# Closure Theories

Symbolic notation:

$$\partial_t u(k) = uu - \nu k^2 u(k)$$

averaging and since $\langle u \rangle = 0 \Longrightarrow 0 = 0$

We want to calculate spectral tensor $\langle u(k)u(k') \rangle$ :

$$\left(\partial_t + \nu\left(k^2 + k^2\right)\right)\left\langle u(k)u\left(k'\right)\right\rangle = \langle uuu \rangle$$

not closed: need evolution of $\langle uuu \rangle$

$$\left(\partial_t + \nu\left(k^2 + p^2 + q^2\right)\right)\langle u(k)u(p)u(q) \rangle = \langle uuuu \rangle$$

also not closed: what's next ?

Try to manipulate $\langle uuuu \rangle$ !

# Closure Theories

proposed by Chou (1940), Millionshtchikov (1941
worked out by Proudman and Reid (1954), Tatsumi (1957)

Consider Gaussian random functions:

Let $X$ be a four-dimensional variable (3 space +1 time), and let $g(X)$ be a random function of $X$ ($g$ might also be a vector) of zero mean. $g$ is a Gaussian random function if, given $N$ arbitrary numbers $\alpha_i$ and $N$ values $X_i$ of $X$, the linear combination $\sum \alpha_i X_i$ is a Gaussian random variable.

If $g(X)$ is a Gaussian random variable, then

- the odd moments of $g$ are zero. (Now you understand why we need the fourth-order moment.)
- the even moments can be expressed in terms of the second-order moments,e.g.

$$
\begin{aligned}
\left\langle g\left(X_1\right) g\left(X_2\right) g\left(X_3\right) g\left(X_4\right)\right\rangle = & \left\langle g\left(X_1\right) g\left(X_2\right)\right\rangle\left\langle g\left(X_3\right) g\left(X_4\right)\right\rangle \\
& +\left\langle g\left(X_1\right) g\left(X_3\right)\right\rangle\left\langle g\left(X_2\right) g\left(X_4\right)\right\rangle \\
& +\left\langle g\left(X_1\right) g\left(X_4\right)\right\rangle\left\langle g\left(X_2\right) g\left(X_3\right)\right\rangle
\end{aligned}
$$

Derivations from the Gaussian behavior are captured in the cummulants.

# Closure Theories

Idea of the Quasi-Normal approximation (Q.N.):

replace $\langle uuuu \rangle$ by the Gaussian values $\sum \langle uu \rangle \langle uu \rangle$

$$\left(\partial_t + \nu\left(k^2 + p^2 + q^2\right)\right)\langle u(k)u(p)u(q)\rangle = \sum \langle uu \rangle \langle uu \rangle$$

integrate in time and plug in equation for the spectral tensor:

$$\left(\partial_t + 2\nu k^2\right) U_{ij}(k,t) = \int_0^t d\tau \int_{p+q=k} dp \exp\left[-\nu\left(k^2 + p^2 + q^2\right)(t-\tau)\right]$$

isotropic turbulence without helicity:

$$\left(\partial_t + 2\nu k^2\right) E(k,t) = \int_0^t d\tau \int_{p+q=k} dp \exp\left[-\nu\left(k^2 + p^2 + q^2\right)(t-\tau)\right]$$

where $b(k,p,q)$ is a known function.

Note: this is an easy equation !!!

# Closure Theories

Numerical simulation of Ogura (1963):
negative energy spectra of large eddies $\Longrightarrow$ USELESS

Reason for failure identified by Orszag (1970, 1977):

Q.N. builds up to high third-order moments

fourth-order cummulants (discarded in Q.N.) provide damping to saturate third-order moments.

This is the motivation of the

**Eddy-Damped Quasi-Normal type theories**

Orszag (1970, 1977): approximate fourth-oder cumulants (neglected in Q.N.) by a linear damping term $\mu_{kpq}$

$$\left(\partial_t + \nu\left(k^2 + p^2 + q^2\right) + \mu_{kpq}\right)\langle u(k)u(p)u(q)\rangle = \sum \langle uu\rangle\langle uu\rangle$$

where $\mu_{kpq}$ is a damping rate associated to the triad $(k, p, q)$ having the dimension of an inverse time.

