). For implicit time discretizations however, it *cannot* be discarded.

Classical-statistical action is *highly nonlocal* in space due to κ_A.

In earlier work we employed an overrelaxation algorithm (with $\kappa_A(k) \propto |k|^{-1}$ that yields a Kolmogorov energy spectrum), which samples the velocity field via successive local (in space-time) updates of the velocity field at successive space-time points.

Here, we propose another approach for this problem – a **Hybrid Monte Carlo (HMC)** algorithm, which makes large steps in configuration space and therefore reduces autocorrelation times.

Our aim is to construct an **improved sampling around optimal fluctuations** (giving the dominant contribution to high-order moments of field differences and gradients).

But first a systematic study of the sampling dynamics, boundary conditions, and stability criteria is crucial . . .

→ *Cross-check with direct numerical methods!*

As with the standard HMC a fictitious Hamiltonian

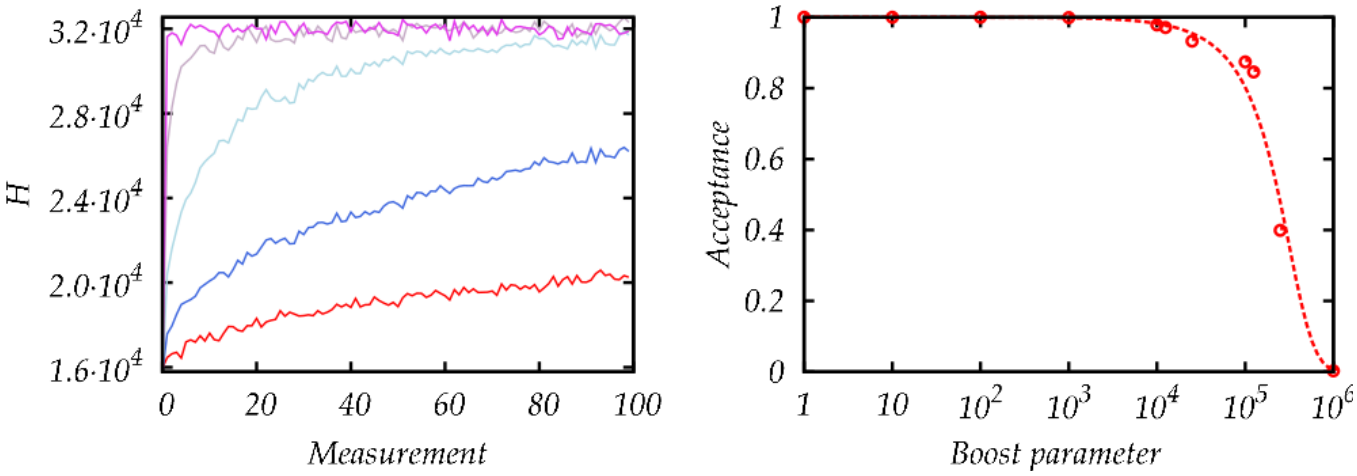
$$H = \frac{1}{2}\langle \pi, \Omega \circ \pi \rangle + S,$$

is introduced, which will be used to suggest new field configurations via the integration of Hamilton's equations of motion in fictitious time τ, i.e.,

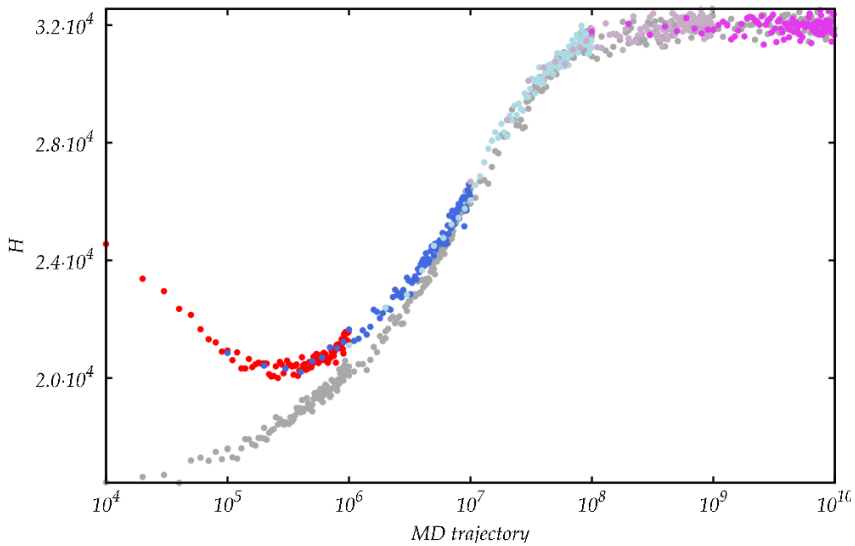
$$\dot{u} = \frac{\delta H}{\delta \pi} = \Omega \circ \pi, \quad \dot{\pi} = -\frac{\delta H}{\delta u} = -\frac{\delta S}{\delta u}.$$

