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Singularities, Turbulence and Instantons

WPI Vienna, May 2015

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T. Grafke, R. Grauer, T. Schäfer
Instanton filtering for the stochastic Burgers equation
Journal of Physics A: Mathematical and Theoretical, 46 (2013) 62002

T. Grafke, R. Grauer, T. Schäfer, E. Vanden-Eijnden
Arclength parametrized Hamilton's equations for the calculation of instantons
SIAM: Multiscale Modeling and Simulation 12 (2014) 566

T. Grafke, R. Grauer, T. Schäfer, E. Vanden−Eijnden
Relevance of instantons in Burgers turbulence
European Physics Letters, 109 (2015) 34003

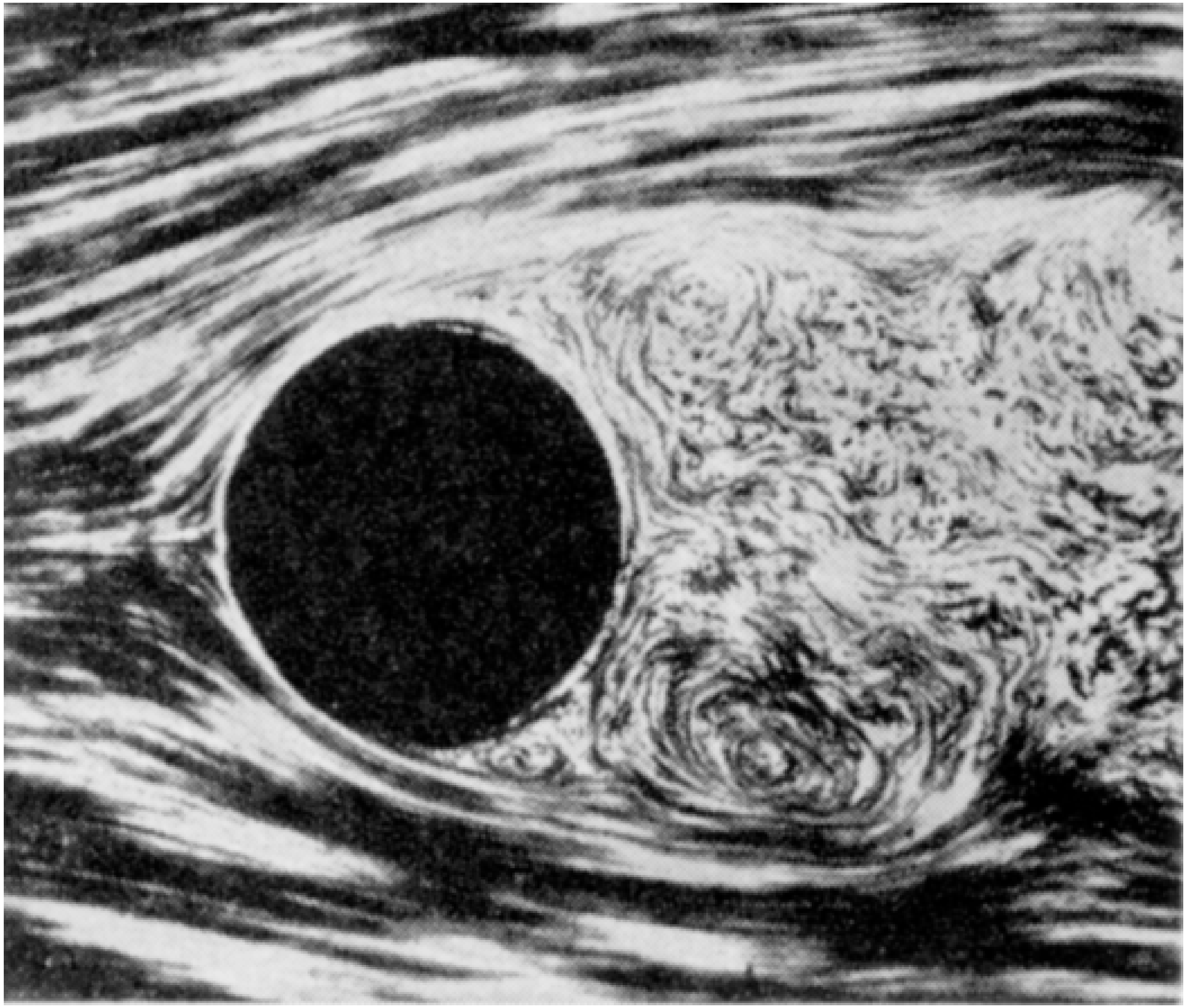
T. Grafke, R. Grauer, St. Schindel
Efficient Computation of Instantons for Multi−Dimensional Turbulent Flows with Large Scale Forcing
to appear in Communications in Computational Physics (2015)

T. Grafke, R. Grauer, T. Schäfer
The instanton method and its numerical implementation in fluid mechanics
under consideration (Topical Review)

Outline

- Turbulence and Singularities
- Martin-Siggia-Rose/Janssen/de Dominicis functional
- Instantons
  - Instanton calculus
  - Why are Instantons promising ? (Singularities and Turbulence)
  - Burgers turbulence
  - Gotoh puzzle
  - 2D/3D memory problem
  - 3D Navier-Stokes (Novikov) instanton
- What's next?
  - Adaptive Mesh Refinement
  - Fluctuations

K41



Flow around a cylinder at high Reynolds number (L. Prandtl)

degrees of freedom: $\approx R^{9/4} \approx 10^{15}$ (at $R = 10^7$)

Navier–Stokes–equations

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \nu \Delta \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0 \quad , \quad \text{boundary conditions}$$

Reynolds number: $R = UL/\nu$

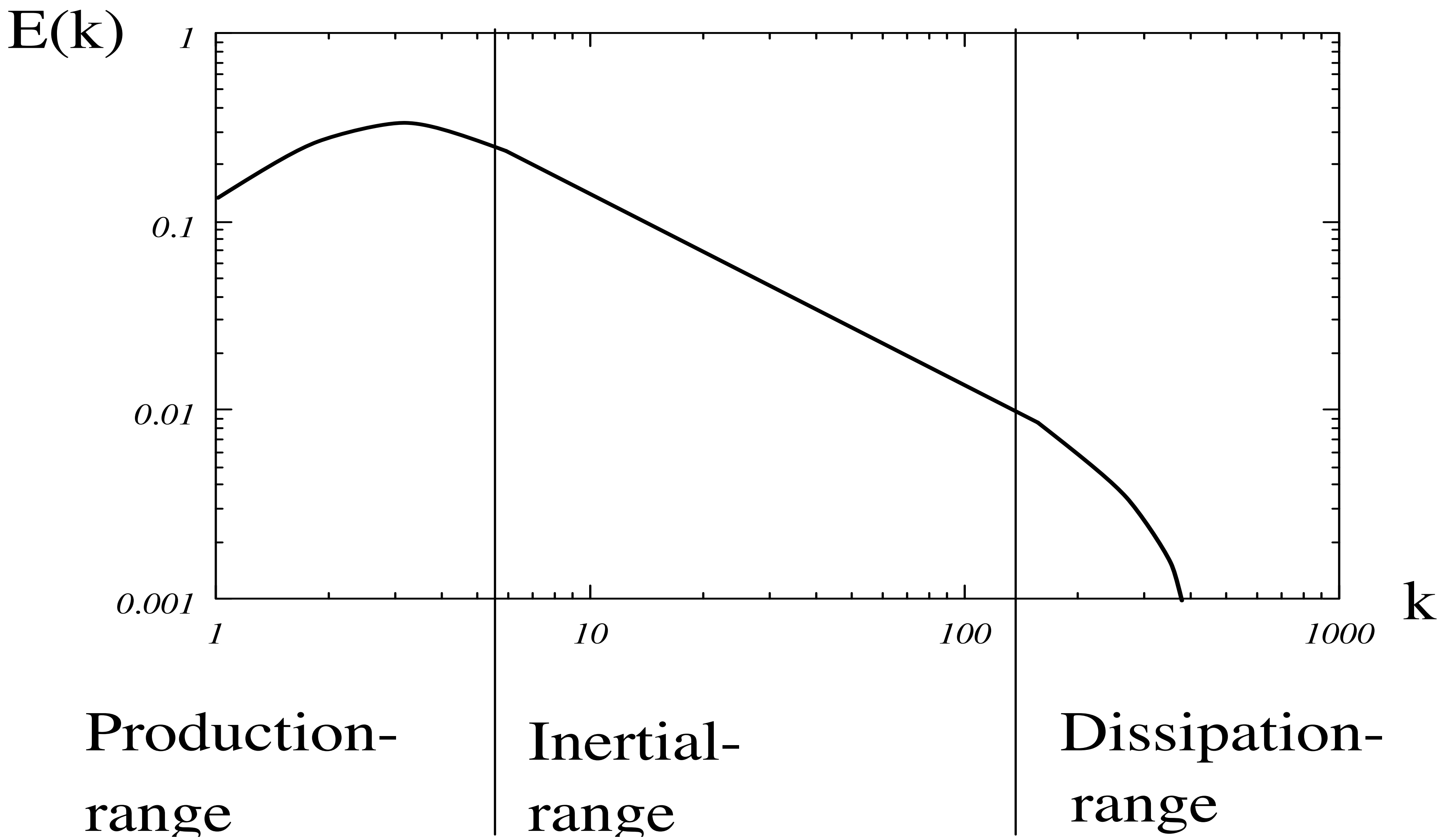
Energy dissipation:

$$\epsilon = \nu \int |\, \nabla \mathbf{u} \,|^2 \, d\Omega$$

independent of ν

$$\Longrightarrow \boldsymbol{\omega} = \nabla \times \mathbf{u} \longrightarrow \infty \quad \text{for} \quad \nu \longrightarrow 0$$

Energy spectra and structure functions



1. cascade
2. scaling–invariance: $(\nu = 0)$
   $\mathbf{r} \longrightarrow \lambda \mathbf{r}\ ,\ \mathbf{u} \longrightarrow \lambda^h \mathbf{u}\ ,\ t \longrightarrow \lambda^{1-h} t$
3. local transfer

ϵ does not depend on the scale: $\Rightarrow$ $\boxed{h = 1/3}$

Structure functions:

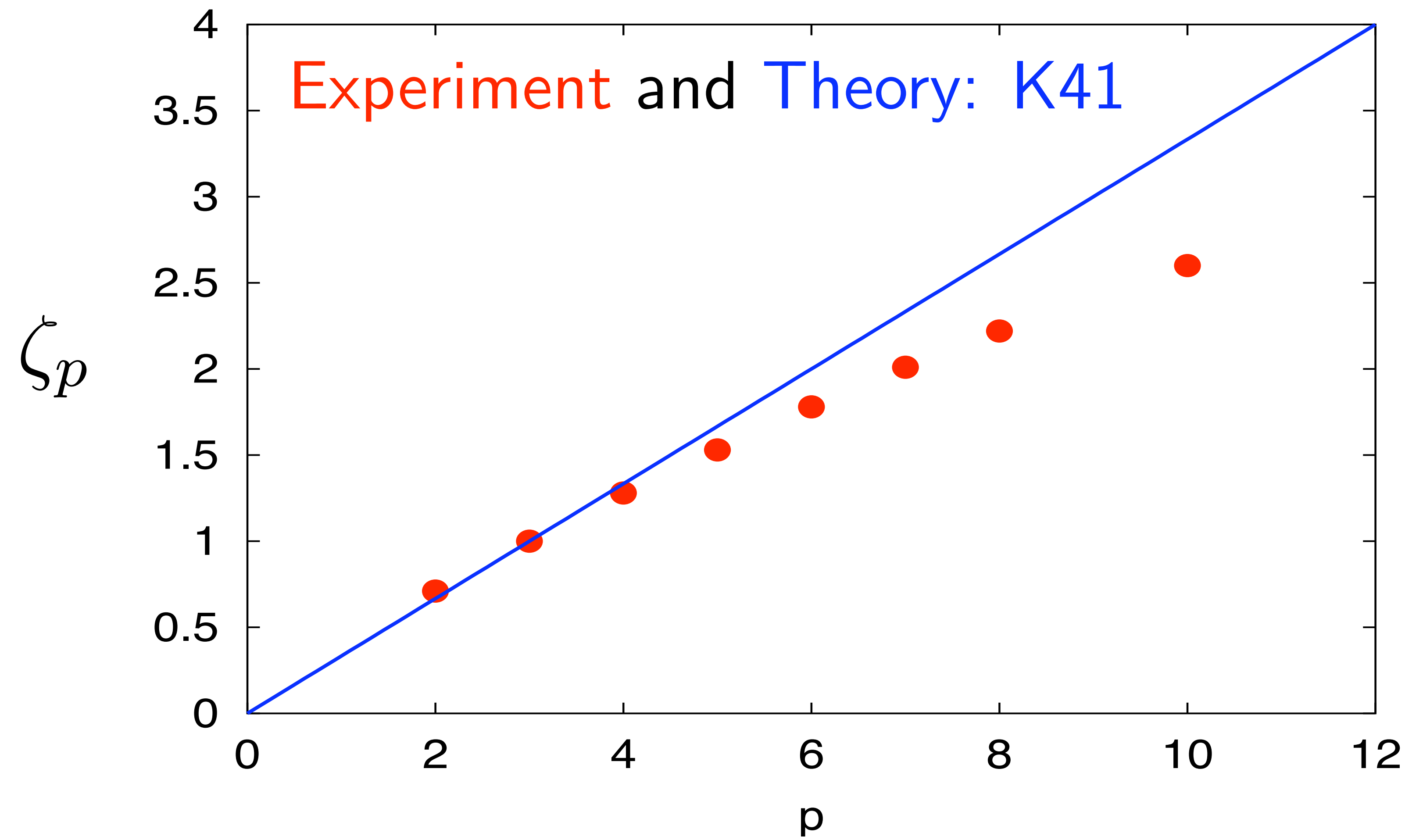
$$<|\, \mathbf{u}(\mathbf{r}+\mathbf{l}) - \mathbf{u}(\mathbf{r})\, |^p> \propto \; l^{\,\zeta_p} \qquad \zeta_p = \frac{p}{3}$$

Fourier transformation for $p = 2 \Rightarrow$

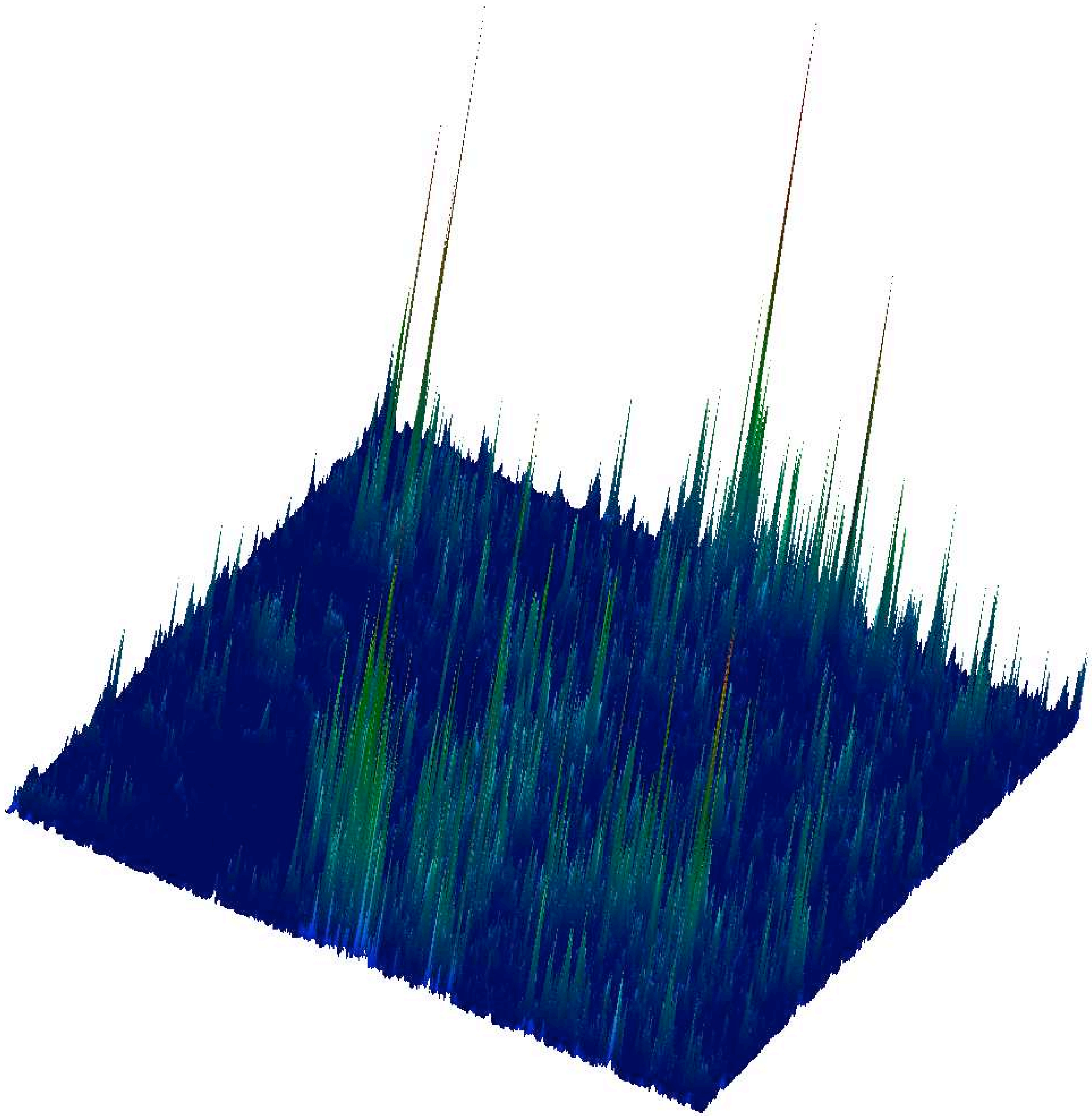
$$\boxed{E(k) \sim k^{-5/3}}$$

Kolmogorov 1941, Obukhov 1941,
Weizsäcker 1948, Heisenberg 1948

What does the experiment show ?



Why ?