# Closure Theories

Isotropic turbulence: $\mu_{kpq} = \mu_k + \mu_p + \mu_q$

Orszag (1970): $\mu_k \sim \left[k^3 E(k)\right]^{1/2}$

$\mu_k$ is kind of frequency, therefore should be higher for higher $k$

$\Longrightarrow$ Does not work for decaying turbulence where spectrum can be rapidly decreasing for large $k$ and thus producing low frequency.

Much better ansatz: Frisch (1974) and Pouquet et al (1975)

$$\mu_k \sim \left[\int_0^k p^2 E(p,t) dp\right]^{1/2}$$

takes into account large eddies and produces always growing $\mu_k$

Eddy-Damped Quasi-Normal approximation (E.D.Q.N)

$$\left(\partial_t + 2\nu k^2\right) U_{ij}(k,t) = \int_0^t d\tau \int_{p+q=k} dp \exp\left[-\mu_{kpq} - \nu\left(k^2 + p^2 + q^2\right)(t-\tau)\right] \sum \langle uu \rangle \langle uu \rangle (\tau)$$

E.D.Q.N. physically more acceptable, but does not guarantee realizability (positivity of energy spectrum)

# Closure Theories

Orszag (1977): minor modification, called Markovianization

exponential term in integrand varies with much smaller time scale than nonlinear term $\sum \langle uu \rangle \langle uu \rangle$ of the order of large eddy turnover time

$\Longrightarrow$ change

$$\sum \langle uu \rangle \langle uu \rangle(\tau) \longrightarrow \sum \langle uu \rangle \langle uu \rangle(t)$$

Energy spectrum of Eddy-Damped Quasi-Normal Markovian approximation (E.D.Q.N.M)

$$\left(\partial_t + 2\nu k^2\right) E(k,t) = \int_{p+q=k} dp \theta_{kpq} \frac{k}{pq} b(k,p,q) \left[k^2 E(p,t) - p^2 E(k,t)\right] E(q,t)$$

with

$$\theta_{kpq} = \int_0^t \exp\left[-\left(\mu_{kpq} + \nu\left(k^2 + p^2 + q^2\right)\right)\right](t-\tau)d\tau$$

Orszag (1977): E.D.Q.N.M has positive energy spectrum

# Renormalized Perturbation Theory

Perturbation expansion of the Navier-Stokes equation

| | |
|---|---|
| Kraichnan (1959): | direct-interaction approximation |
| Wyld (1961): | partial summation for a simplified scalar model |
| Lee (1965): | partial summation for Navier-Stokes and MHD |

The zero-order isotropic propagators

$$\left(\frac{\partial}{\partial t} + \nu k^2\right) u_\alpha(\mathbf{k}, t) = \lambda M_{\alpha\beta\gamma}(\mathbf{k}) \sum_j u_\beta(\mathbf{j}, t) u_\gamma(\mathbf{k} - \mathbf{j}, t) + D_{\alpha\beta}(\mathbf{k}) f_\beta(\mathbf{k}, t)$$

$\lambda$: bookkeeping parameter, $D_{\alpha\beta}$: projector on divergence free part

zero-order Green tensor: $$\left(\frac{\partial}{\partial t} + \nu k^2\right) G^{(0)}_{\alpha\beta}(\mathbf{k}; t, t') = D_{\alpha\beta}(\mathbf{k}) \delta(t - t')$$

with $$G^{(0)}_{\alpha\beta}(\mathbf{k}; t, t') = D_{\alpha\beta}(\mathbf{k}) G_0\left(k; t, t'\right)$$

so that $$\left(\frac{\partial}{\partial t} + \nu k^2\right) G_0\left(k; t, t'\right) = \delta(t - t')$$

# Renormalized Perturbation Theory

zero-order velocity:

$$u_\alpha^{(0)}(\mathbf{k},t) = \int \mathrm{d}t' G_{\alpha\beta}^{(0)}(\mathbf{k};t,t') f_\beta(\mathbf{k},t') = D_{\alpha\beta}(\mathbf{k}) \int \mathrm{d}t' G_0\left(k;t,t'\right) f_\beta(\mathbf{k},t')$$

