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Monte Carlo approach to turbulence*

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The behavior of the one-dimensional random-force-driven Burgers equation is investigated in the path integral formalism on a discrete space-time lattice. We show that by means of Monte Carlo methods one may evaluate observables, such as structure functions, as ensemble averages over different field realizations. The regularization of shock solutions to the zero-viscosity limit (Hopf-equation) eventually leads to constraints on lattice parameters required for the stability of the simulations. Insight into the formation of localized structures (shocks) and their dynamics is obtained.

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1. Introduction

Besides tremendous research having been done since Kolmogorov's famous publication in 1941 [1], hydrodynamic turbulence essentially remains an unsolved problem of modern physics. This is especially remarkable as the fundamentals seem to be fairly easy – the Navier-Stokes equations for the velocity field u_α and pressure p

$$\partial_t u_\alpha + u_\beta \partial_\beta u_\alpha - \nu \nabla^2 u_\alpha + \frac{1}{\rho} \partial_\alpha p = 0 \tag{1.1}$$

with the additional constraint

$$\partial_\alpha u_\alpha = 0 \tag{1.2}$$

simply express the conservation of momentum in a classical, incompressible fluid of viscosity ν and density ρ. For laminar flows it is well known that the Navier-Stokes equations reproduce realistic flows very accurately; in the turbulent regime, it is still an open question how the universal characteristics of turbulent flow, characterized by the scaling exponents ξ_p of structure functions S_p of order p, defined by

$$S_p(x) := \overline{|u(r+x) - u(r)|^p} \sim |x|^{\xi_p}, \tag{1.3}$$

can be extracted from first principles. Here the bar corresponds to a spatial averaging.

Monte Carlo simulations in the path integral formulation enable us to gain direct insight into the formation of localized structures and their behavior, and to measure observables as, e.g. structure functions and their scaling exponents [2 – 4].

2. Burgers' Equation

We decided to elaborate the methods using the stochastically forced Burgers equation [5] in 1+1 dimensions

$$\partial_t u + u \partial_x u - \nu \partial_x^2 u = f\,, \tag{2.1}$$

which may be interpreted as the flow equation for a fully compressible fluid. The stochastic force is modeled to be Gaussian with correlation

$$\chi(x,t;x',t') := \left\langle f(x,t) f(x',t') \right\rangle = \varepsilon\, \delta(t-t') \exp\left(-\frac{|x-x'|}{\Lambda} \right), \tag{2.2}$$

where Λ defines the correlation length of the forcing and the $\langle \cdots \rangle$ denotes the ensemble average. A finite viscosity ν and energy dissipation ε provide a dissipation length scale λ corresponding to the Kolmogorov-scale in Navier-Stokes turbulence:

$$\lambda := \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}}. \tag{2.3}$$

We can furthermore identify the Reynolds-number as

$$Re := (\varepsilon \Lambda^4 / \nu^3)^{1/3}. \tag{2.4}$$

The fundamental solutions to the Burgers equation are well-known – in the limit of vanishing viscosity (Hopf-equation) these form singular shocks. A finite dissipation scale $\lambda \sim \nu/U$, where U is the characteristic velocity, provides an UV-regularization of the shock structures:

$$u = -U \tanh \frac{U}{2\nu} x. \tag{2.5}$$

Most interestingly, the exponents ξ_p as defined in (1.3) are non-trivial for Burgers turbulence; for the forcing (2.2) and in the regime $x \sim \lambda$ we have the analytic result [6]

$$\xi_p = \min(1, p). \tag{2.6}$$

3. Path Integral Formulation

Following the method of Martin, Siggia and Rose [7], we established a path integral for Burgers' equation

$$Z \propto \int \mathscr{D}u \exp\left(-\frac{1}{2} \int dt dx \left(\partial_t u + u\partial_x u - \nu\partial_x^2 u\right) \chi^{-1} * \left(\partial_t u + u\partial_x u - \nu\partial_x^2 u\right) \right), \tag{3.1}$$

where $*$ denotes the convolution.

It has been shown by Falkovich et al. [8, 9] on the basis of an equivalent sum of states that the fundamental solutions of Burgulence can be understood as instantons.

