Lattice Monte Carlo methods for systems far from equilibrium

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Universality and anomalous scaling far from equilibrium

Systems out-of-equilibrium displaying scaling phenomena are typically characterized by constant flux conditions

$\rightarrow$ Strong nonlocal interactions transfer excitations from the injection to the damping scale

Nonperturbative approach to determine the universal scaling properties in the strongly-correlated inertial regime

Lattice Monte Carlo methods via MSR/Schwinger-Keldysh action

Generally applicable to systems where classical-statistical fluctuations dominate the dynamics

A simple model – Burgers' equation

One-dimensional hydrodynamic turbulence without pressure

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

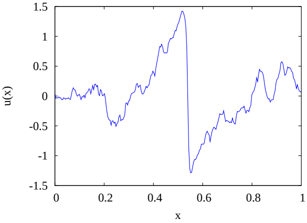
System driven by a (non-analytic) self-similar forcing that is white in time

$$\langle f(k,t) f(k',t') \rangle = \Gamma(k,t;k',t')$$
$$\Gamma(k,t;k',t') \propto |k|^{-y} \delta(k+k') \delta(t-t')$$

$\exists$ nonequilibrium steady state with constant energy flux in the inertial range

$\rightarrow$ Kolmogorov energy spectrum ($y = 1$)

Physical picture: shocks with finite dissipative width



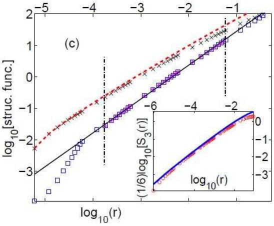
Scaling spectrum and anomalous scaling

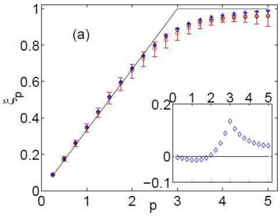
In the limit $\nu \to 0^+$ a fast Legendre transform algorithm for the velocity potential ($u = -\partial_x \psi$) is applicable:

$$\psi(x,t) = \max_y \left[\psi(y,t') - \frac{(x-y)^2}{2(t-t')} \right], \quad t > t'$$

Noullez & Vergassola, J. Sci. Comp. **9**, 259 (1994)

$\boldsymbol{y = 1}$:





Mitra, Bec, Pandit & Frisch, Phys. Rev. Lett. **94**, 194501 (2005)

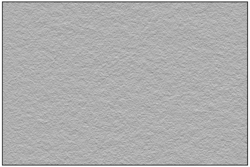
Useful benchmark to test new analytical and numerical methods

From equilibrium to nonequilibrium

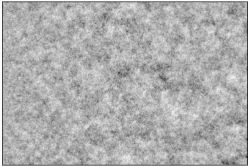
$y = -2$: thermal noise (KPZ class) $\to$ perturbative UV dominated regime

$0 < y < 3$: system is strongly driven at all scales $\to$ complex interplay nearly Gaussian background and coherent structures

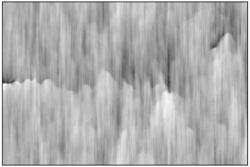
$y > 3$: large-scale forcing dominated regime (universality)



$y = -2$
UV dominated



$y = 0$
Intermediate regime



$y = 2$
Strong scaling

Lattice MC via MSR/Janssen-de Dominicis functional integral

Martin-Siggia-Rose (MSR) action

$$S = \frac{1}{2}(\mu, \Gamma * \mu) - i(\mu, \chi(u))$$

Martin, Siggia & Rose, Phys. Rev. A**8**, 423 (1973)
Janssen, Z. Phys. B**23**, 377 (1976)
de Dominicis, J. Phys. Colloques **37**, 247 (1976)

$\chi(u) \equiv \partial_t u + u\partial_x u - \nu\partial_x^2 u$ and force spectrum Γ completely characterize the dynamics of the theory

Itō prescription (i.e. pre-point/backward-time discretization)

$$-i(\mu, \chi(u)) \;\rightarrow\; -i\epsilon \sum_n (\mu_n, \chi_n(u)) = -i\epsilon \sum_n \left(\mu_n, \frac{1}{\epsilon}(u_n - u_{n-1}) + f(u_{n-1})\right)$$

$\rightarrow$ Check if discretized dynamics admits globally regular solutions!

Lattice action

$u(x,t)$ is defined on a regular space-time lattice

$\rightarrow$ UV cutoff eliminates details of processes in the dissipative regime

Lattice action

$$S = \frac{1}{2}\left(\chi(u), \Gamma^{-1} * \chi(u)\right)$$

and $\chi(u)$ defined in terms of the finite-difference equation with backward-time discretization:

$$\partial_t u + u\partial_x u \;\rightarrow\; \frac{1}{\epsilon}(u_n - u_{n-1}) + \frac{1}{2}\partial_x u_{n-1}^2$$

May discretize nonlinear advection and viscous terms any way we like (provided correct continuum limit and globally regular solutions)

$\rightarrow$ Improved algorithms, e.g., local overrelaxation algorithm with Chebyshev acceleration (for multiquadratic actions)

Mesterházy & Jansen, New. J. Phys. **13**, 103028 (2011)

Quasi-local HMC with adaptive FACC

Quasi-local HMC with even-odd updating in physical time

Periodic boundary conditions in spatial direction and initial condition in time (free boundary at final time)

MD Hamiltonian

$$H = \frac{1}{2}\,(\pi, \Omega * \pi) + \frac{1}{2}\,\big(\chi(u), \Gamma^{-1} * \chi(u)\big)$$

Typical choices for the force spectrum Γ^{-1} will strongly emphasize high-momentum modes and lead to large fluctuations in the HMC force spectrum