Fourier transform in time:

$$u_\alpha(\mathbf{x},t) = \sum_{\mathbf{k}} \sum_{\omega} u_\alpha(\mathbf{k},\omega) \exp\{i\mathbf{k}\cdot\mathbf{x} + i\omega t\}$$

$\Longrightarrow$ Navier-Stokes

$$\left(\mathrm{i}\omega + \nu k^2\right) u_\alpha(\mathbf{k},\omega) = \lambda M_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{j}} \sum_{\omega'} u_\beta\left(\mathbf{j},\omega'\right) u_\gamma\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right) + D_{\alpha\beta}(\mathbf{k}) f_\beta(\mathbf{k},\omega)$$

zero-order propagator is given by

$$G_0(\mathbf{k},\omega) = \frac{1}{\mathrm{i}\omega + \nu k^2}$$

# Renormalized Perturbation Theory

## The primitive perturbation expansion

Stirring force $$\left(\frac{L}{2\pi}\right)^3 \left\langle f_\alpha(\mathbf{k},t) f_\beta(-\mathbf{k},t')\right\rangle = D_{\alpha\beta}(\mathbf{k}) w\left(k;t,t'\right)$$

after Fourier-trafo $$\left(\frac{L}{2\pi}\right)^3 \left(\frac{T}{2\pi}\right) \left\langle f_\alpha(\mathbf{k},\omega) f_\beta(-\mathbf{k},\omega')\right\rangle = D_{\alpha\beta}(\mathbf{k}) w\left(k;\omega,\omega'\right)$$

zero-order velocity field after in Fourier-space $$u_\alpha^{(0)}(\mathbf{k},\omega) = D_{\alpha\beta}(\mathbf{k}) G_0(k,\omega) f_\beta(\mathbf{k},\omega)$$

which is the zero-order term in expansion

$$u_\alpha(\mathbf{k},\omega) = u_\alpha^{(0)}(\mathbf{k},\omega) + \lambda u_\alpha^{(1)}(\mathbf{k},\omega) + \lambda^2 u_\alpha^{(2)}(\mathbf{k},\omega) + \cdots + -\lambda^n u_\alpha^{(n)}(\mathbf{k},\omega) + \cdots$$

correlation $Q_{\alpha\beta}(\mathbf{k};\omega,\omega')$

$$\left\langle u_\alpha^{(0)}(\mathbf{k},\omega) u_\beta^{(0)}(-\mathbf{k},\omega')\right\rangle = D_{\alpha\gamma}(\mathbf{k}) D_{\beta\sigma}(-\mathbf{k}) G_0(k,\omega) G_0\left(-k,\omega'\right) \left\langle f_\gamma(\mathbf{k},\omega) f_\sigma(-\mathbf{k},\omega')\right\rangle$$

$$= D_{\alpha\gamma}(\mathbf{k}) D_{\beta\sigma}(\mathbf{k}) D_{\gamma\sigma}(\mathbf{k}) G_0(k,\omega) G_0\left(k,\omega'\right) \left(\frac{2\pi}{L}\right)^3 w\left(k;\omega,\omega'\right)$$

$$= \left(\frac{2\pi}{L}\right)^3 D_{\alpha\beta}(\mathbf{k}) G_0(\mathbf{k},\omega) G_0\left(k,\omega'\right) w\left(k;\omega,\omega'\right)$$

# Renormalized Perturbation Theory

homogeneous isotropic turbulence

$$\left(\frac{L}{2\pi}\right)^3 \left\langle u_\alpha^{(0)}(\mathbf{k},\omega) u_\beta^{(0)}(-\mathbf{k},\omega')\right\rangle = D_{\alpha\beta}(\mathbf{k}) Q_0\left(k;\omega,\omega'\right)$$

and

$$Q_0\left(k;\omega,\omega'\right) = G_0(k,\omega) G_0\left(k,\omega'\right) w\left(k;\omega,\omega'\right)$$