DNS 1024^3: Homann, Grauer (2006)

Structures imply:

order

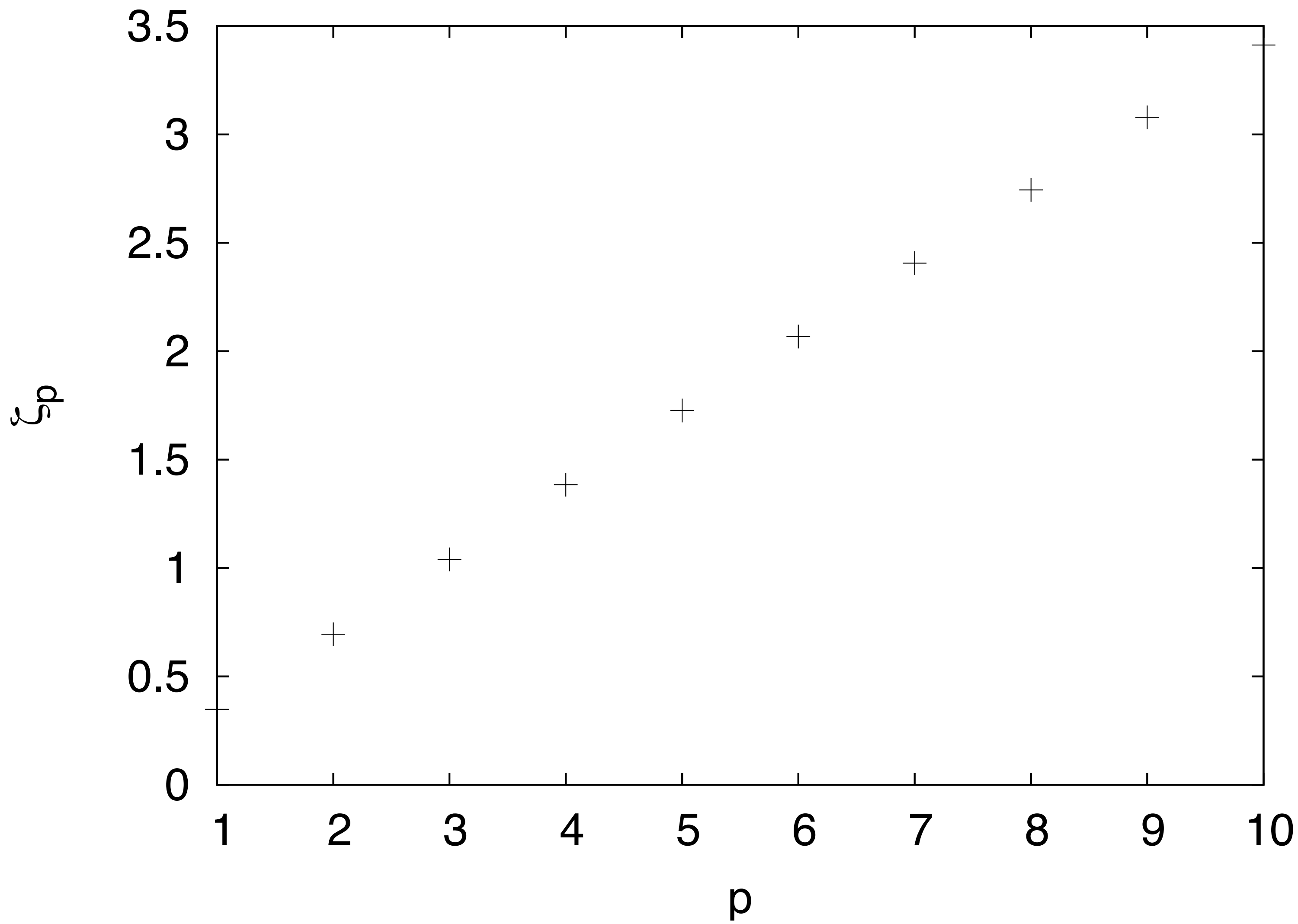
correlations

non-Gaussian

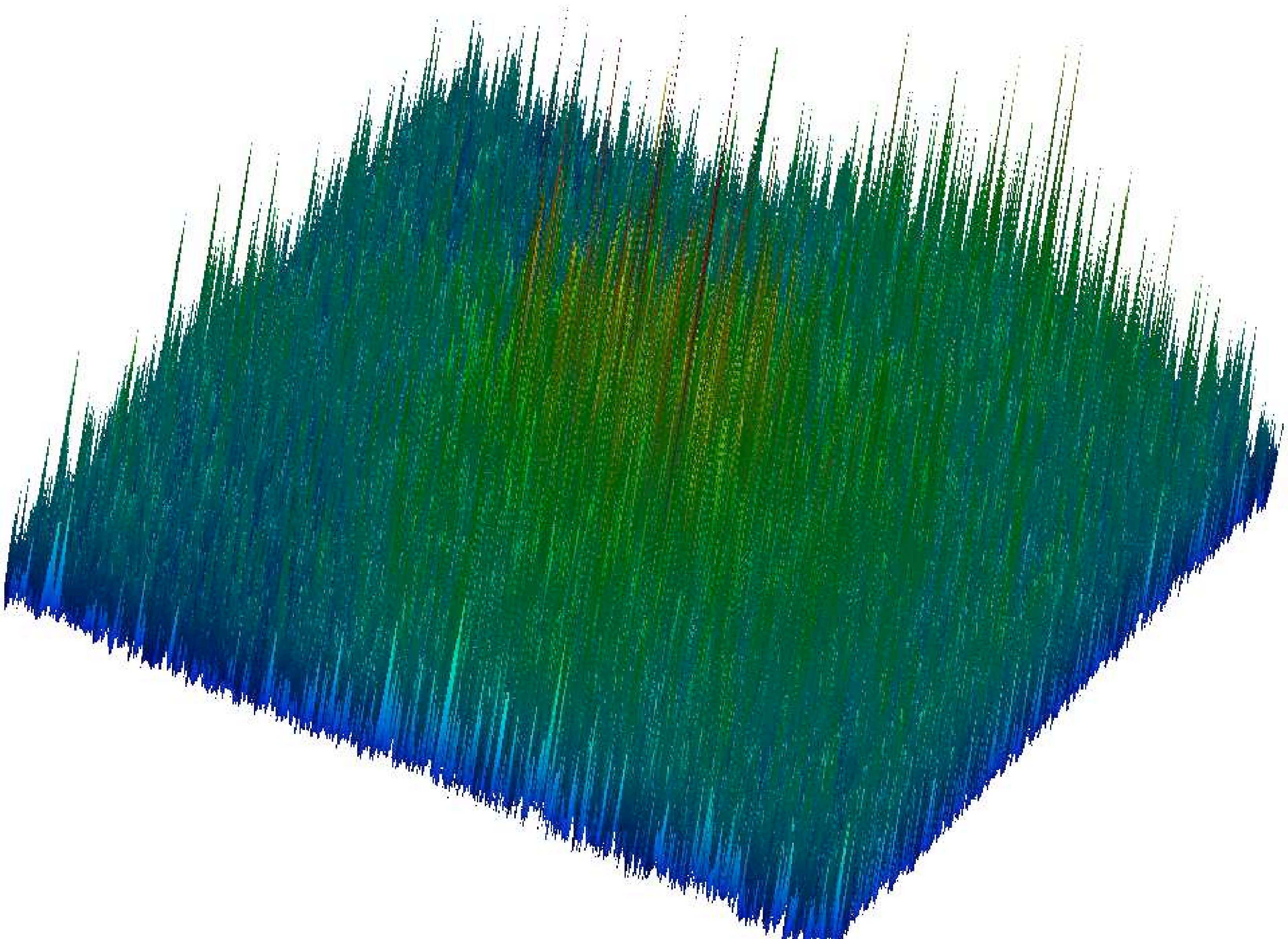
Decorrelated turbulence

- add additional field $\tilde{\mathbf{u}}$
- rotate modes of $\tilde{\mathbf{u}}$ in Fourier space with k-dependent speed
- conserves energy and enstrophy of $\tilde{\mathbf{u}}$
- keeps $div\tilde{\mathbf{u}} = 0$

Result: perfect K41 scaling of $\tilde{\mathbf{u}}$



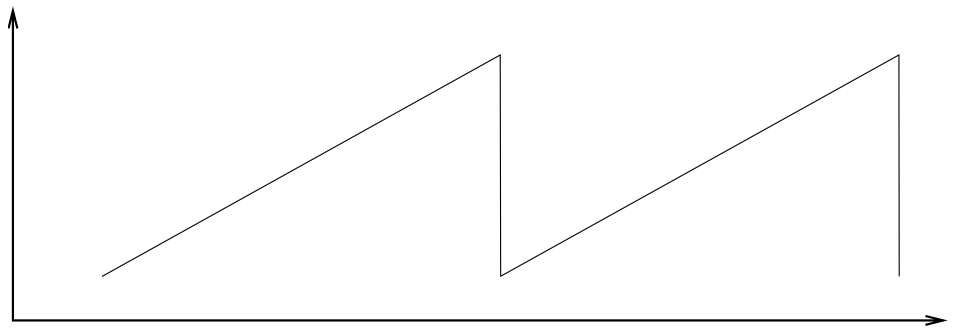
dissipation field

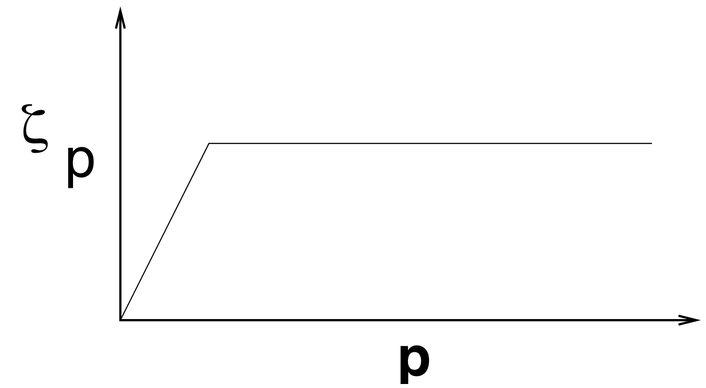


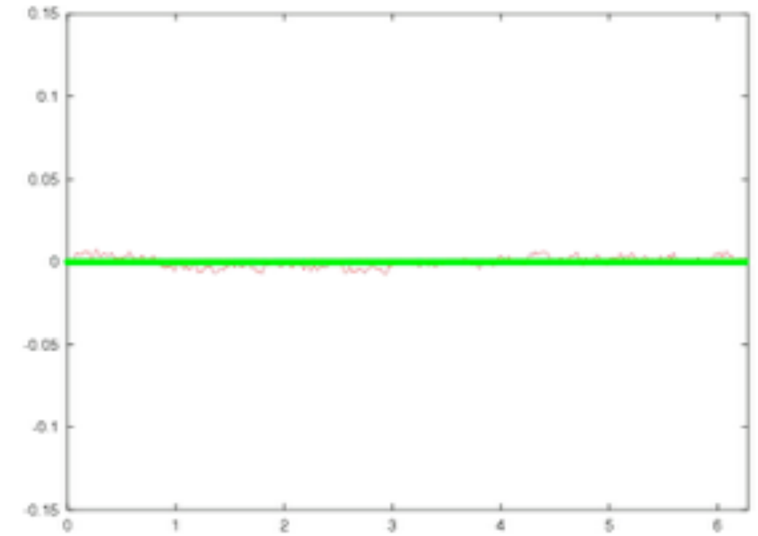
DNS 1024^3: Homann, Grauer (2006)

Locality in real space versus Fourier space

Burgers turbulence: $u_t + uu_x - \nu u_{xx} = f$



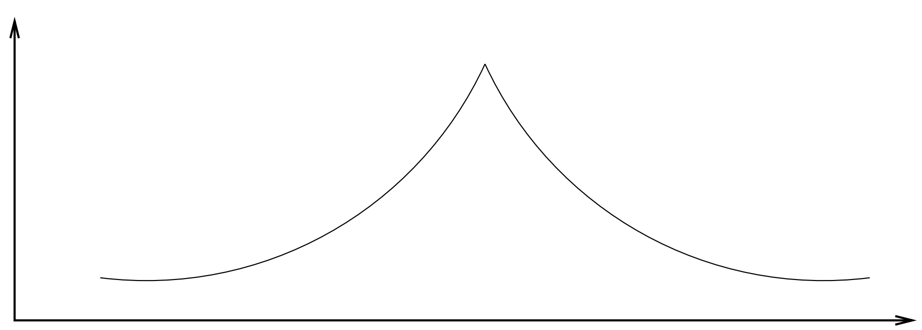


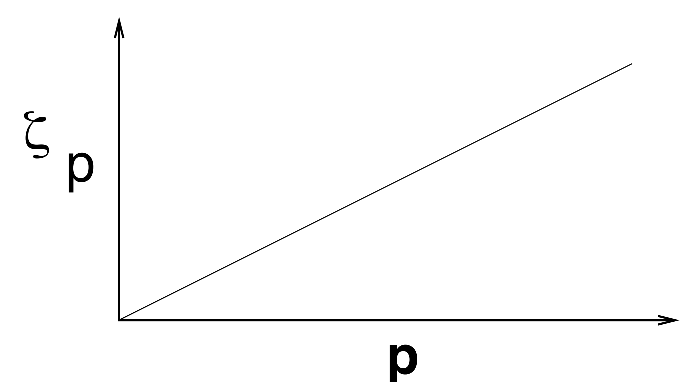


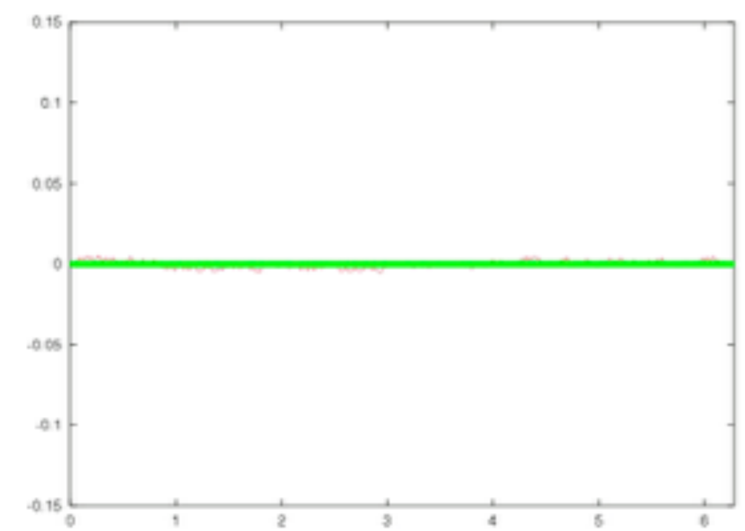
Hilbert-Burgers turbulence: $u_t + \mathrm{H}[u]u_x - \nu u_{xx} = f$

with Zikanov, Thess

$$\mathrm{H}[u] = \frac{1}{\pi} P.V. \int \frac{u(y)}{x-y} dy \quad , \quad \mathrm{H}[u_k] = i \; sign(k) u_k$$







Martin-Siggia-Rose/Janssen/de Dominicis functional

P. C. Martin, E. D. Siggia, and H. A. Rose
Statistical Dynamics of Classical Systems
Phys. Rev. A **8** (1973) 423

H.K. Janssen
On a Lagrangean for Classical Field Dynamics and Renormalization Group Calculations of Dynamical Critical Properties
Z. Physik B **23** (1976) 377

C. de Dominicis
Techniques de renormalisation de la théorie des champs et dynamique des phénomènes critiques
J. Phys. C **1** (1976) 247

R. Phythian
The functional formalism of classical statistical dynamics
J. Phys. A **10** (1977) 777

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Martin-Siggia-Rose àla Phythian

(see also E.V. Ivashkevich, J. of Phys. A **30** (1997) L525)

$$\partial_t u + N[u, x] = \eta(x, t)$$

(stochastic diff. eqn.)

↑

gaussian noise with
covariance-operator K

$$\langle \eta(x, t)\eta(x + r, t + s)\rangle = \chi(r)\delta(s)$$

keep in mind: the field u is a functional $u[\eta]$ of the forcing η

$$\begin{aligned}\langle O[u]\rangle &= \text{expectation value of an observable}\\ &= \text{average over all path} = \text{possible noise realization}\\ &= \int \mathcal{D}\eta\, O[u[\eta]] e^{-\int(\eta,\chi^{-1}\eta)/2\,dt}\end{aligned}$$

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coordinate transformation $\eta \to u$

Jacobian: $\mathcal{D}\eta = J[u]\mathcal{D}u$ with $J[u] = \det \left\| \frac{\delta \eta}{\delta u} \right\| = \det \left\| \partial_t - \frac{\delta N}{\delta u} \right\|$

↑ Jacobi determinant

↑ functional derivative

Onsager-Machlup functional

$$\langle O[u] \rangle = \int \mathcal{D}u\, O[u] J[u] \mathrm{e}^{-\int (\dot{u} - N[u], \chi^{-1}(\dot{u} - N[u]))/2\, dt}$$

starting point for directly minimizing the Lagrangian action

$$S_{\mathcal{L}}[u, \dot{u}] = \frac{1}{2} \int (\dot{u} - N[u], \chi^{-1}(\dot{u} - N[u]))\, dt$$

Martin-Siggia-Rose/Janssen/de Dominicis (MSRJD) response functional

Hubbard-Stratonovich transformation, Keldysh action

working with the original correlation function χ instead of working with its inverse (by virtue of the Fourier transform, completion of the square):

$$\langle O[u] \rangle = \int \mathcal{D}\eta \, \mathcal{D}\mu \, O[u[\eta]] \, \mathrm{e}^{-\int [(\mu,\chi\mu)/2 - i(\mu,\eta)] \, dt}$$

again coordinate change $\eta \to u$

$$\langle O[u] \rangle = \int \mathcal{D}\eta \, \mathcal{D}\mu \, O[u] J[u] \, \mathrm{e}^{-S[u,\mu]}$$

with the action function $S[u, \mu]$ given by

$$S[u, \mu] = \int \left[-i(\mu, \dot{u} - N[u]) + \frac{1}{2}(\mu, \chi\mu) \right] \, dt$$

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Instanton calculus

The instanton calculus consists basically of 4 steps:

1. calculation of the instanton as a classical solution (minima of the corresponding action S): the instanton provides the exponential decay term $\exp(-S)$ in the transition amplitude.

2. calculation of zero modes that leave the action invariant: finding the zero modes closely related with finding the symmetries of the underlying system. Once the zero modes are determined and if, as usually, their number is finite, the contribution from the zero modes results from a finite dimensional integral and often takes the form $(\sqrt{S})^p$, where p is the number of zero modes.