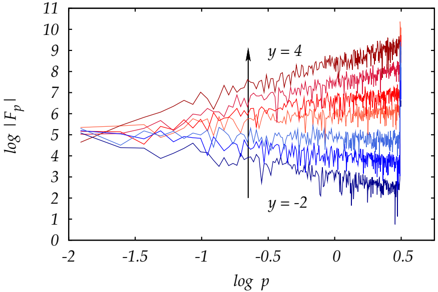
Need to stabilize the simulation by adapting the stepsizes via Ω (Fourier acceleration)

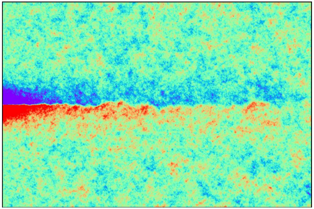
Iterative procedure, $\Omega_i = \Omega(u_i)$ and held fixed during the MD and final accept/reject step

$$u_j \leftarrowtail \Omega_i \pi_i \ , \quad \pi_j \leftarrowtail -\frac{1}{\epsilon}\Gamma^{-1} * \chi(u_i)$$

Performance of Quasi-local HMC

HMC force spectrum $\|F_p\|$ evaluated for fixed time in a single configuration (512×1024 space-time lattice, with $-2 < y < 4$):





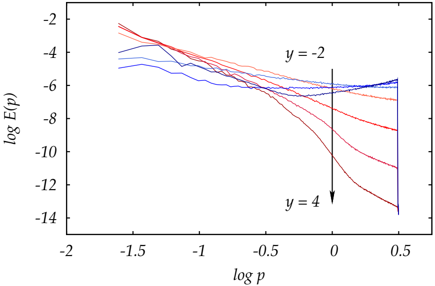
HMC with nontrivial initial conditions
(512×1024 lattice, $\boldsymbol{y = 0}$)

QL-HMC update dynamics

Start movie

Transition to large-scale forcing dominated regime

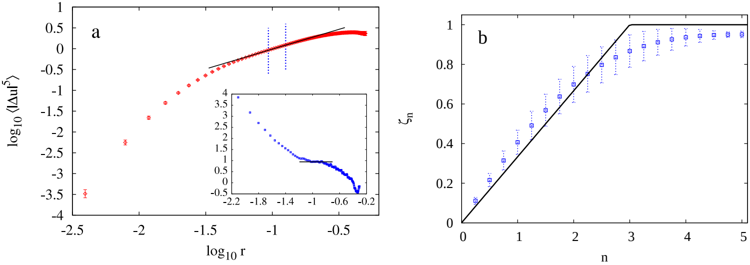
Energy spectrum $E(p)$ evaluated on a small sample of configurations (512×1024 lattice, with $-2 < y < 4$):



Transition roughly at $\boldsymbol{y \simeq 3}$ – high-momentum modes effectively decouple from forcing mechanism

Structure functions and scaling behavior

$\boldsymbol{y = 1}$:



a log-log plot of the structure function of order $n = 5$ with a linear scaling function plotted for comparison

b scaling exponents ζ_n versus order n

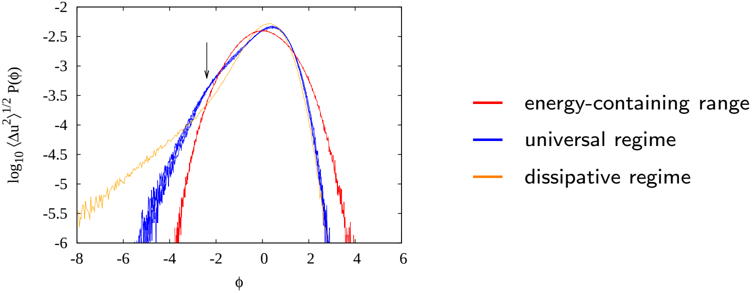
Mesterházy & Jansen, New. J. Phys. **13**, 103028 (2011)

Subtle interplay between leading and subleading scaling contributions

High-order moments require large sample-size ($\boldsymbol{y \neq 1}$ in preparation) . . .

Probability distribution functions

Probability distribution functions $\mathcal{P}(\Delta u, r)$ as a function of the dimensionless variable $\phi = \Delta u / [\langle \Delta u^2 \rangle]^{1/2}$:



Universal scaling form

For $|\Delta u| \ll u_{rms}$ and $r \ll L$ the PDF of velocity differences has a universal scaling form

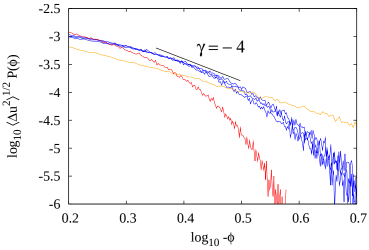
$$\mathcal{P}(\Delta u, r) = \frac{1}{r^z} f\left(\frac{\Delta u}{r^z}\right)$$

where z the dynamic exponent

In the asymptotic region $-\Delta u / r^z \gg 1$ where $\Delta u < 0$ we expect the algebraic scaling

$$\mathcal{P}(\Delta u, r) \sim (\Delta u)^\gamma$$

scaling region
for the left tail of the PDF:



Outlook

Lattice MC simulations as a unique approach to determine the universal scaling behavior, dynamic critical scaling, etc.

$\rightarrow$ Generally applicable to other systems of interest, e.g., Navier Stokes

Improved actions (unconditional stability)? Constraints on lattice geometry to reach the stationary regime? Possible initial conditions (quenching)?

Statistics of extreme events on the attractor (instantons) $\rightarrow$ sample strong fluctuations that contribute to high order moments