Perturbation expansion for $Q$

$$D_{\alpha\beta}(\mathbf{k}) Q\left(k;\omega,\omega'\right) = \left(\frac{2\pi}{L}\right)^3 \left\langle u_\alpha(\mathbf{k},\omega) u_\beta(-\mathbf{k},\omega')\right\rangle$$

$$= \left(\frac{2\pi}{L}\right)^3 \left\{ \left\langle u_\alpha^{(0)}(\mathbf{k},\omega) u_\beta^{(0)}(-\mathbf{k},\omega')\right\rangle + \right.$$

$$\left. + \lambda^2 \left[ \left\langle u_\alpha^{(0)} u_\beta^{(2)} \right\rangle + \left\langle u_\alpha^{(1)} u_\beta^{(1)} \right\rangle + \left\langle u_\alpha^{(2)} u_\beta^{(0)} \right\rangle \right] + O\left(\lambda^4\right) \right\}$$

$$= D_{\alpha\beta}(\mathbf{k}) Q_0\left(k;\omega,\omega'\right) + \left(\frac{2\pi}{L}\right)^3 \left\{ \lambda^2 \left[ \left\langle u_\alpha^{(0)} u_\beta^{(2)} \right\rangle + \right.\right.$$

$$\left.\left. + \left\langle u_\alpha^{(1)} u_\beta^{(1)} \right\rangle + \left\langle u_\alpha^{(2)} u_\beta^{(0)} \right\rangle \right] + O\left(\lambda^4\right) \right\}$$

# Renormalized Perturbation Theory

Take Fourier transformed NS-equation, invert linear part and substitute

forcing by $u^{(0)}$

$$u_\alpha(\mathbf{k},\omega) = u_\alpha^{(0)}(\mathbf{k},\omega) + \lambda G_0(k,\omega) M_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{j}} \sum_{\omega'} u_\beta\left(\mathbf{j},\omega'\right) u_\gamma\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right)$$

Now substitute perturbation expansion for $u$

$$\begin{aligned} &u_\alpha^{(0)}(\mathbf{k},\omega) + \lambda u_\alpha^{(1)}(\mathbf{k},\omega) + \lambda^2 u_\alpha^{(2)}(\mathbf{k},\omega) + \cdots \\ &\quad = u_\alpha^{(0)}(\mathbf{k},\omega) + \lambda G_0(k,\omega) M_{\alpha\beta\gamma}(\mathbf{k}) \times \sum_{\mathbf{j}} \sum_{\omega'} \Big\{ u_\beta^{(0)}\left(\mathbf{j},\omega'\right) u_\gamma^{(0)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right) \\ &\quad + \lambda \left[ u_\beta^{(0)}\left(\mathbf{j},\omega'\right) u_\gamma^{(1)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right) + u_\beta^{(1)}\left(\mathbf{j},\omega'\right) u_\gamma^{(0)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right) \right] + O\left(\lambda^2\right) \Big\} \end{aligned}$$

equating coefficients:

$$u_\alpha^{(1)}(\mathbf{k},\omega) = G_0(k,\omega) M_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{j}} \sum_{\omega'} u_\beta^{(0)}\left(\mathbf{j},\omega'\right) u_\gamma^{(0)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right)$$

$$u_\alpha^{(2)}(\mathbf{k},\omega) = 2G_0(k,\omega) M_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{j}} \sum_{\omega'} u_\beta^{(1)}\left(\mathbf{j},\omega'\right) u_\gamma^{(0)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right)$$

# Renormalized Perturbation Theory

$u^{(2)}$ can be expressed by $u^{(0)}$

$$u_\alpha^{(2)}(\mathbf{k},\omega) = 2G_0(k,\omega)M_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{j}} \sum_{\omega'} G_0\left(\mathbf{j},\omega'\right) M_{\beta\rho\sigma}(\mathbf{j}) \times$$

$$\times \sum_{\mathbf{l}} \sum_{\omega''} u_\rho^{(0)}\left(\mathbf{l},\omega''\right) u_\sigma^{(0)}\left(\mathbf{j}-\mathbf{l},\omega'-\omega''\right) u_\gamma^{(0)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right)$$

stirring Gaussian $\Longrightarrow$ $u^{(0)}$ Gaussian

$\Longrightarrow \left\langle u^{(0)}u^{(0)}u^{(0)}u^{(0)}\right\rangle$ can be factored as in Quasi-Normal approximation