3. calculation of the path integral of fluctuations around the instanton which change the action: this is normally done in the Gaussian approximation.

4. summation over the instanton gas.

observable $O[u] = \delta(F[u(x, t = 0)] - a)$ at time $t = 0$ comming from $-T < 0$

path integral representation of the PDF $\mathcal{P}(a)$ for the events that $F[u] = a$ at $t = 0$:

$$\begin{aligned} \mathcal{P}(a) &= \langle \delta(F[u]\delta(t) - a) \rangle \\ &= \int \mathcal{D}\eta\, \mathcal{D}\mu\, \frac{1}{2\pi} \int_{-\infty}^{\infty} d\lambda J[u]\, \mathrm{e}^{-S[u,\mu]}\, \mathrm{e}^{-i\lambda(F[u]\delta(t)-a)} \end{aligned}$$

Instanton $=$ saddle point

$$\begin{aligned} \dot{u} &= N[u] + i\chi\mu \\ \dot{\mu} &= -(\nabla N[u])^T \mu - i\lambda \nabla F[u]\delta(t)\,. \end{aligned}$$

Instanton = rare extreme event = “singularity”

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Burgers turbulence

smooth right tails:

V. Gurarie, A. Migdal
Instantons in the Burgers equation
Phys. Rev. E **54** (1996) 4908

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general instantons:

G. Falkovich, I. Kolokolov, V. Lebedev, A. Migdal
Instantons and intermittency
Phys. Rev. E **54** (1996) 4896

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left tails:

E. Balkovsky, G. Falkovich, I. Kolokolov, V. Lebedev
Intermittency of Burgers' Turbulence
Phys. Rev. Lett. **78** (1997) 1452

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numerics:

A.I. Chernykh, M.G. Stepanov
Large negative velocity gradients in Burgers turbulence
Phys. Rev. E 64 (2001) 026306

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A.I. Chernykh, M.G. Stepanov (2001): consider strong gradients

we will use notation from paper

$$u_t + uu_x - \nu u_{xx} = \phi \qquad \langle \phi(x_1, t_1)\phi(x_2, t_2)\rangle = \delta(t_1 - t_2)\chi(x_1 - x_2)$$

$$\begin{aligned} \mathcal{P}(a) &= \langle \delta[u_x(0,0) - a]\rangle_\phi \\ &= \int \mathcal{D}u\mathcal{D}p \int_{-i\infty}^{i\infty} d\mathcal{F}\ \exp\{-S + 4\nu^2 \mathcal{F}[u_x(0,0) - a]\} \end{aligned}$$

with action

$$\begin{aligned} S &= \frac{1}{2}\int_{-\infty}^{0} dt \int dx_1 dx_2\, p(x_1, t)\chi(x_1 - x_2)p(x_2, t) \\ &\quad - i\int_{-\infty}^{0} dt \int dx\, p\,(u_t + uu_x - \nu u_{xx}) \end{aligned}$$

interested in strong gradients: saddle point (or instanton or optimal fluctuation)

variation with respect to u and p vanishes

instanton equations:

$$u_t + uu_x - \nu u_{xx} = -i \int dx' \chi(x - x') p(x', t)$$ integration forward in time

$$p_t + up_x + \nu p_{xx} = i4\nu^2 \mathcal{F} \delta(t) \delta'(x)$$ integration backward in time

boundary conditions:

$$\lim_{t \to -\infty} u(x,t) = 0 \qquad \lim_{t \to +0} p(x,t) = 0$$

$$\lim_{|x| \to \infty} u(x,t) = 0 \qquad \lim_{|x| \to \infty} p(x,t) = 0$$

initial condition for μ:

$$p(x, t = -0) = i4\nu^2 \mathcal{F} \delta'(x)$$

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$\mathcal{F}$ given $\Longrightarrow u_x(0,0) = a$ thus: $a = a(\mathcal{F})$ or $\mathcal{F} = \mathcal{F}(a)$

normalization: $t = \frac{T}{2\nu}$, $u = 2\nu U$, $p = 4i\nu^2 P$, $a = 2\nu A$, $S_{\text{extr}}(a) = 8\nu^3 S(a/2\nu) = (2\nu)^3 S(A)$

$$U_T + UU_x - \frac{1}{2}U_{xx} = \int dx'\, \chi(x-x')P(x')$$

$$P_T + UP_x + \frac{1}{2}P_{xx} = \mathcal{F}\delta(T)\delta'(x)$$

$$\begin{aligned} S(A) &= -\frac{1}{2}\int_{-\infty}^{0} dT \int dx_1 dx_2\, P(x_1,T)\chi(x_1-x_2)P(x_2,T) \\ &\quad + \int_{-\infty}^{0} dT \int dx\, P\left(U_T + UU_x - \frac{1}{2}U_{xx}\right) \end{aligned}$$

action at instanton S_{extr} gives the tail of PDF $\mathcal{P}(A) \simeq e^{-S(A)}$

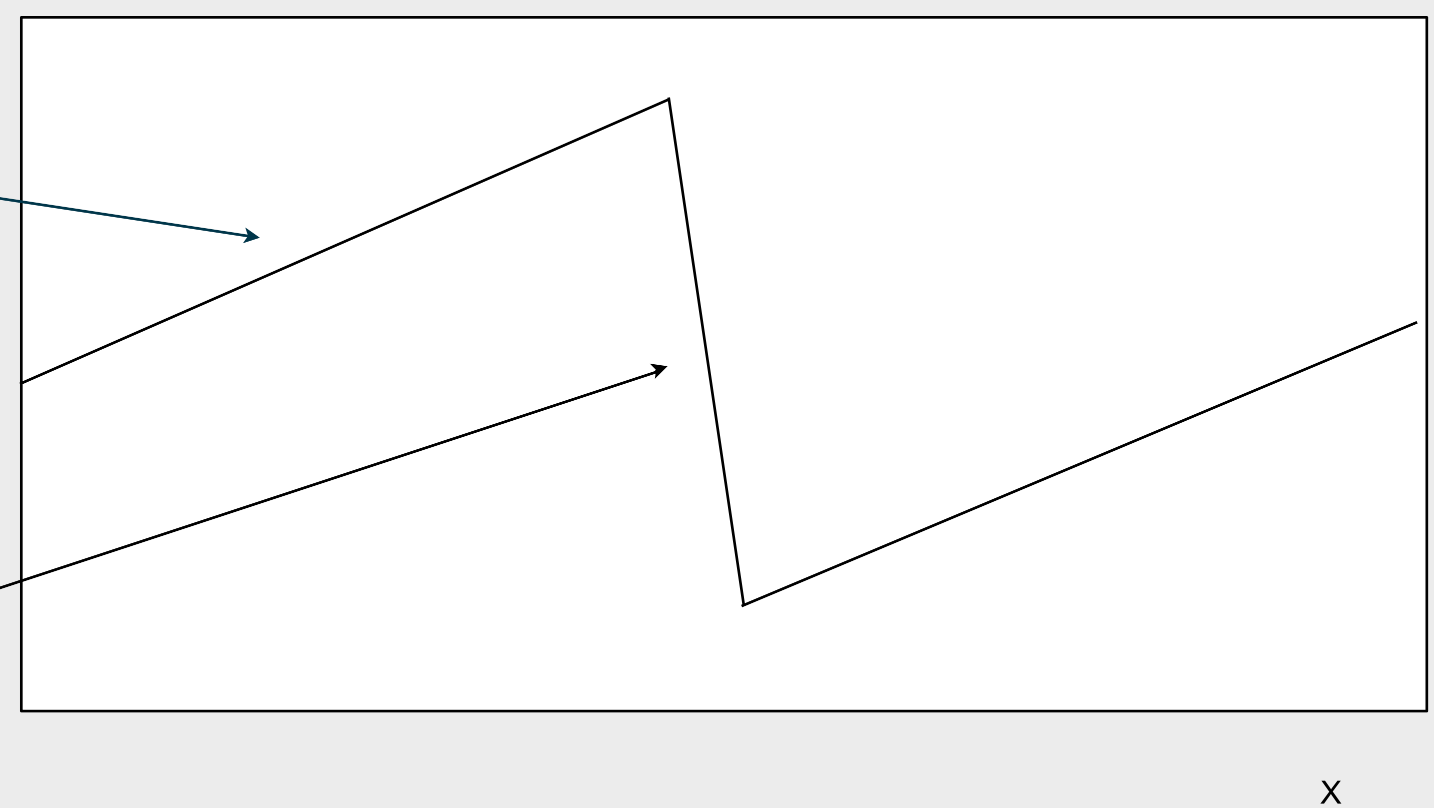
action at instanton S_{extr} gives the tail of PDF

$$\mathcal{P}(A) \simeq e^{-S(A)}$$

It holds: $$\mathcal{F} = \frac{dS(A)}{dA} \Longrightarrow \frac{\mathcal{F}A}{S} = \frac{d\ln S}{d\ln A}$$

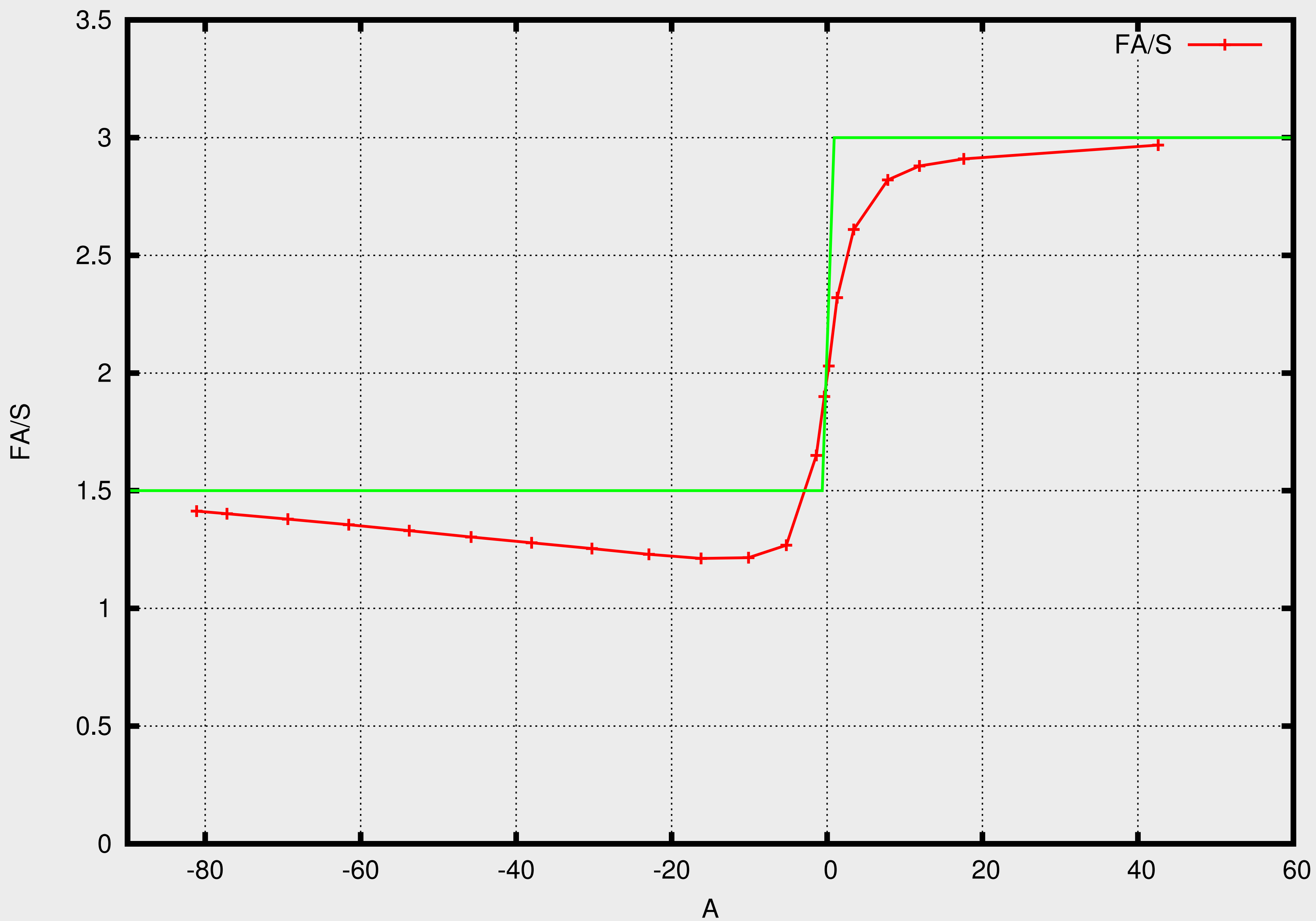
If $\frac{\mathcal{F}A}{S} = \gamma$ then $\mathcal{P}(A) \simeq e^{-\alpha|A|^\gamma}$

right tail: $\gamma = 3$
Gurarie, Migdal (1996)
easy



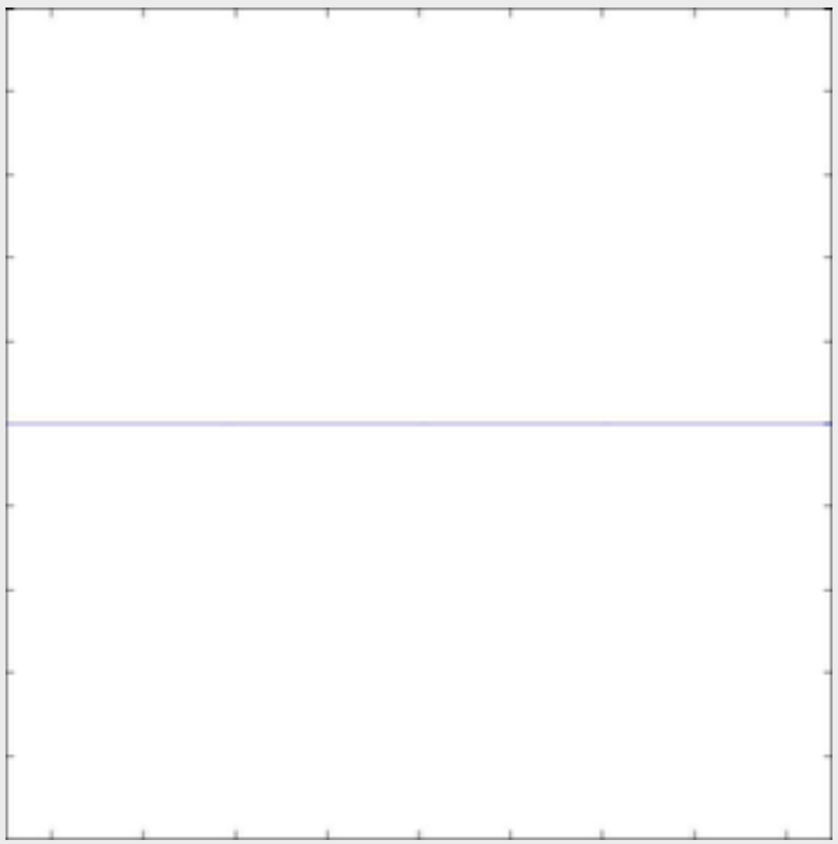
left tail: $\gamma = 3/2$
Balkovsky, Falkovich et al (1997)
using Cole-Hopf

everything coded in $\frac{\mathcal{F}A}{S}$ curve:



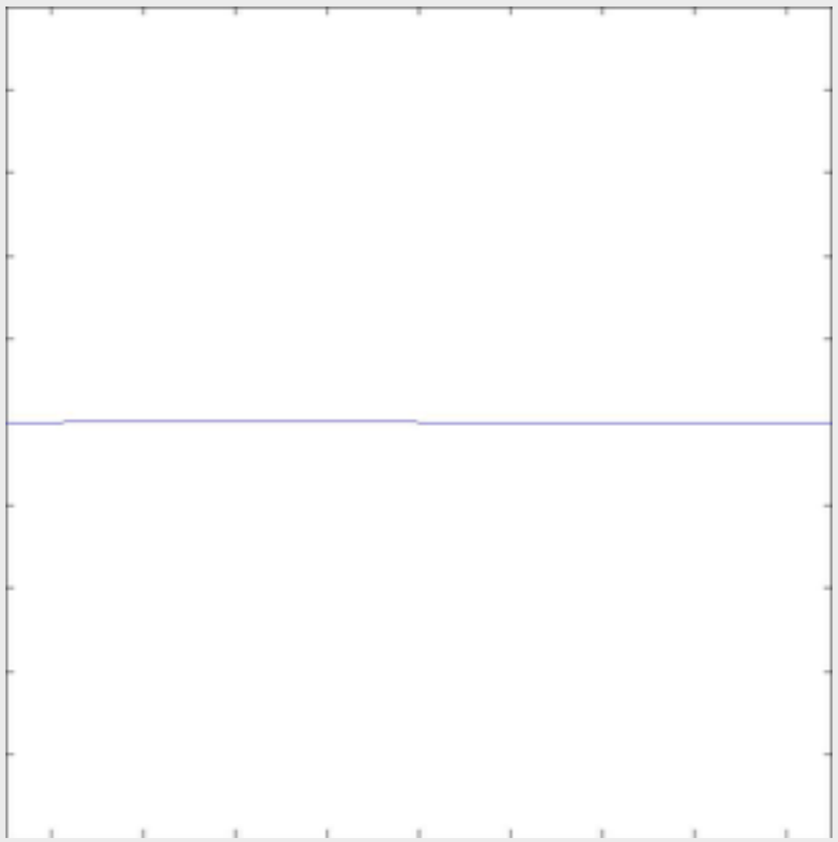
X

u



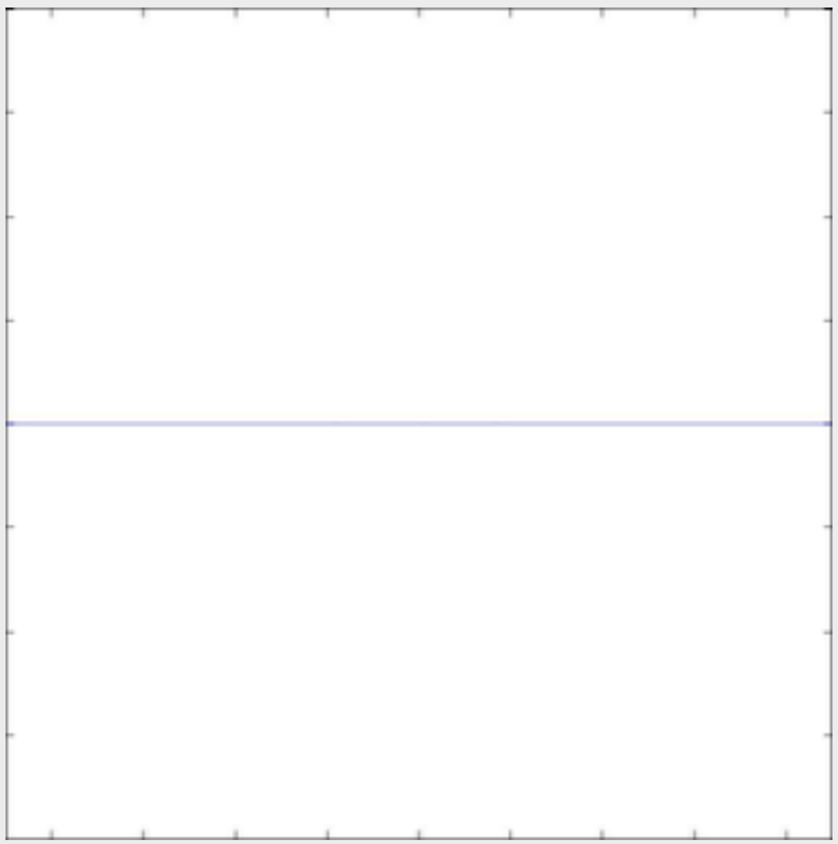
instanton

p



auxiliary field

f



optimal force

Gotoh puzzle

Gotoh 1999: high resolution numerics

no indication of 3/2 exponential decay

In the case of the velocity-gradient PDF, however, these tails are long enough that the invisibility of the asymptotic behavior predicted by instanton analysis requires an explanation.