4. Monte Carlo Simulations

For 1+1 dimensional Burgulence, a large number of stable simulations could be performed; we are working on the final analysis. Typical lattice sizes range from $(N_x = 16) \times (N_t = 16)$ up to $(N_x = 4096) \times (N_t = 128)$ lattice points.

4.1 Boundary Conditions

To be in general agreement with literature and analytic calculations, we started with lattices periodic both in time and space direction. In an attempt to reduce autocorrelation times, we dropped these boundary conditions. While autocorrelation times did not change much, simulating with free boundaries effectively doubles the spatial lattice extent and gives access to excitations of the Burgers vacuum state.

4.2 Lattice Discretization

Once having discretized the path integral on a Euclidean lattice of spacings Δx and Δt, we get for ν:

$$\nu = \alpha \frac{(\Delta x)^2}{\Delta t}. \tag{4.1}$$

The continuum limit of our lattice theory is reached by holding ν and Re constant while increasing the number of lattice sites. α is an a priori arbitrary constant that can be interpreted as a measure for Δt depending on Δx and also has to be kept fixed while performing the continuum limit.

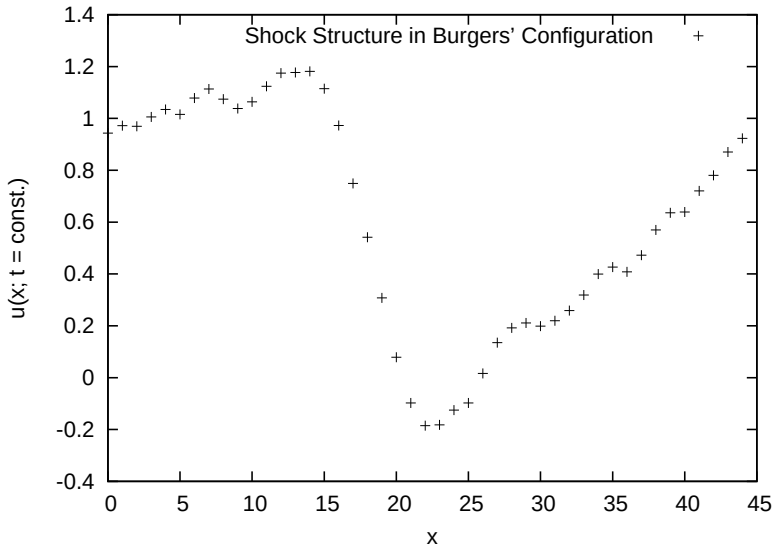

Figure 1: Time-slice of a $(N_x = 256) \times (N_t = 45)$-lattice at $Re = 4$, $\nu = 1/32$, showing the velocity $u(x,t = const)$ as a function of x. The typical shock structure is clearly visible.

4.3 Algorithms

We use a local heat bath algorithm with successive over-relaxation (SOR) for the Monte Carlo evaluation of the partition function [11]. The use of certain acceleration techniques with SOR, specifically Chebyshev acceleration [12], significantly accelerates the thermalization process.

Though suiting our purposes so far, it poses certain restrictions on parallelization. We therefore started employing a Hybrid Monte Carlo algorithm that we expect to scale better with the number of parallel processors.

4.4 Autocorrelation Times

With χ being a nonlocal operator one would expect long autocorrelation times in the simulation of stochastically forced differential equations. However, with the over-relaxed heat bath algorithm and an appropriate definition of structure functions on the lattice (where the reference point for evaluation is chosen randomly for each configuration) the integrated autocorrelation time is reduced to $\tau \sim O(1)$.

4.5 Resources

For testing purposes small lattices may easily be simulated on desktop PCs. However, high resolution simulations on large lattices require massively parallel architectures. We have run our simulations on the IBM p690 cluster JUMP at FZ Jülich and on the Linux cluster at Humboldt University Berlin with up to 256 processors in parallel. In July 2009 we continued our simulations on the new supercomputer JUROPA at FZ Jülich.