# Renormalized Perturbation Theory

second-order correlation tensor:

$$D_{\alpha\beta}(\mathbf{k})Q\left(k;\omega,\omega'\right) = D_{\alpha\beta}(\mathbf{k})Q_0\left(k;\omega,\omega'\right)+$$

$$+\lambda^2\Big[4G_0\left(k,\omega'\right)M_{\beta\delta\gamma}(-\mathbf{k})\int \mathrm{d}^3j\int \mathrm{d}\omega''\int \mathrm{d}\omega'''G_0\left(j,\omega''\right)\times$$

$$\times M_{\delta\rho\sigma}(\mathbf{j})D_{\alpha\rho}(\mathbf{k})D_{\gamma\sigma}(\mathbf{k}+\mathbf{j})\times Q_0\left(k;\omega,\omega'''\right)Q_0\left(|\mathbf{k}+\mathbf{j}|;\omega'-\omega'',\omega''-\omega'''\right)+$$

$$+2G_0(k,\omega)M_{\alpha\delta\gamma}(\mathbf{k})\int \mathrm{d}^3j\int \mathrm{d}\omega''\int \mathrm{d}\omega'''G_0\left(k,\omega'\right)\times$$

$$\times M_{\beta\rho\sigma}(-\mathbf{k})D_{\delta\sigma}(\mathbf{j})D_{\gamma\rho}(\mathbf{k}-\mathbf{j})\times Q_0\left(|\mathbf{k}-\mathbf{j}|;\omega-\omega'',\omega'''\right)Q_0\left(j;\omega'',\omega'-\omega'''\right)+$$

$$+4G_0(k,\omega)M_{\alpha\delta\gamma}(\mathbf{k})\int \mathrm{d}^3j\int \mathrm{d}\omega''\int \mathrm{d}\omega'''G_0\left(j,\omega''\right)\times$$

$$\times M_{\delta\rho\sigma}(\mathbf{j})D_{\beta\rho}(\mathbf{k})D_{\sigma\gamma}(\mathbf{k}-\mathbf{j})\times Q_0\left(k;\omega',\omega'''\right)Q_0\left(|\mathbf{k}-\mathbf{j}|;\omega-\omega'',\omega''-\omega'''\right)\Big]+O\left(\lambda^4\right)$$

# Renormalized Perturbation Theory

**Graphical representation of the perturbation series**

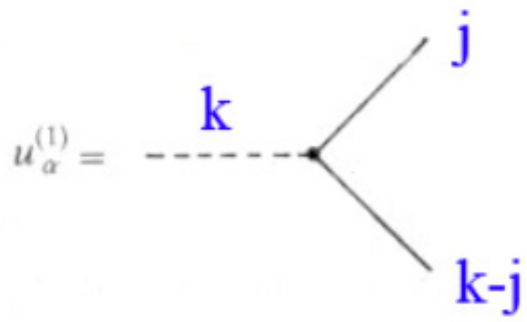
all orders can be expressed by zero-order terms, but possible divergent series

three main constituents: $u^{(0)}$, $G_0$ and $M$

| | |
|---|---|
| full line | $\leftrightarrow u^{(0)}$ |
| broken line | $\leftrightarrow G_0$ |
| point (vertex) | $\leftrightarrow M$ |