An important modification to the standard kinetic term appears due to the nature of our action which is nonlocal. If $\Omega \propto 1$ highly inefficient update!

Tuning the wave-number dependence by hand we obtain an *order of magnitudes improvement*:



We confirm that the Monte Carlo dynamics (relaxation of the algorithm) is universal and reaches a unique fixed point, if started from different initial conditions:



We can do much better by **automated adaption of Ω to Molecular Dynamics forces**, which are measured in the relaxation stage of the HMC.

In practice we apply a **multi-stage Fourier acceleration** (multiple resets of Ω by measuring MD forces).

What about lattice discretization and boundary conditions?

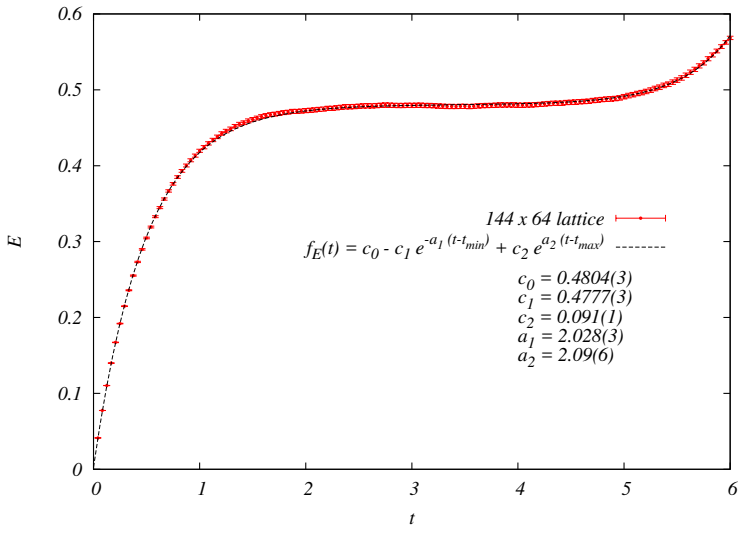
Due to a direct correspondence between the classical-statistical action and the classical (stochastic) equation of motion, different choices discretization schemes can be adapted and allows us to cross-check the HMC with other direct numerical methods.

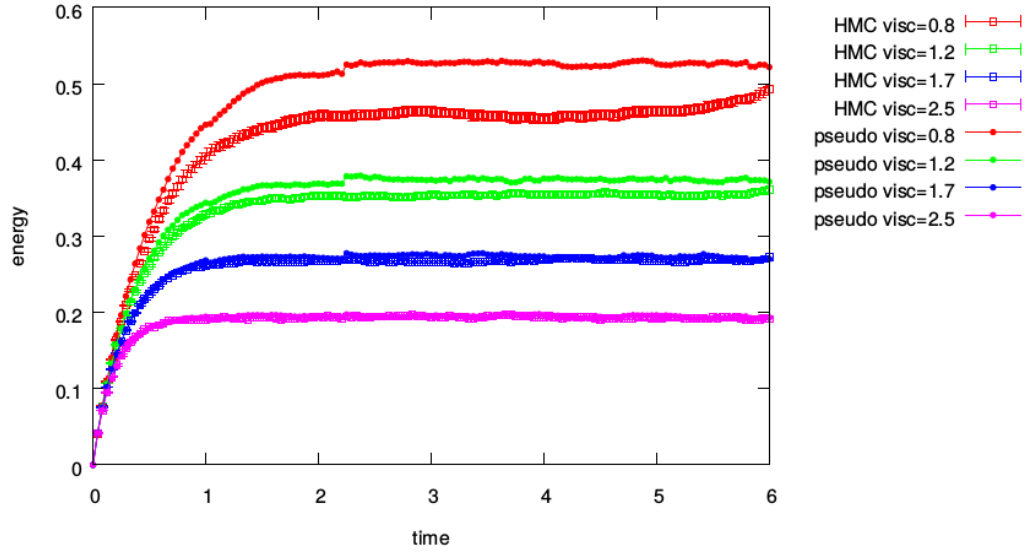
It is well-known that finite-difference approximations approximate the true solution of the random-force-driven Burgers' equation only poorly. **Pseudospectral methods** with **explicit Adams-Bashforth time-step integration** or **strongly-stable Runge-Kutta schemes** are typically used to solve the SPDE directly.