The instanton was dead.

Reincarnation of the instanton: Grafke, Grauer, Schäfer (2013)

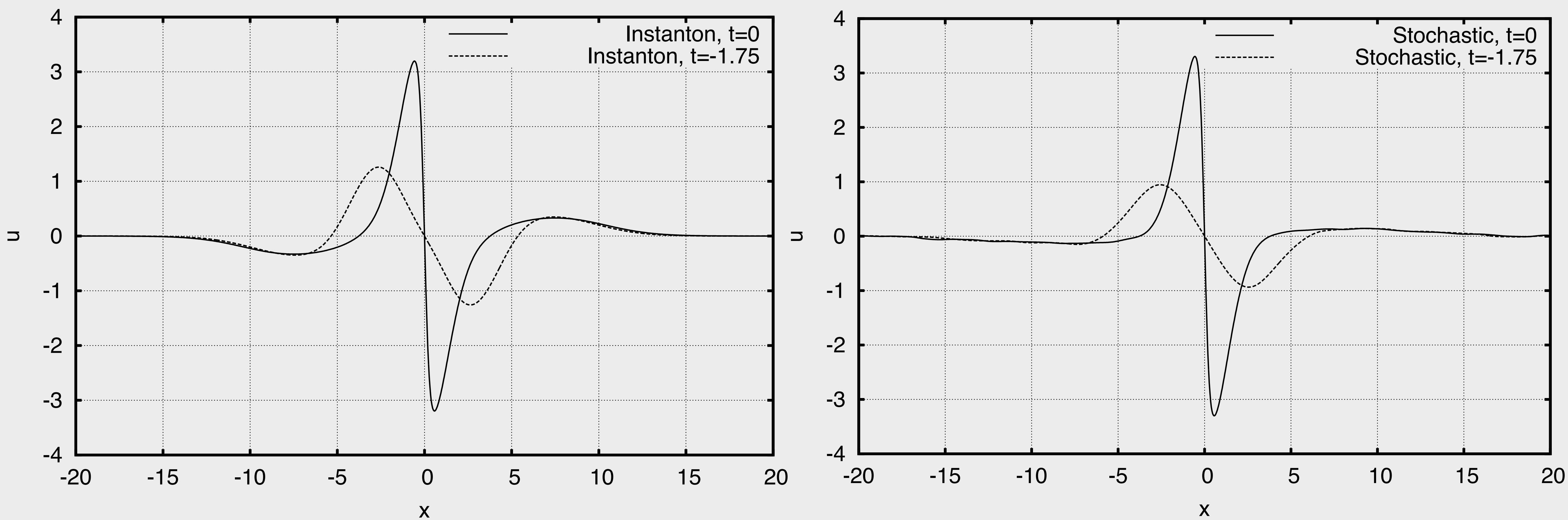
Can we see Instantons in Turbulence:

Instanton filtering

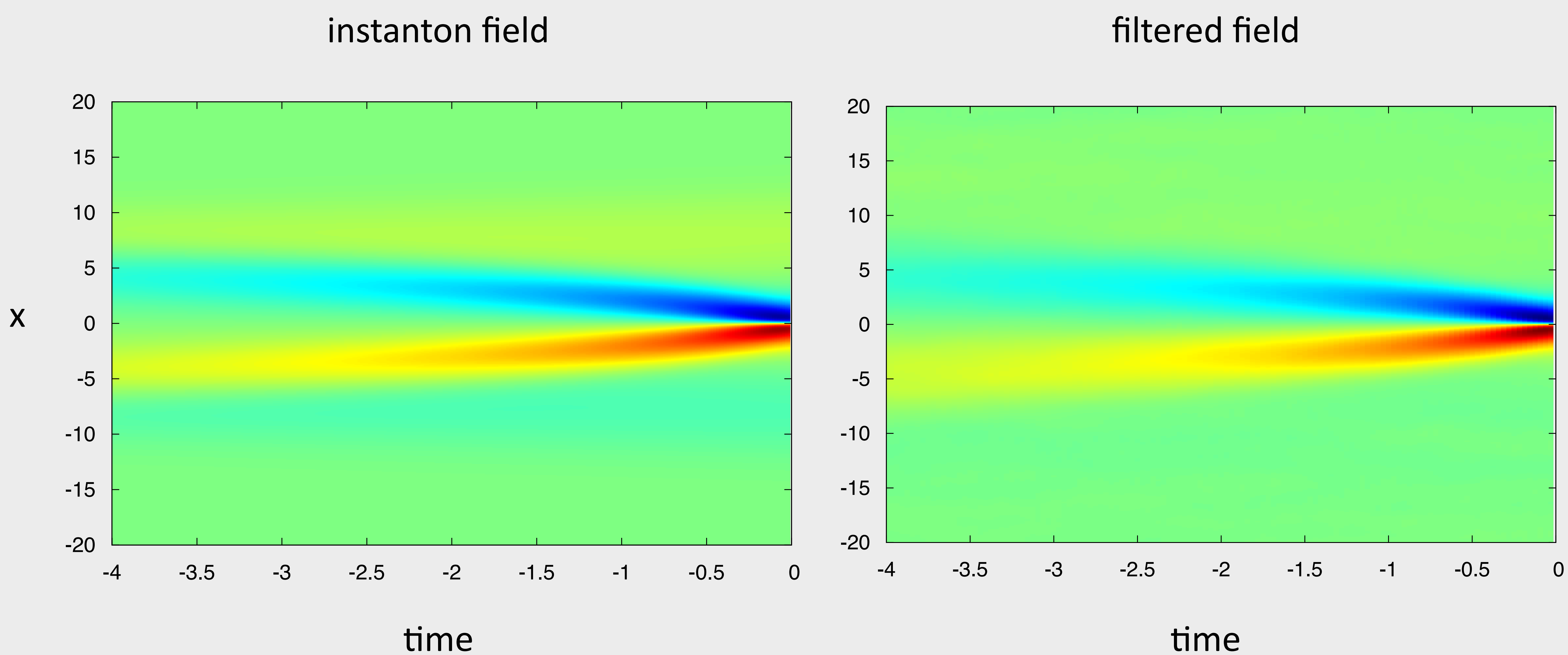
- massive simulations of Burgers turbulence
  using a cluster of CUDA cards:
  starting with u=0 from some fixed time -T to time 0
  (T ~ 10 integral times)
  performing 10^7 full simulation (~ 10^8 integral times)
- search for a prescribed u_x in each simulation
- shift velocity field u and force field
- average over all simulations

	N	dx	η	L	L_{box}	ν	ϵ_{k}	T_L	#hits (%)
Run 1	1024	0.039	0.406	1	40	0.3	4.586	0.99	10.5
Run 2	1024	0.039	0.464	1	40	0.38	2.691	0.97	0.410
Run 3	1024	0.039	0.481	1	40	0.41	2.33	0.95	0.052

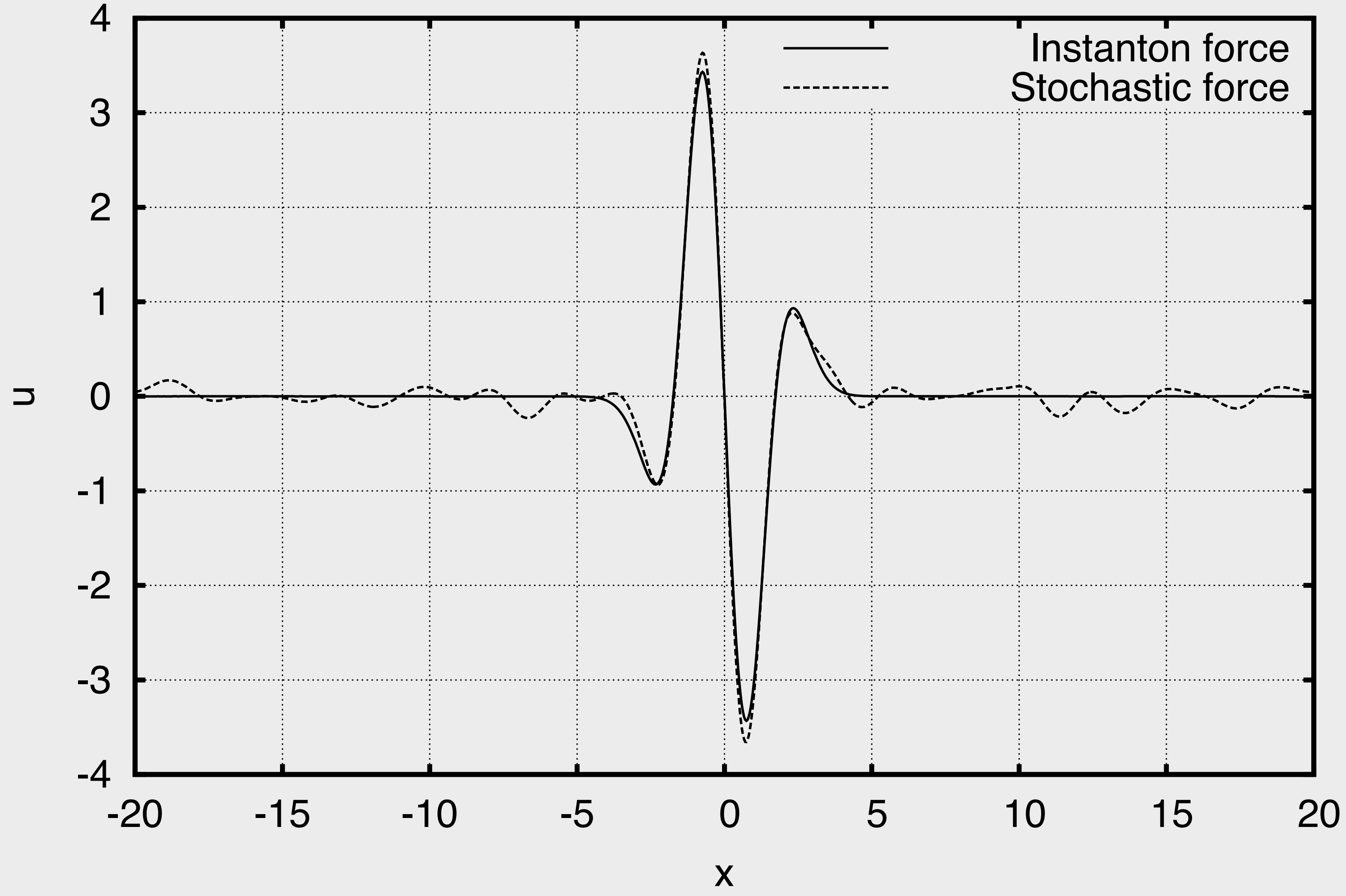
Table 1: Parameters of the numerical simulations. N: number of collocation points, dx: grid-spacing, $\eta = (\nu^3/\epsilon_{\mathrm{k}})^{1/4}$: Kolmogorov dissipation length scale, L: correlation length of forcing, L_{box}: domain length, ν: kinematic viscosity, ϵ_{k}: mean kinetic energy dissipation rate, $T_L = L/u_{\mathrm{rms}}$: large-eddy turnover time, #hits (%): percentage of hits with prescribed velocity derivative.



Temporal evolution

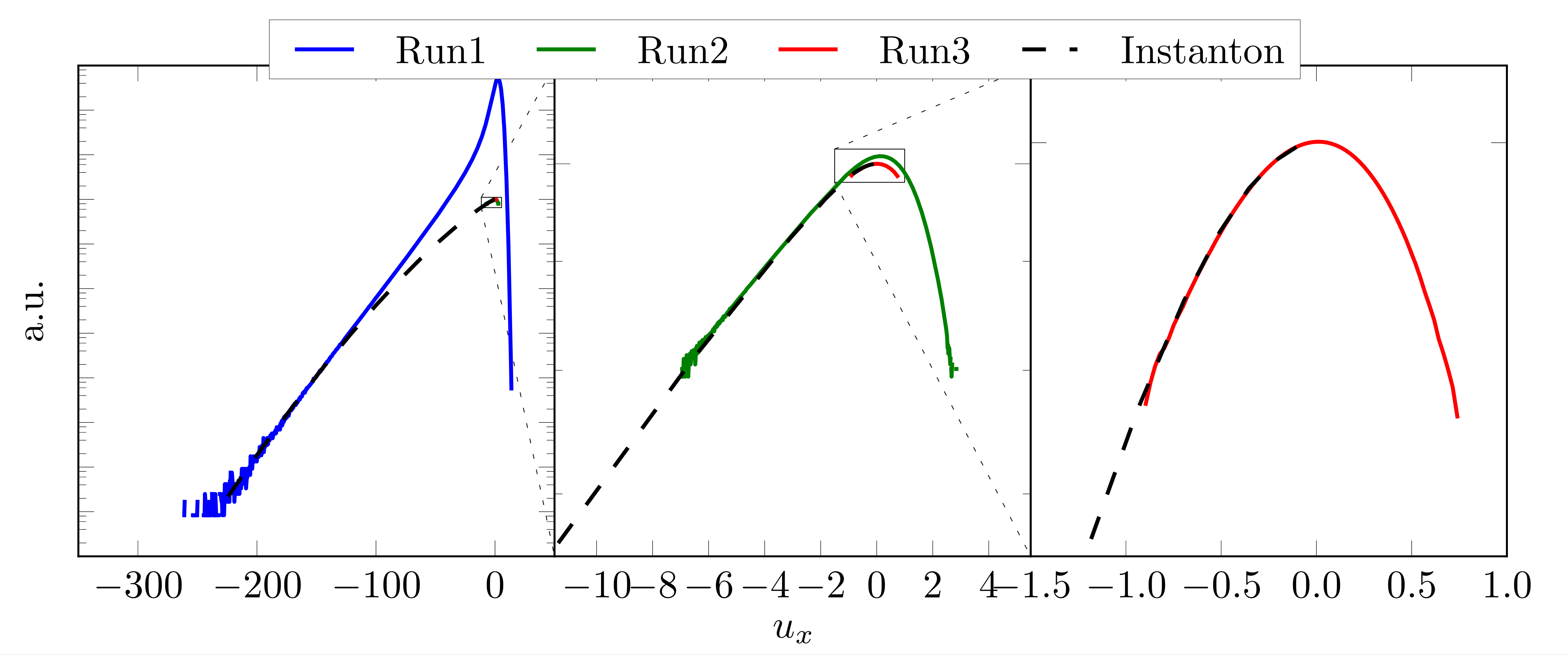


$$\langle \phi_{\text{shifted}}(t,x) \rangle = -i \int \chi(x-x')p(x',t)dx'$$

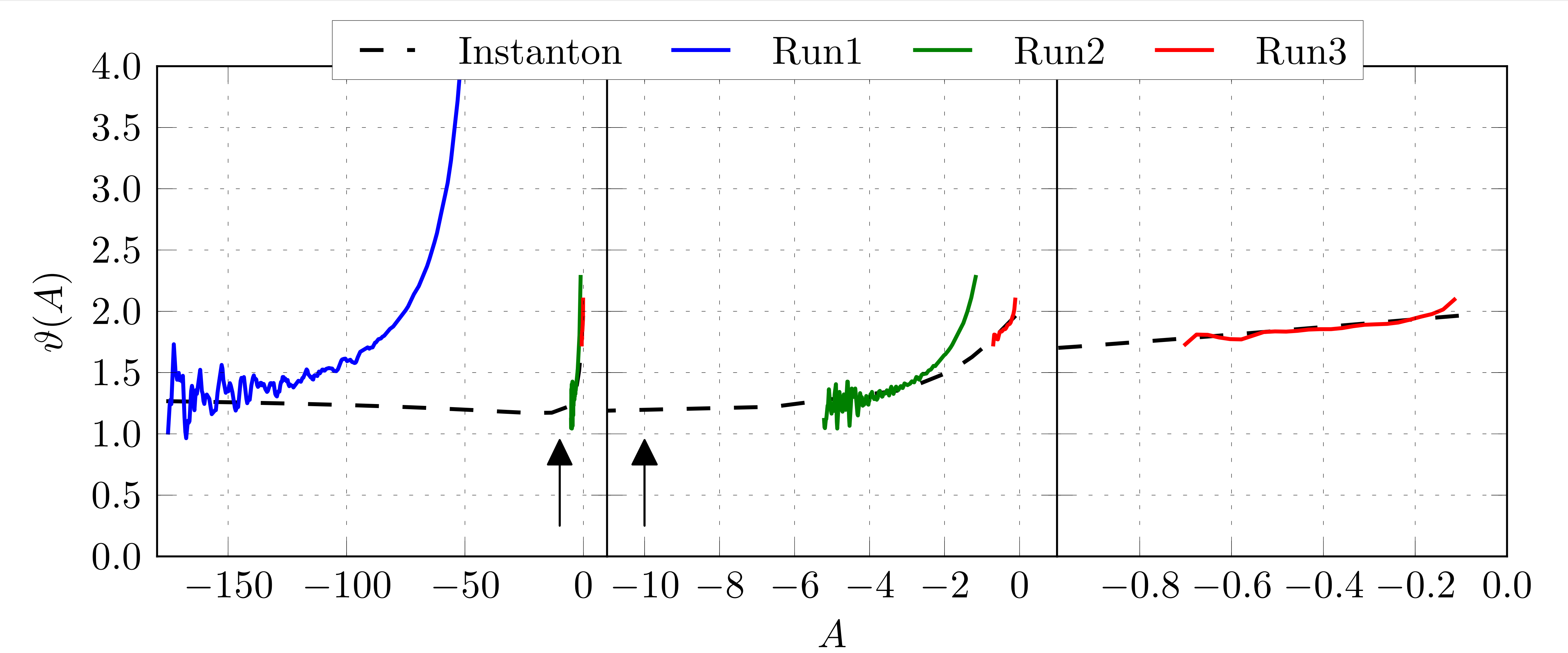


The filtered force field $\langle \phi_{\text{shifted}}(t,x) \rangle$ (dashed) and the analytical force field $4\nu^2 \mathcal{F} \chi'(x)$ (solid) at time $t = 0$.