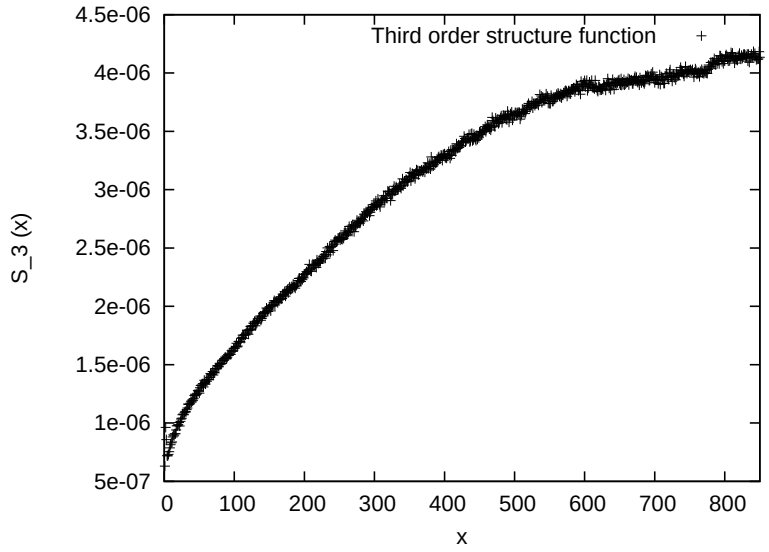

Figure 2: Third order structure function $S_3(x)$ as a function of space separation x.

5. First Results

First results include further constraints that have to be imposed in order to ensure stable numerics. Most constricting is the need to resolve the Kolmogorov-length scale λ on the lattice. We can in this way show the effect of λ as UV-regularization of the otherwise singular shocks. This translates into a relation for the Reynolds-number:

$$Re < \frac{\Lambda}{\Delta x}. \tag{5.1}$$

This will become crucial for Navier-Stokes turbulence enforcing us to simulate big lattices.

5.1 Structure Functions

From analytic calculations [6] we have

$$S_p(x) \sim C_p|x|^p + C'_p|x|, \tag{5.2}$$

for small seperations in the inertial range.

Though our results are in general agreement with this, the extraction of scaling exponents is far from trivial and very sensitive to statistical errors.

5.2 Extended Self-Similarity (ESS)

Rather than measuring the scaling exponents ξ_p directly, there have been attempts to measure the scaling behavior of ratios of structure functions [10]. It was shown that this greatly enhances

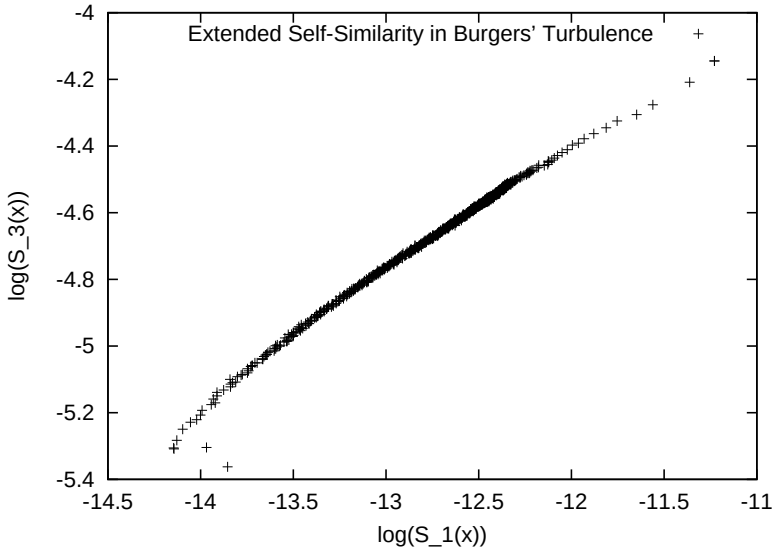

Figure 3: $\log[S_3(x)]$ as function of $\log[S_1(x)]$ clearly showing the linear ESS-dependence.

the inertial range not only at high but also moderate Reynolds numbers. However, we must stress that up to now it is not clear if there are any systematic effects in the evaluation of the structure function exponents via ESS.

5.3 Outlook

After completing the analysis of 1+1 dimensional Burgulence, we will proceed to 3+1 dimensions. The ultimate challenge will be the simulation and analysis of 2+1 and 3+1 dimensional Navier-Stokes turbulence.

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