We capitalize on this knowledge from direct solvers and design corresponding *"improved actions"*.

Another issue that arises in the context of SPDEs is the time-step error, which is more difficult to control in the standard time-integration schemes(due to the necessity to evaluate multiple stochastic integrals). Typically only single-step explicit methods are used . . .

We benchmarking the HMC with a pseudospectral code using an explicit single-step Adams-Bashforth method. We compare the time-dependence (physical time) of the kinetic energy $E \propto \sum_k \overline{|u(k)|^2}$:



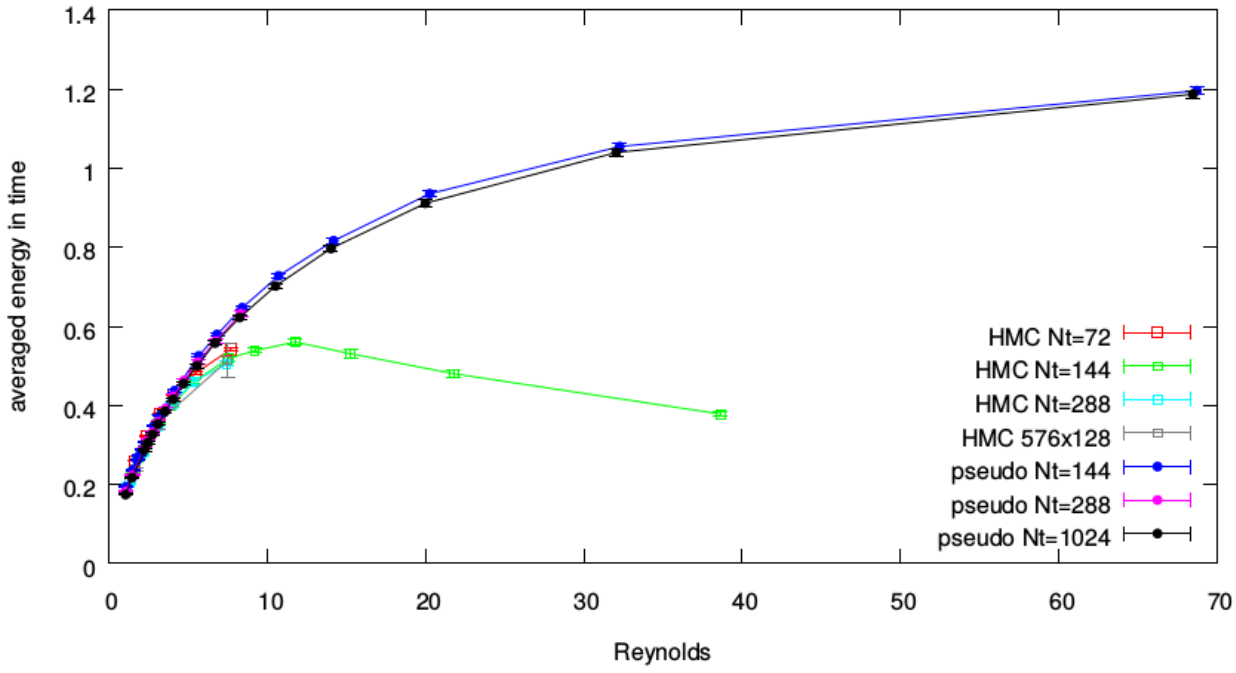


Choice of **open boundary conditions** at final time yields a **localized boundary mode**.

It would seem that this mode is unphysical, but remarkably a similar effect can be induced with direct numerical solvers using post-selection (sifting out space-time histories that feature a "blow up"). *Can we interpret the boundary mode as an indicator for finite-time blow up?*

In direct numerical simulations and Monte Carlo simulations this effect is more pronounced at smaller viscosity (i.e., Re $\gg$ 1).