The “Gotoh” puzzle



PDFs fit very well



clarifies the problem

- 2D/3D memory problem

2D Problems

issue: memory

let's try 2048x2048x4096 on a GPU

- need to u and p in space and time
- store only $\chi * p$ (reduction from 2048 --> 64)
- multigrid in time
- use biorthogonal wavelets to store u

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2D Burgers

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} - \nu\Delta\mathbf{u} = \mathbf{f}$$

$$\langle f_i(\mathbf{x}+\mathbf{r}, s+t) f_j(\mathbf{x}, s)\rangle = \delta(t)\chi_{ij}(r)$$

$$\chi_{ij}(r) = \alpha\chi_{ij}^{\mathrm{irr}}(r) + (1-\alpha)\chi_{ij}^{\mathrm{sol}}(r)$$

$$\chi_{ij}^{\mathrm{irr}}(r) = g(r)\delta_{ij} + r g'(r)\frac{r_i r_j}{r^2}$$

$$\chi_{ij}^{\mathrm{sol}}(r) = f(r)\delta_{ij} + \frac{r f'(r)}{d-1}\left(\delta_{ij} - \frac{r_i r_j}{r^2}\right)$$

2D Burgers

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} = \chi \star \mathbf{p}$$

forward in time

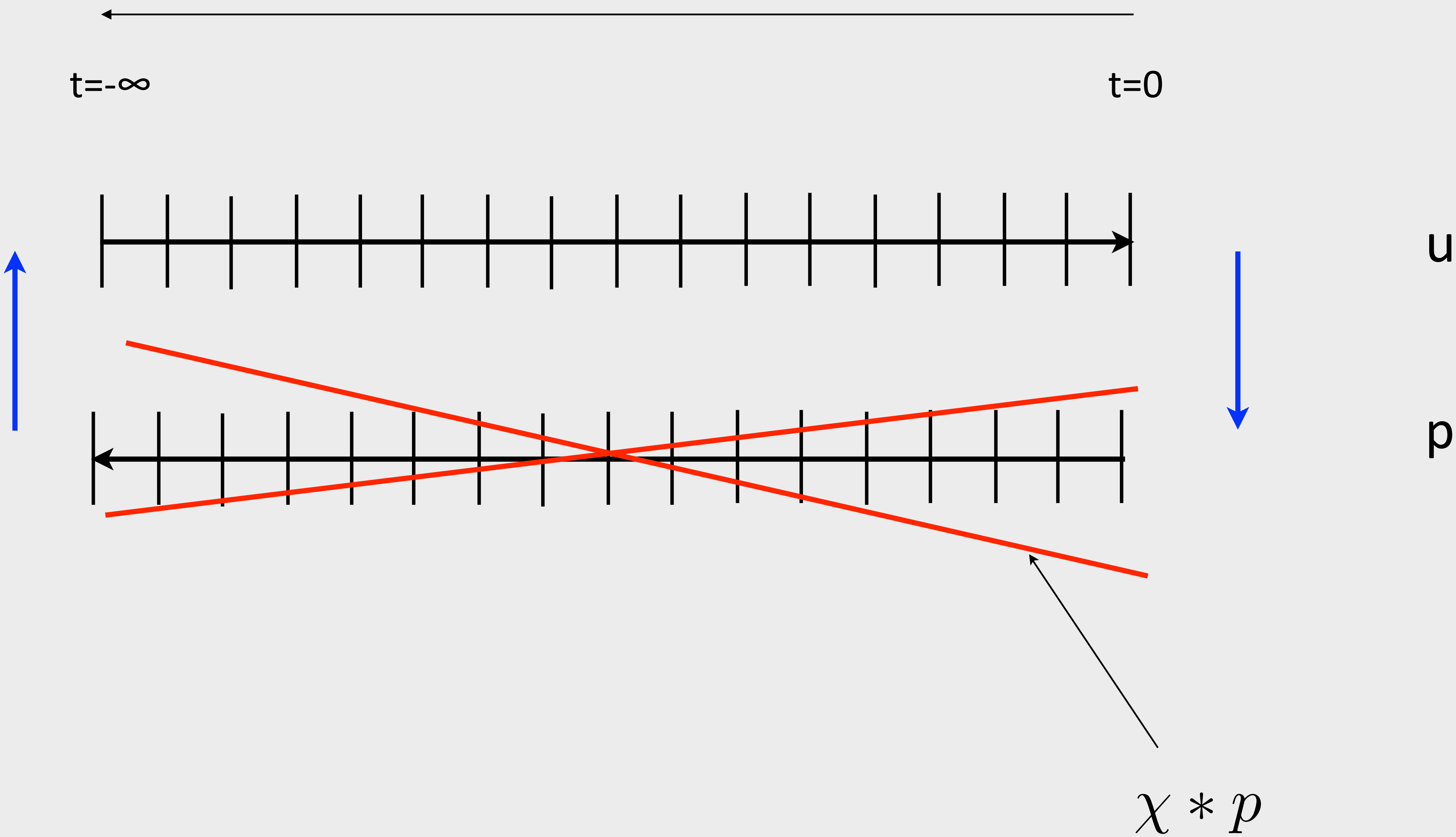
$$\partial_t \mathbf{p} + \mathbf{u} \cdot \nabla \mathbf{p} - (\mathbf{p} \times \nabla)\mathbf{u}^{\perp} + \nu \Delta \mathbf{p} = 0$$

backward in time

$\mathbf{u}^{\perp} = (-u_y, u_x)$ $\quad\quad$ $\chi \star \mathbf{p} = \sum_j \chi_{ij} \star p_j$

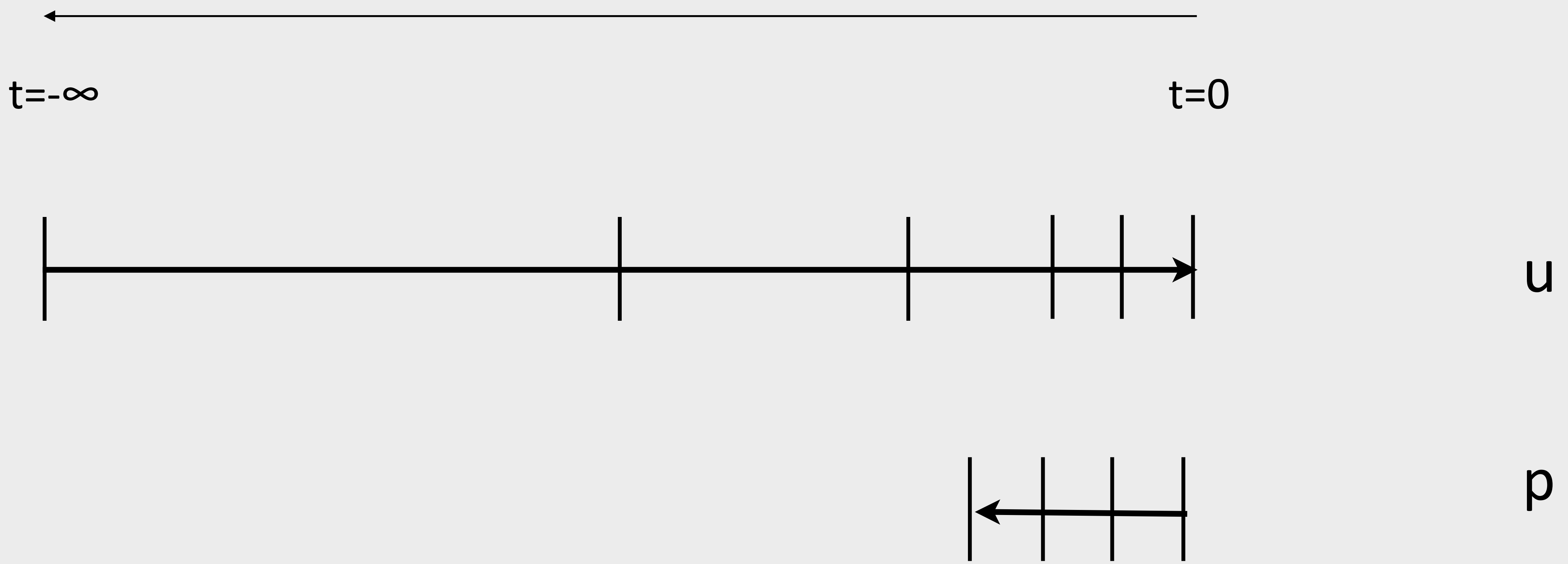
initial condition for p at time t=0

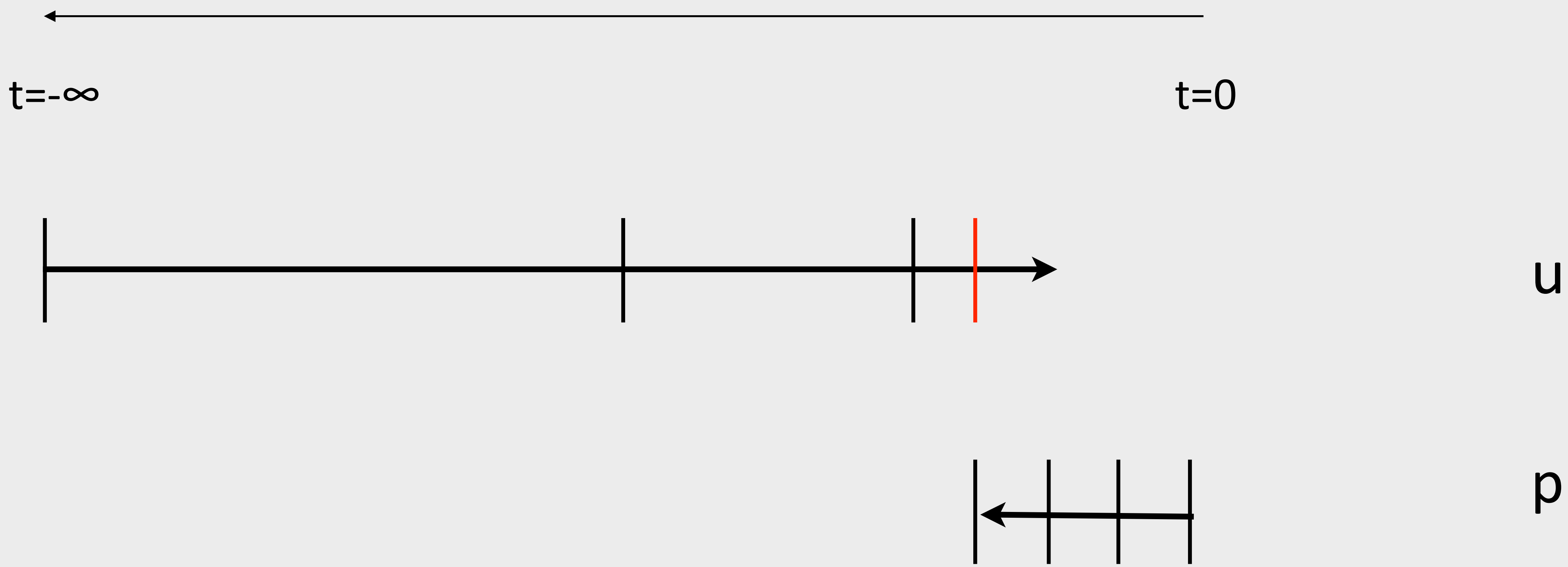

t=-∞
t=0
u
p


t=-∞
t=0
u
p
$\chi * p$

Passive scalar (slightly different)

A. Celani, M. Cencini, and A. Noullez, Physica D 195(3):283–291, 2004


t=-∞
t=0
u
p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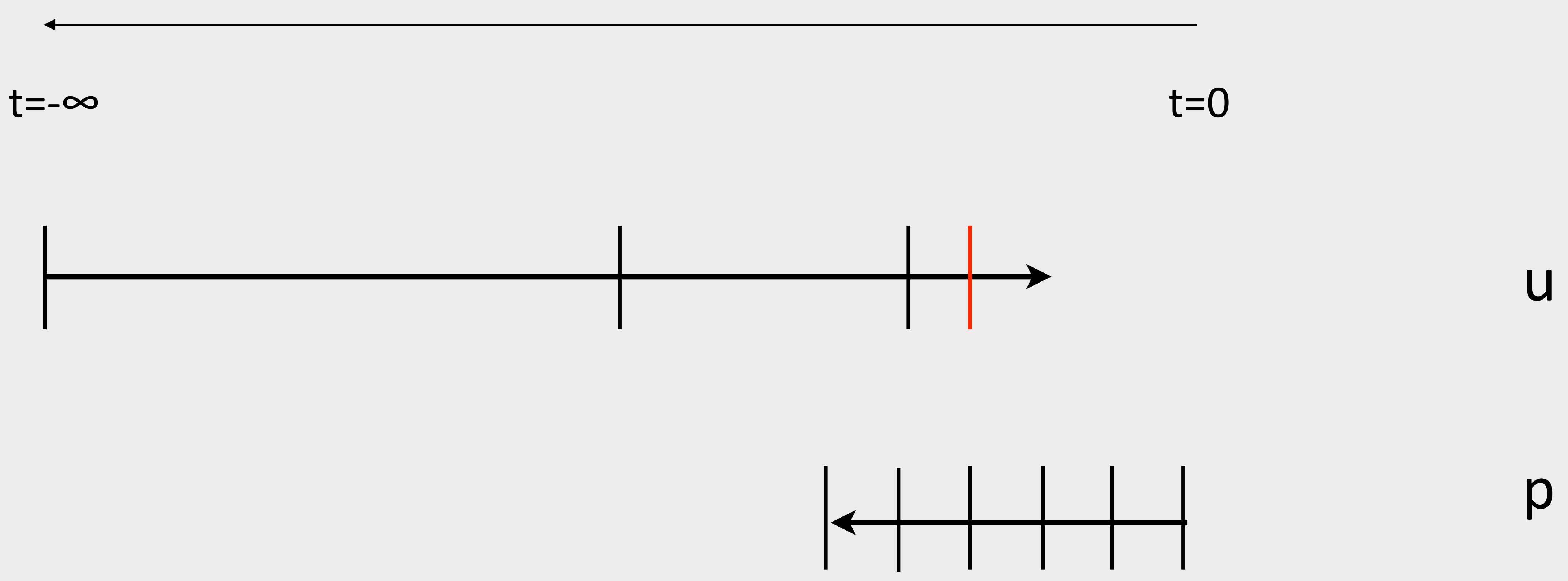
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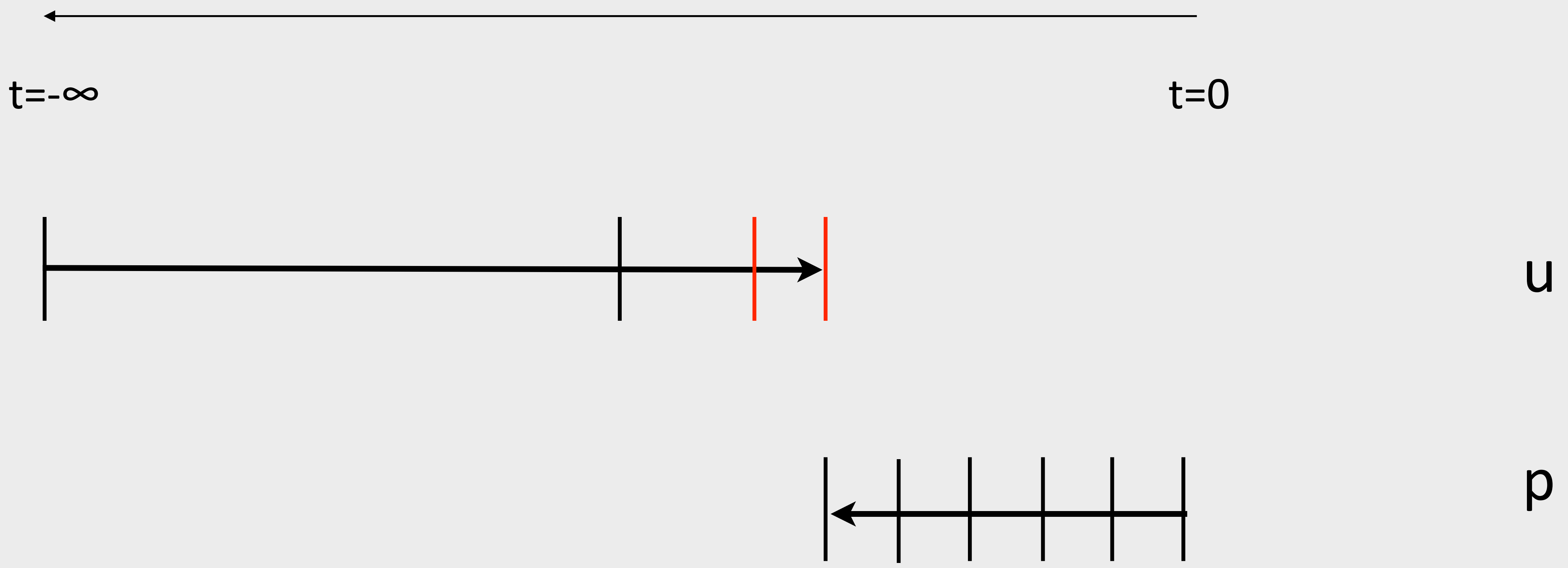
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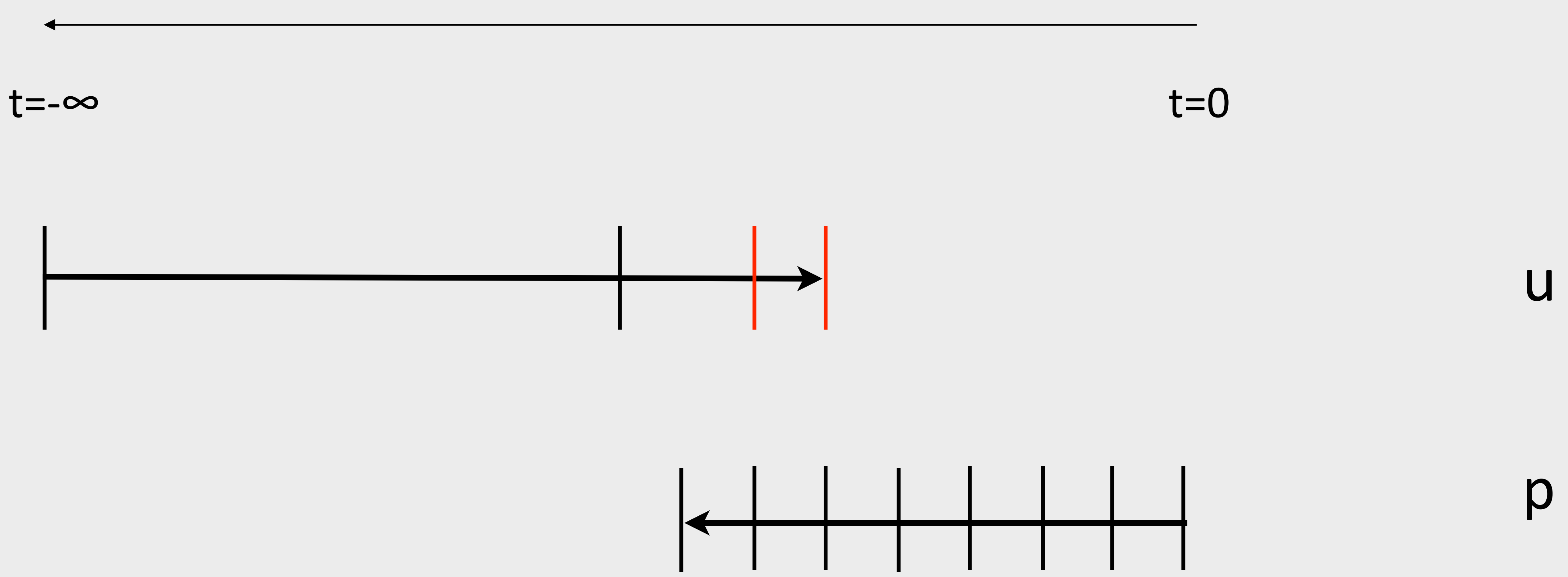
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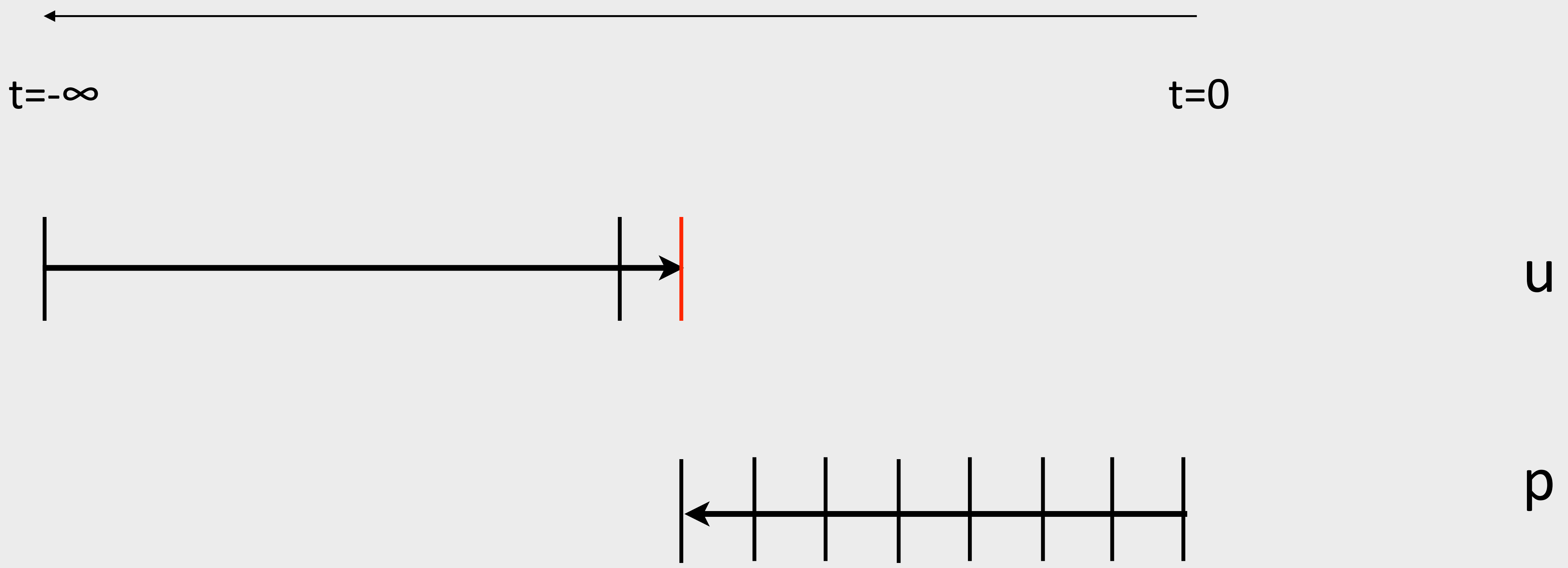
t=0
u
p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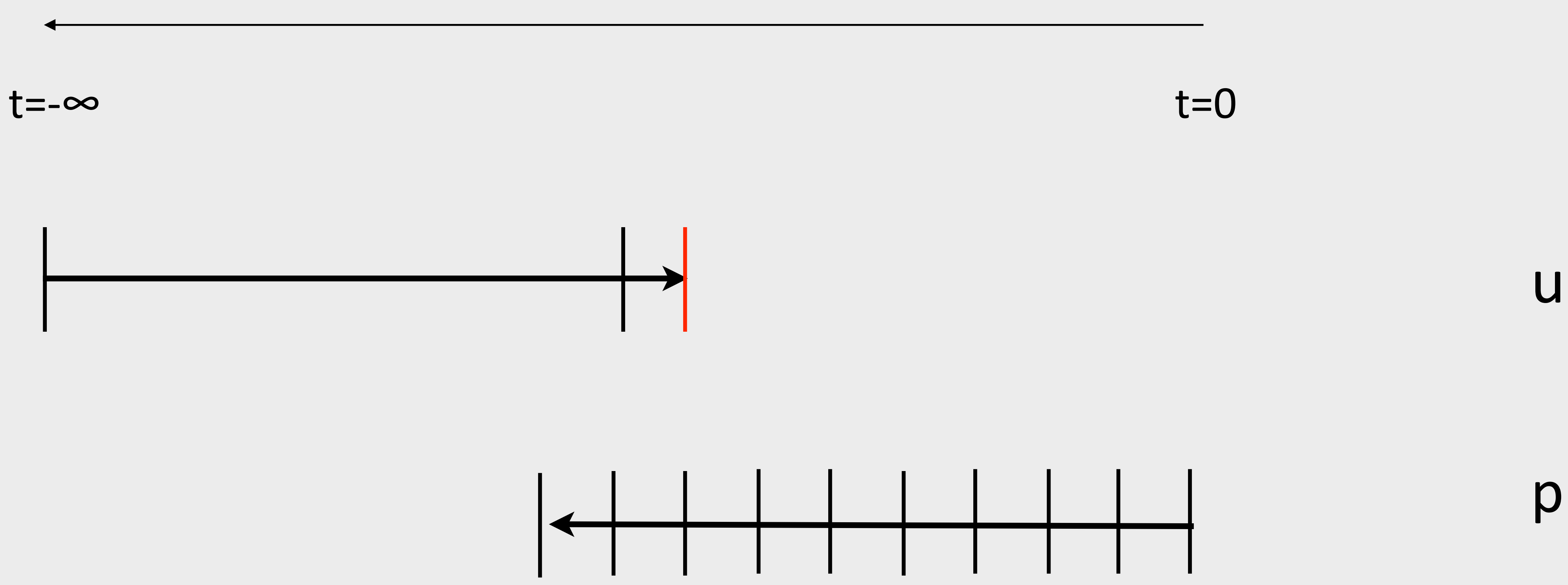
t=0
u
p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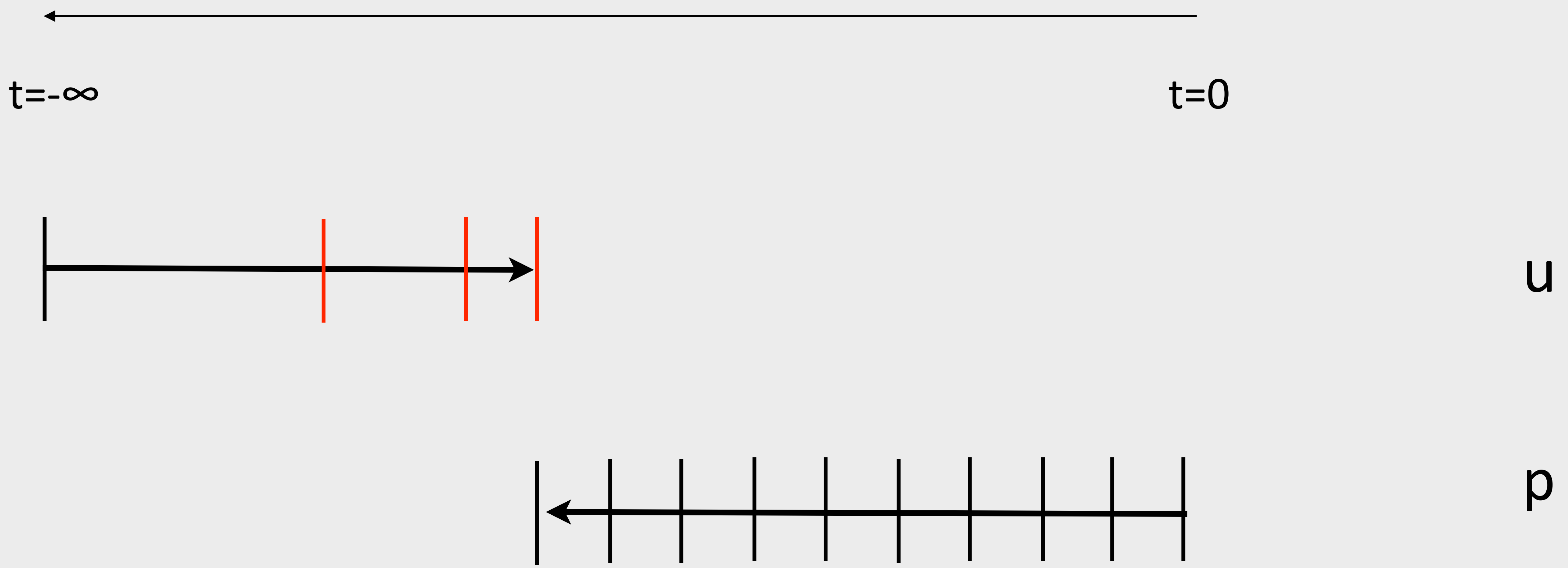
u
p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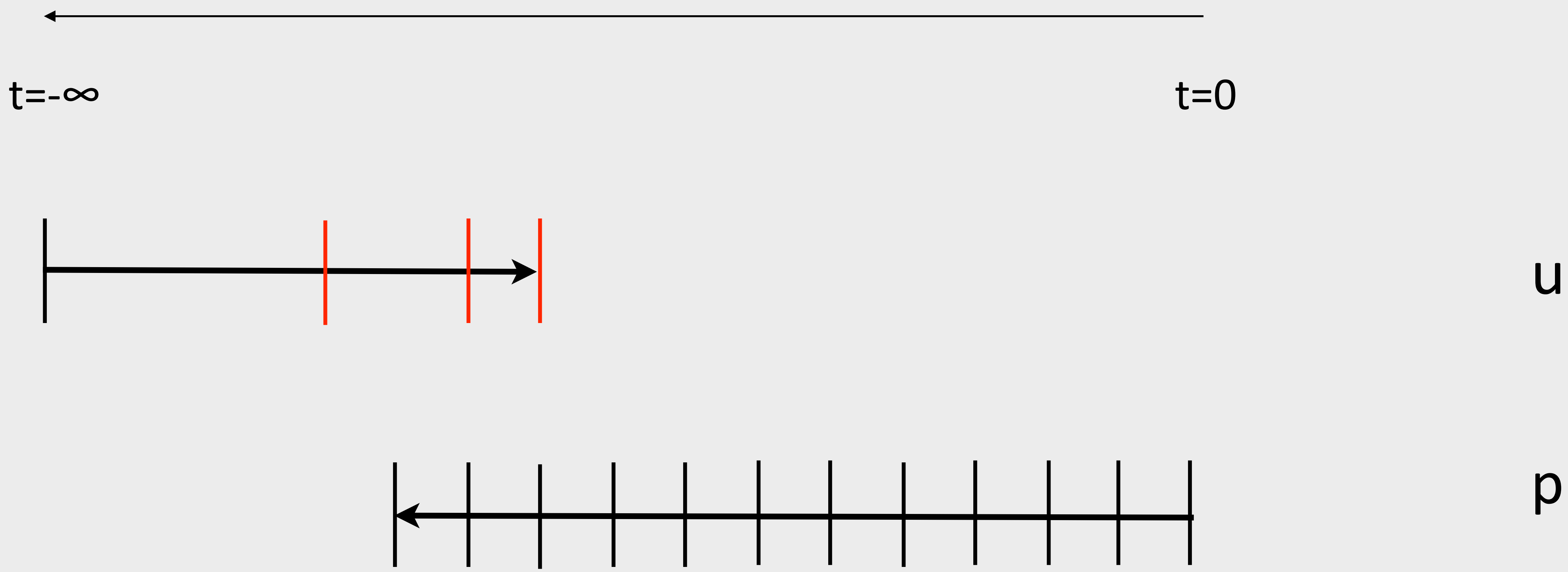
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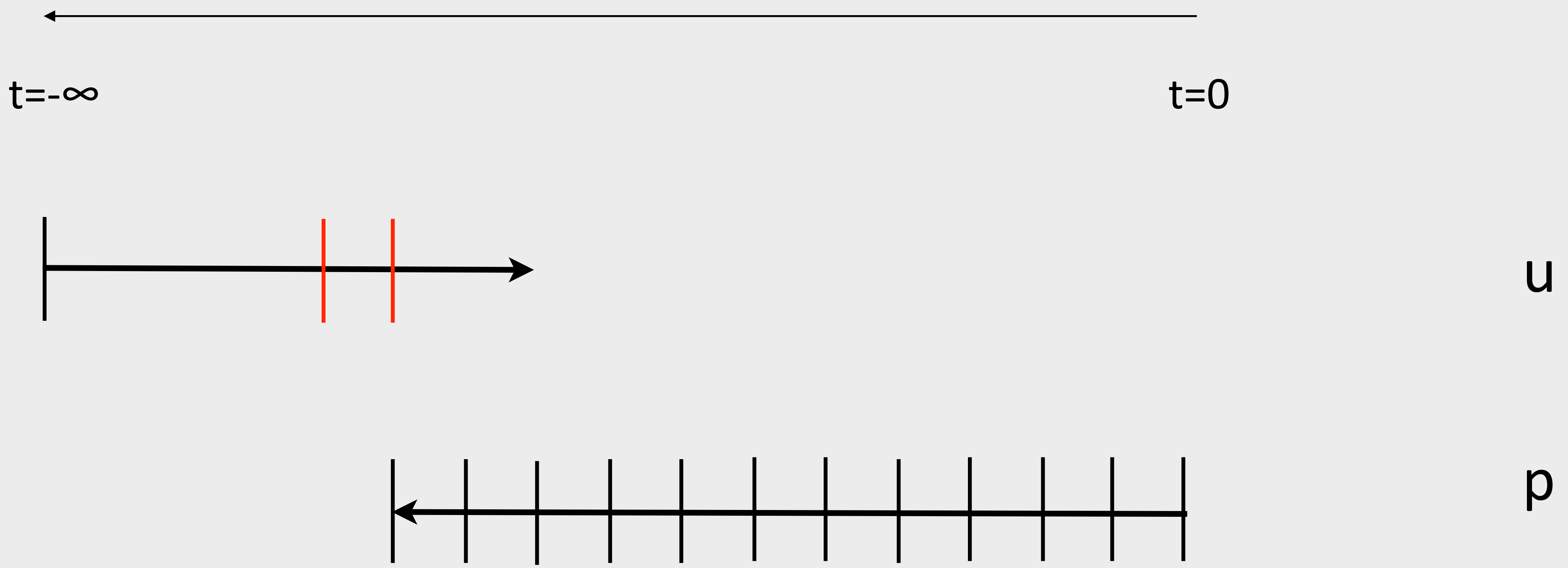
u
p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u
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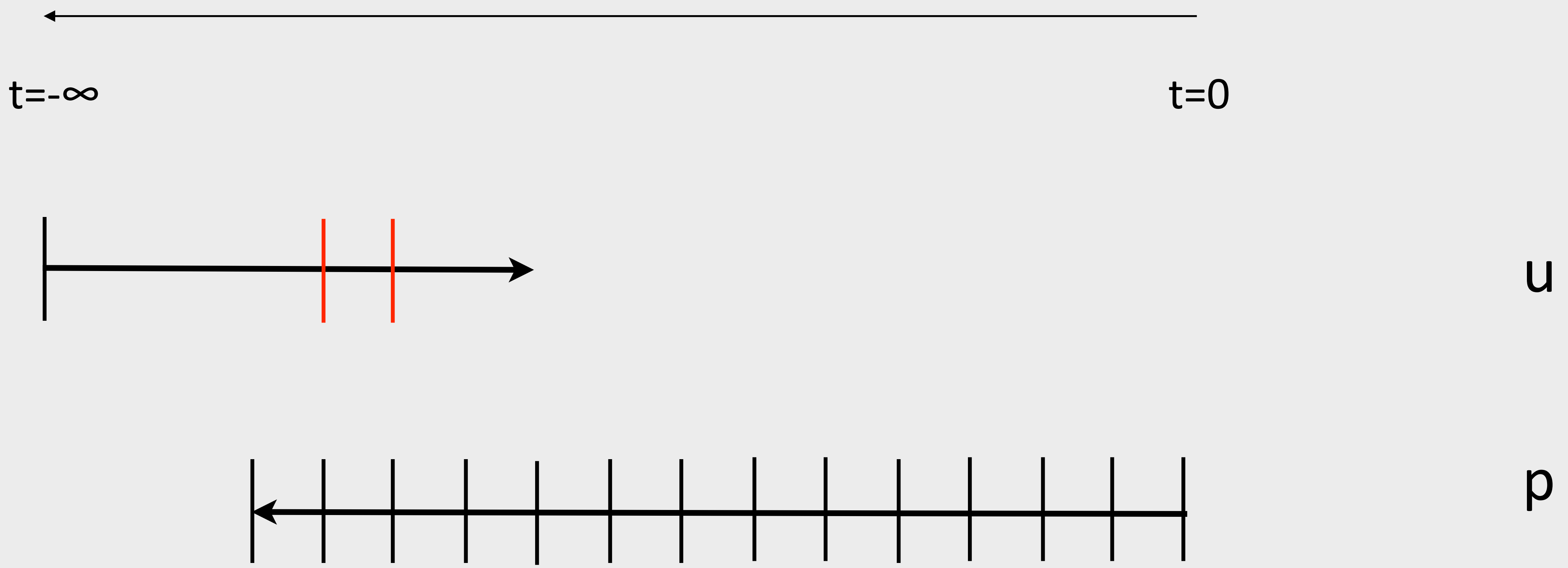