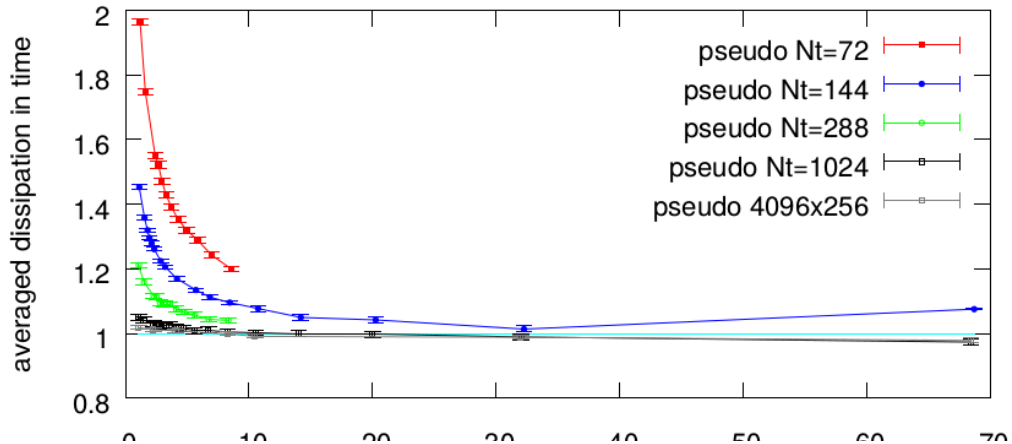
Towards the "physical point" ($\mathrm{Re} \to \infty$*)!*

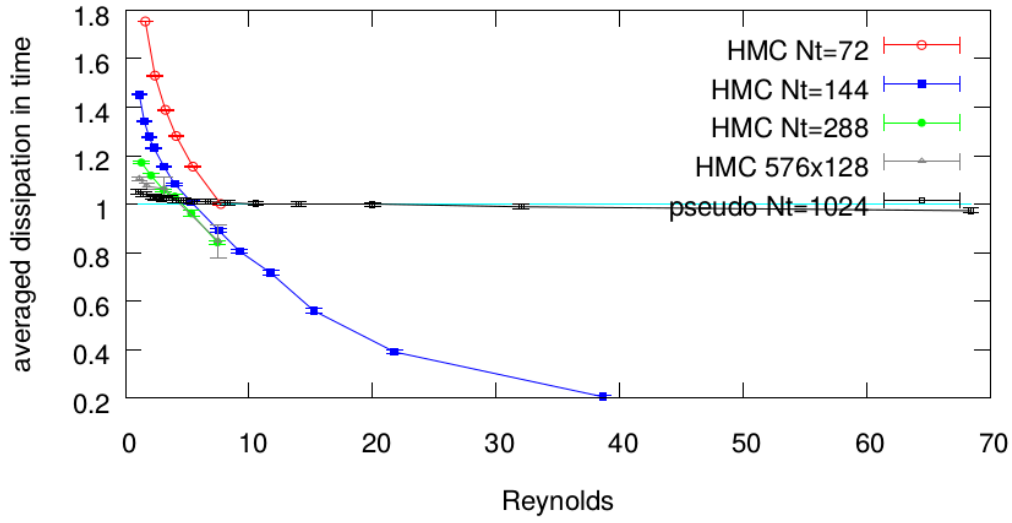


Results from the pseudospectral code and HMC start to diverge at a critical Reynolds number, but things are fine at small viscosity (high spatial resolution not required due to smoothing effect).

This problem is largely due to a limited spatial resolution, which leads to finite-time blow-up in standard integration schemes.

The same picture appears if we look at the average dissipation $\propto \nu \sum_k k^2 \overline{|u(k)|^2}$ in the ensemble:





Outlook

To conclude we can confirm . . . Turbulence is *still* hard!

Nevertheless, the functional integral approach to hydrodynamic turbulence holds quite a number of surprises for us. It provides us (and other practitioners in the field) with new and interesting insights, e.g., regarding viable lattice discretization schemes, on accessibility of the "physical region" of parameter space, etc.

But these are only first steps. Necessary groundwork, before addressing more challenging problems.

HMC sampling is on its way with targeted sampling of rare events currently being explored.
Stay tuned!