t=-∞
t=0
u
p

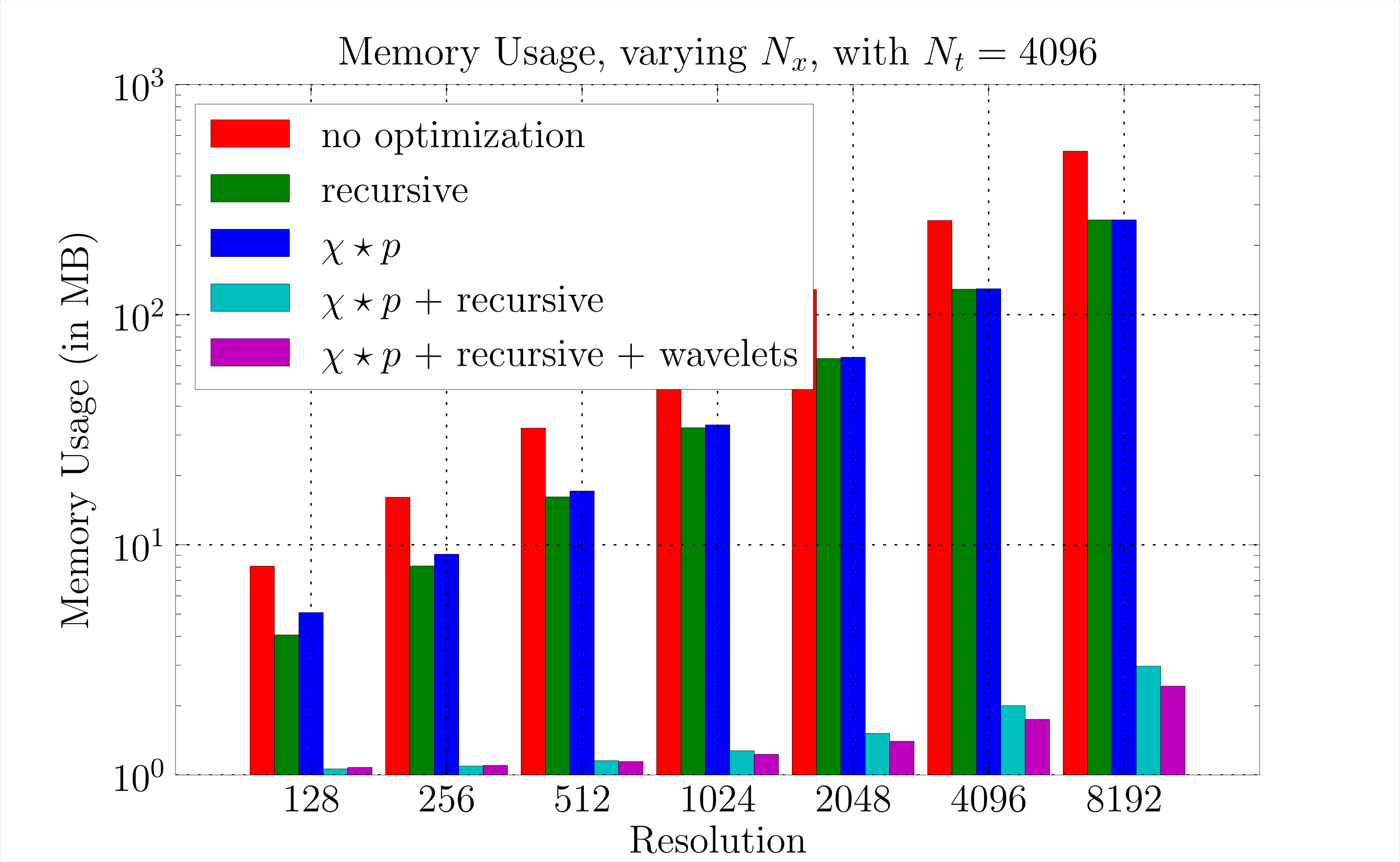

t=-∞
t=0
u
p


t=-∞
t=0
u
p


t=-∞
t=0
u
p

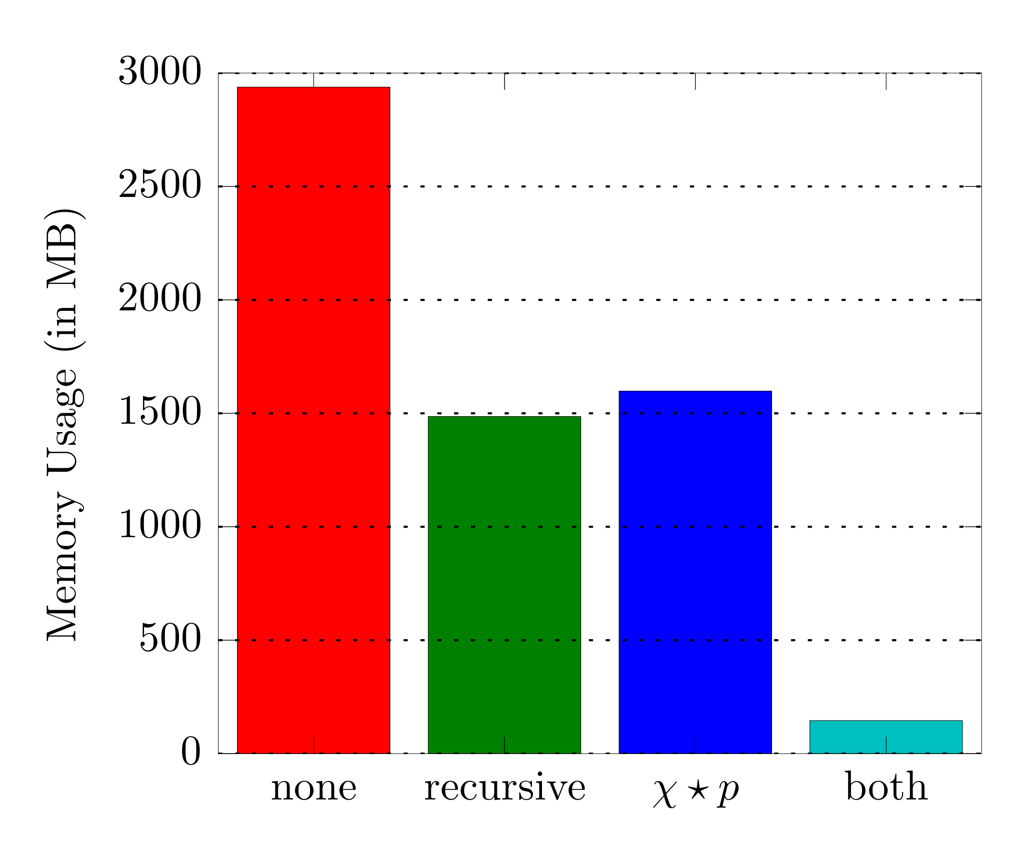
done

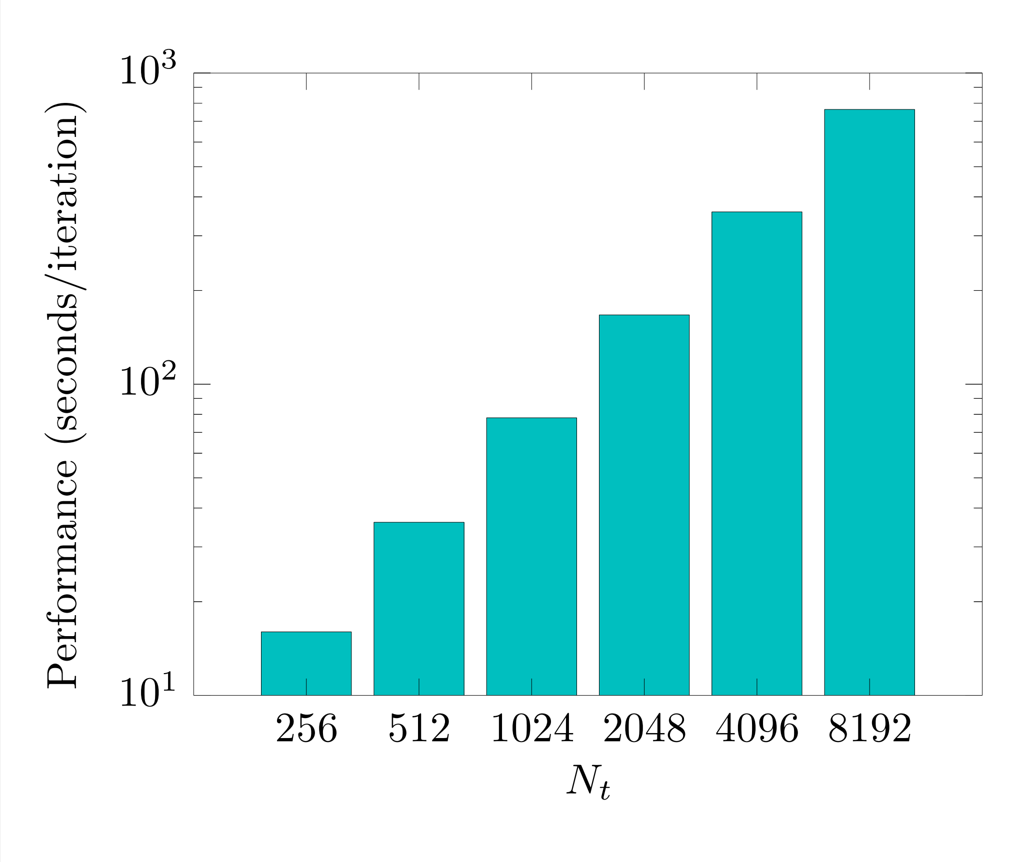
1D Burgers



257MB naive vs. 2MB optimized

2D Burgers

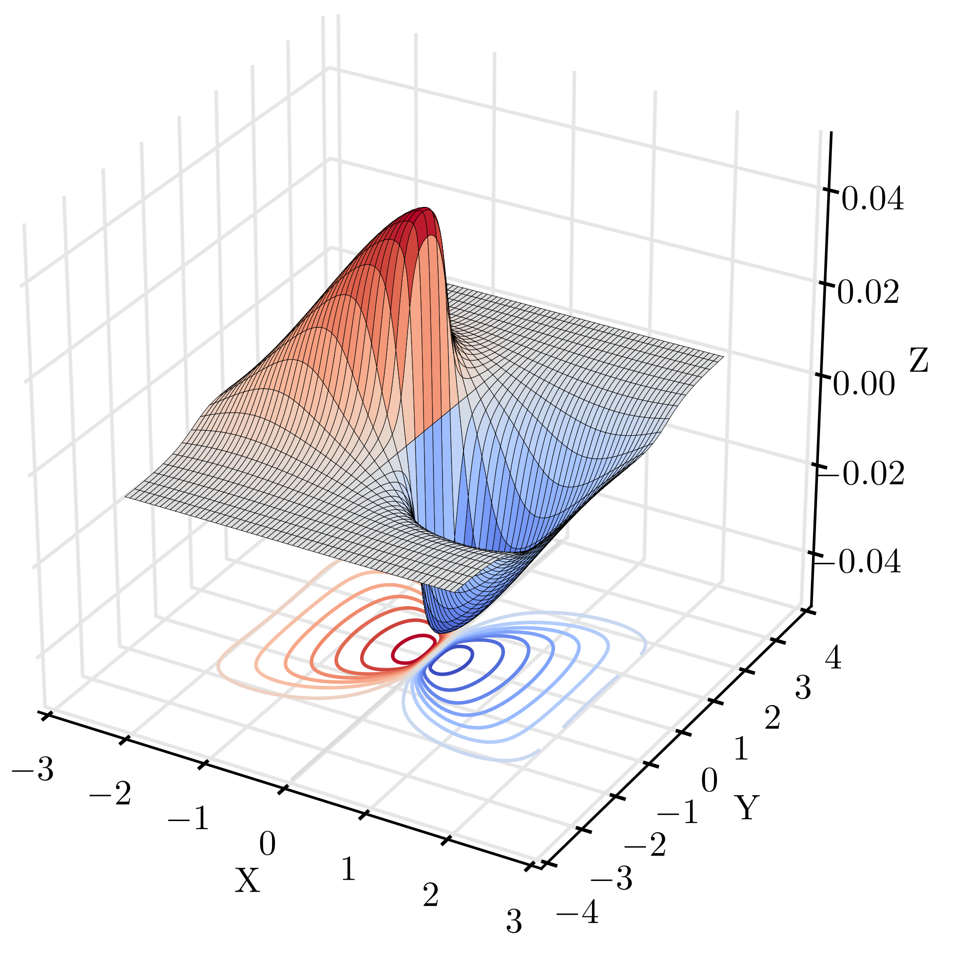




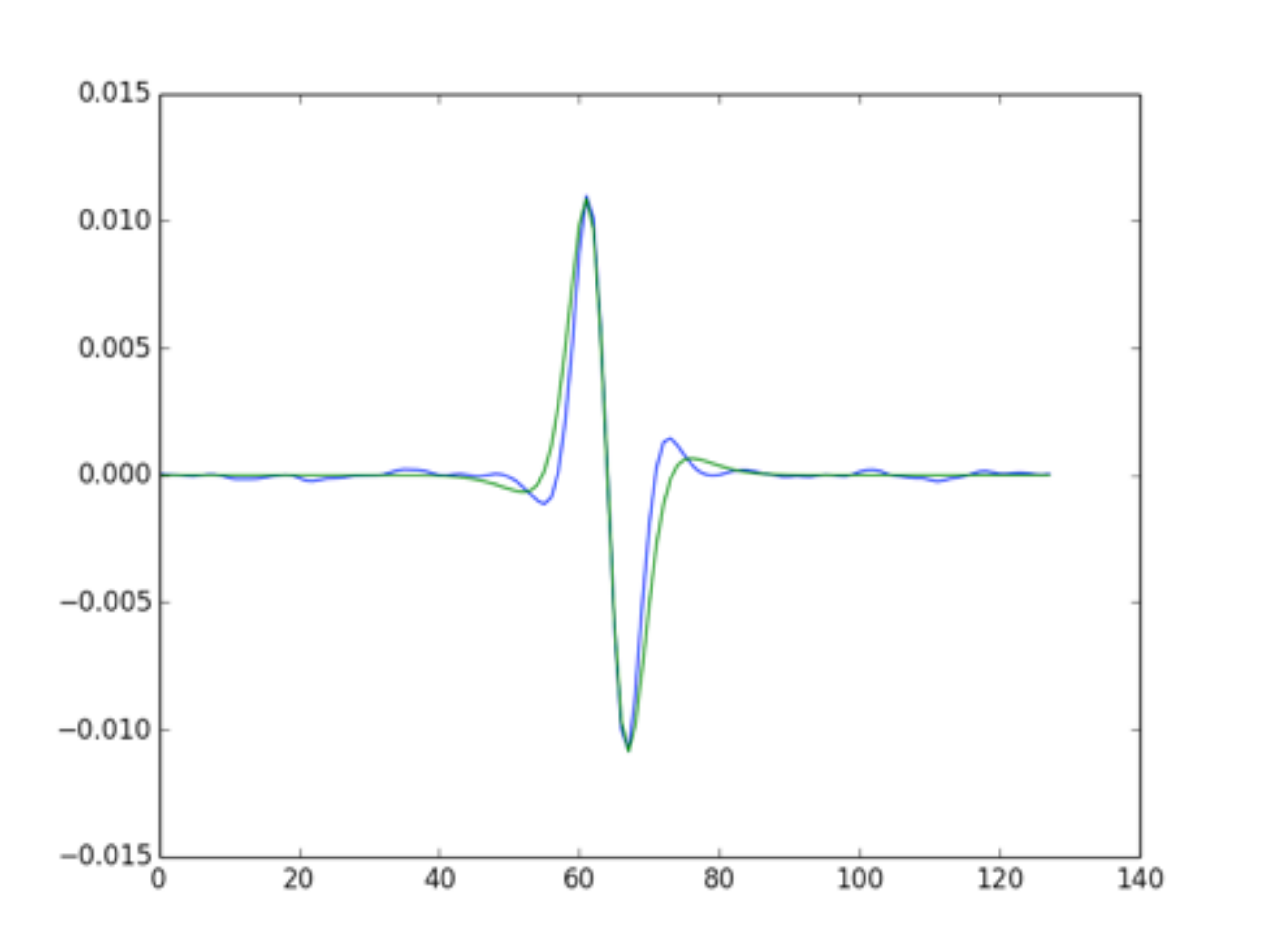
Left: The total memory saving of the combined algorithm exceeds a factor of 200.

Right: Performance of the optimized algorithm for N_x =1024×1024 and varying N_t scales as $O(N_t \log N_t)$.

2D Burgers



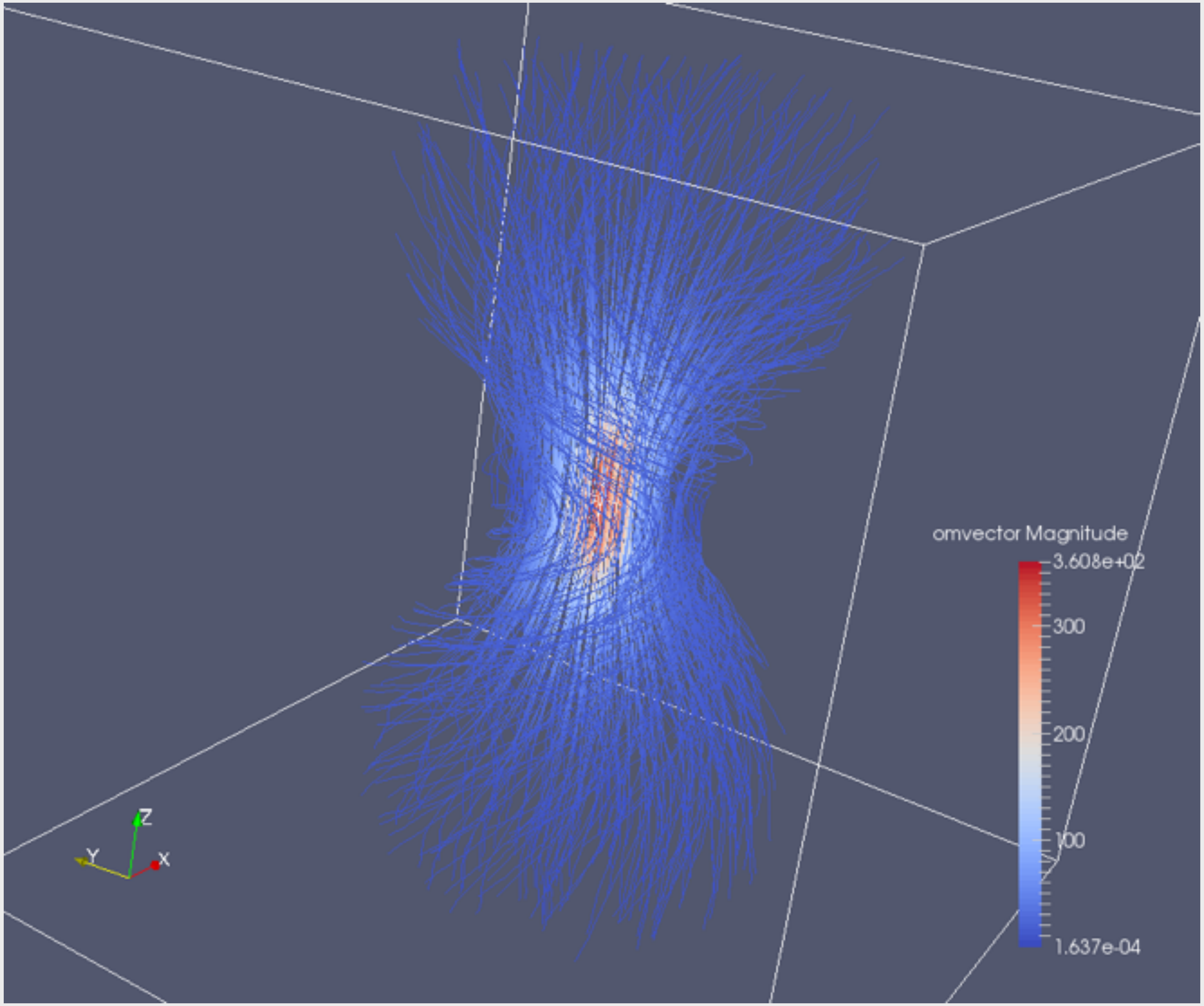
Solution of Instanton equations

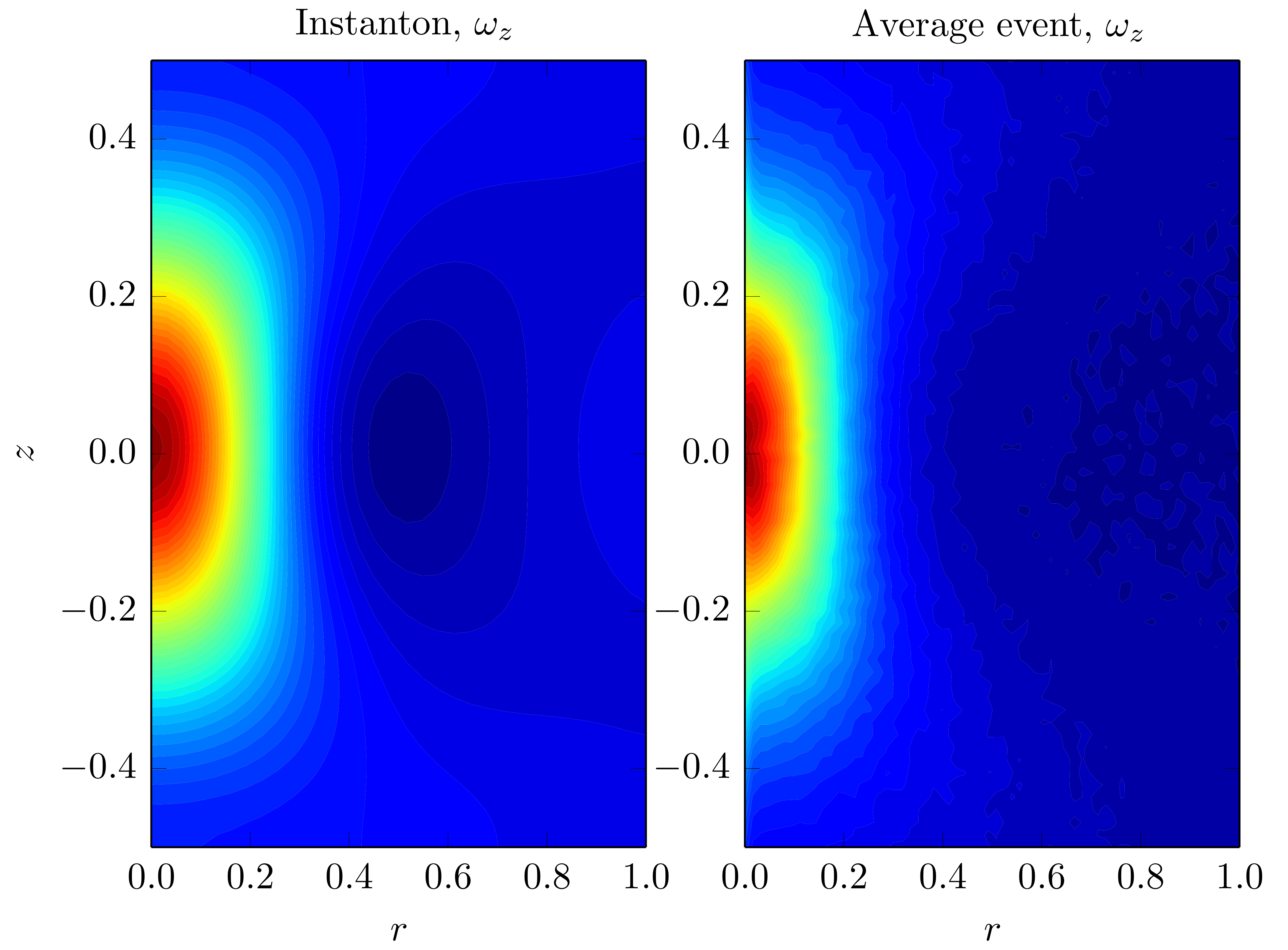


Filtering: shifting and rotating

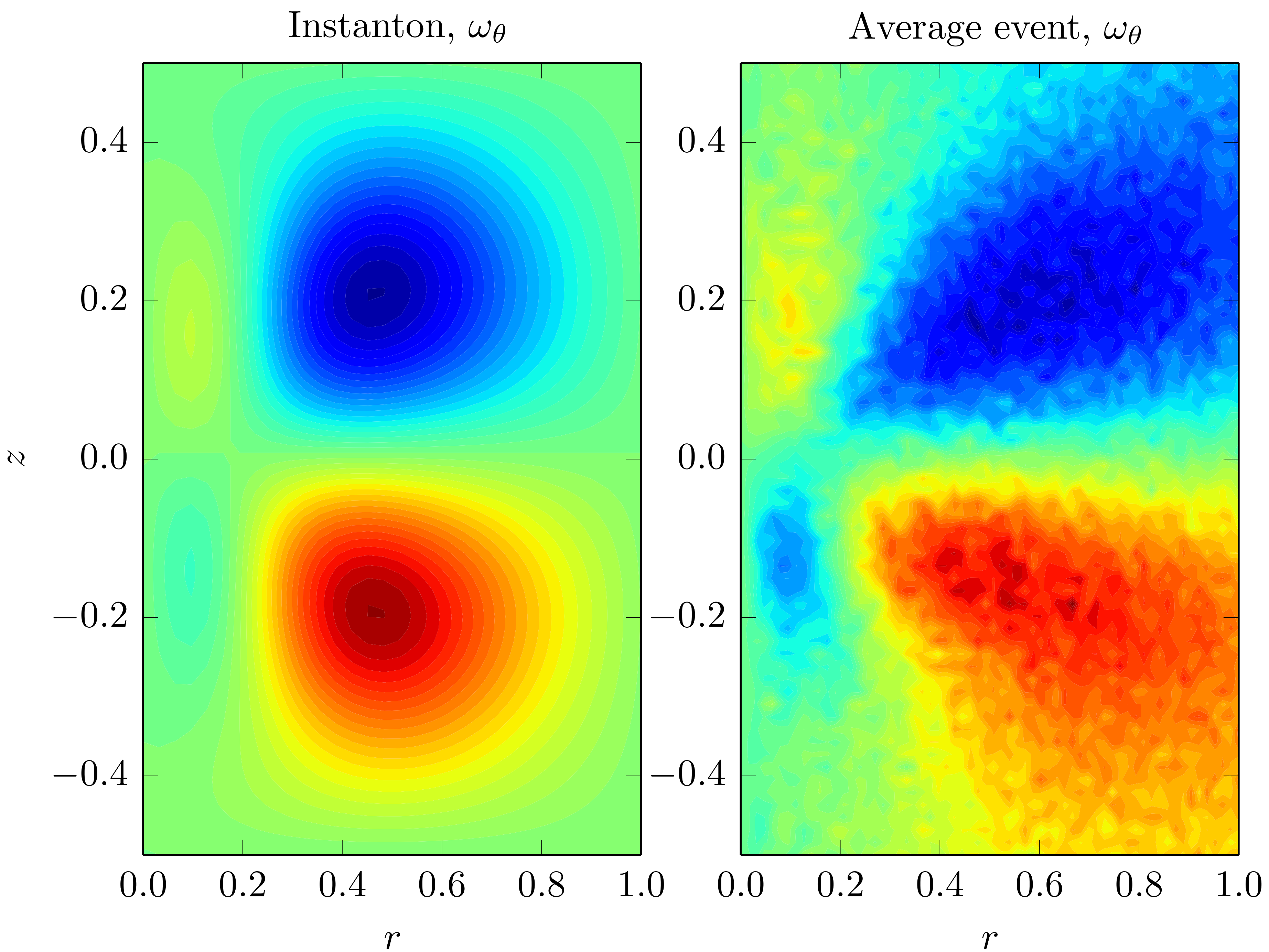
3D Navier-Stokes Instanton

see Mui, Dommermuth, Novikov 1996
Wilczek 2011

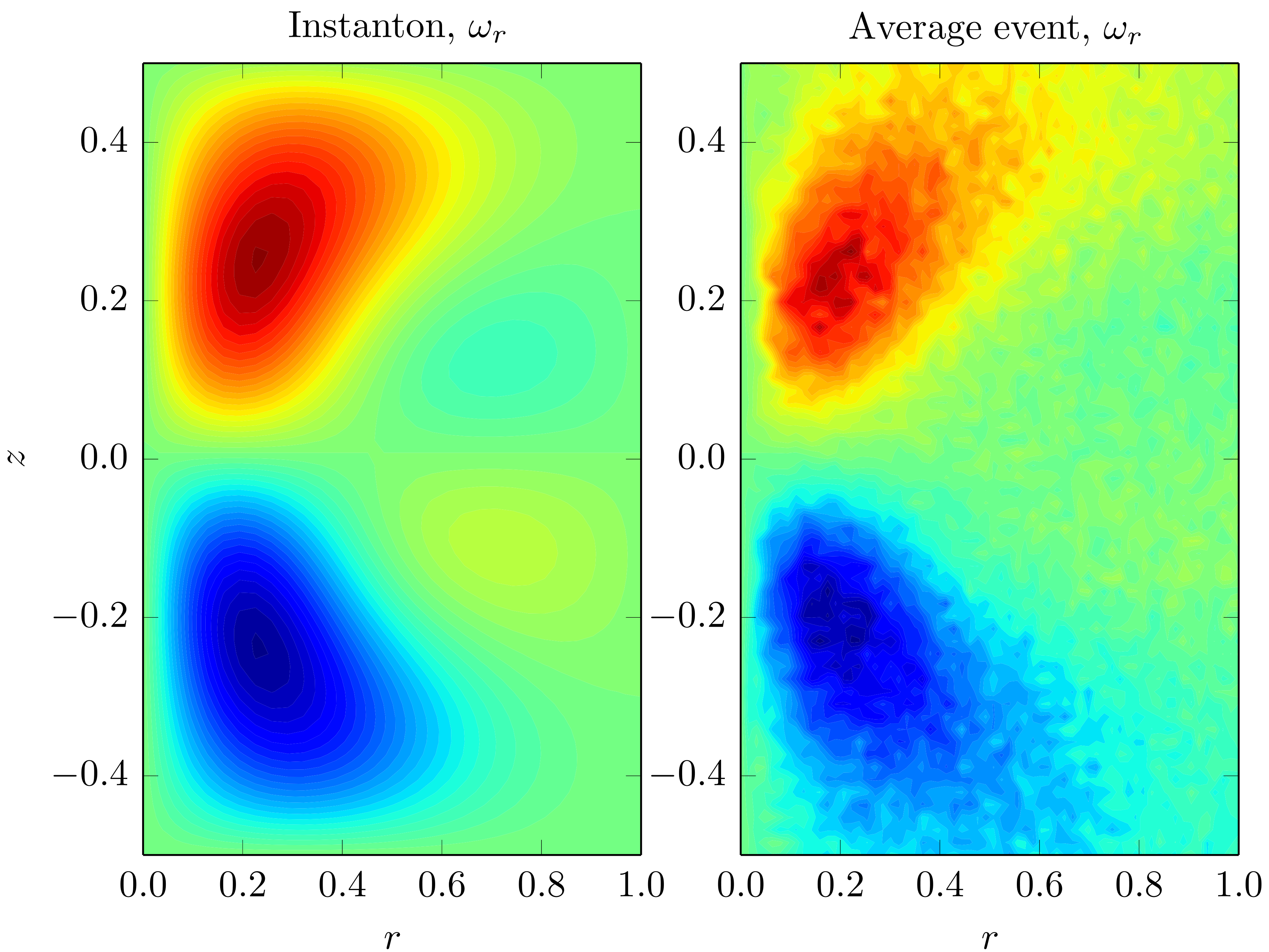



Instanton, ω_z
Average event, ω_z
0.4
0.2
0.0
−0.2
−0.4
z
0.0
0.2
0.4
0.6
0.8
1.0
r

Instanton for the 3D Navier-Stokes equations

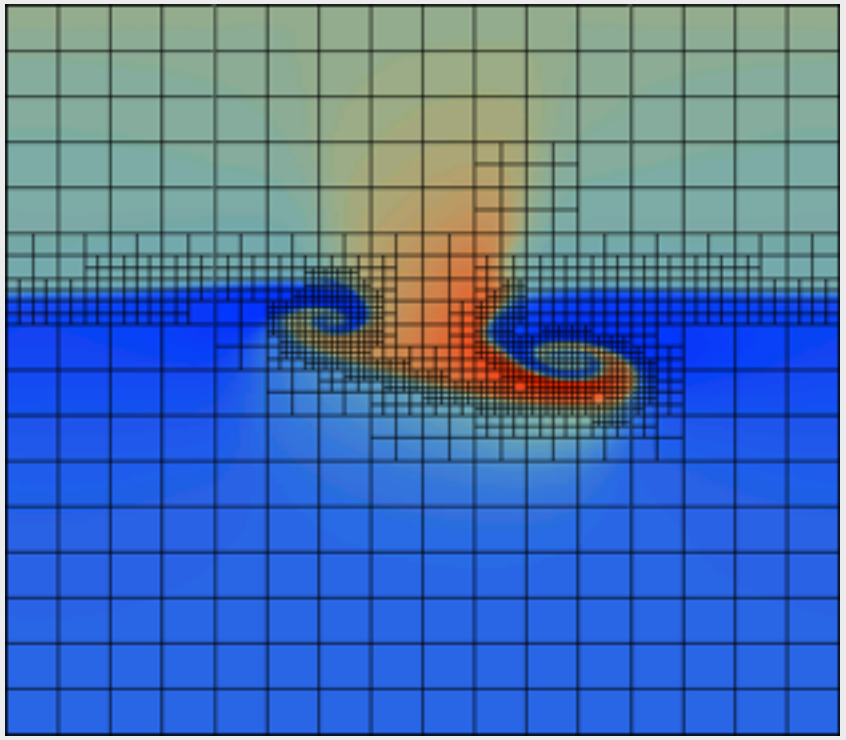


Instanton for the 3D Navier-Stokes equations



- What's next?

- Adaptive Mesh Refinement
- 3D Experiments ???
- fluctuations around the instanton
  - calculate fluctuation determinant



eigenvalues of a matrix of size

in 1D: (2048x4096)x(2048x4096)

in 2D: (2048x2048x4096)x(2048x2048x4096)

the matrix is very, very sparse

need only eigenvalues near zero

Thank You