zero-order: $u_\alpha^{(0)}(\mathbf{k}, t) =$ 

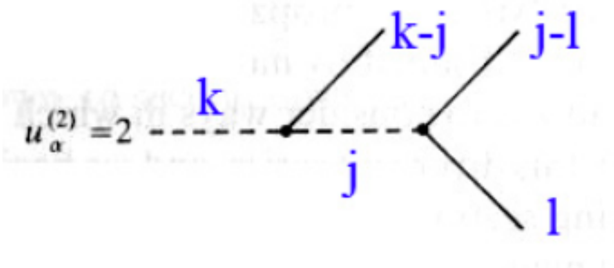
first-order: wavenumber conservation




$$u_\alpha^{(1)}(\mathbf{k}, \omega) = G_0(k, \omega) M_{\alpha\beta\gamma}(\mathbf{k}) \sum_{\mathbf{j}} \sum_{\omega'} u_\beta^{(0)}\left(\mathbf{j}, \omega'\right) u_\gamma^{(0)}\left(\mathbf{k} - \mathbf{j}, \omega - \omega'\right)$$

# Renormalized Perturbation Theory

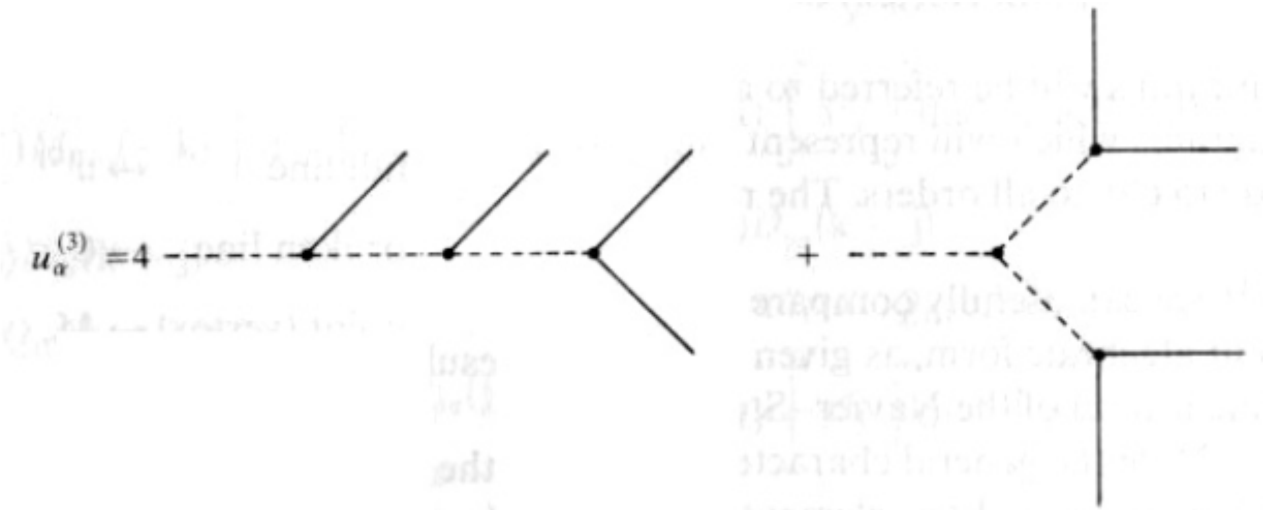
second-order: two $M$ factors:




$$u_\alpha^{(2)}(\mathbf{k},\omega) = 2G_0(k,\omega)M_{\alpha\beta\gamma}(\mathbf{k})\sum_{\mathbf{j}}\sum_{\omega'} G_0\left(\mathbf{j},\omega'\right) M_{\beta\rho\sigma}(\mathbf{j}) \times$$

$$\times \sum_{\mathbf{l}}\sum_{\omega''} u_\rho^{(0)}\left(\mathbf{l},\omega''\right) u_\sigma^{(0)}\left(\mathbf{j}-\mathbf{l},\omega'-\omega''\right) u_\gamma^{(0)}\left(\mathbf{k}-\mathbf{j},\omega-\omega'\right)$$

third-order: three $M$ factors:

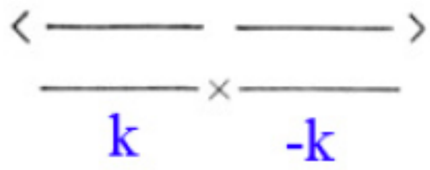


# Renormalized Perturbation Theory

graphical expansion for correlation tensor

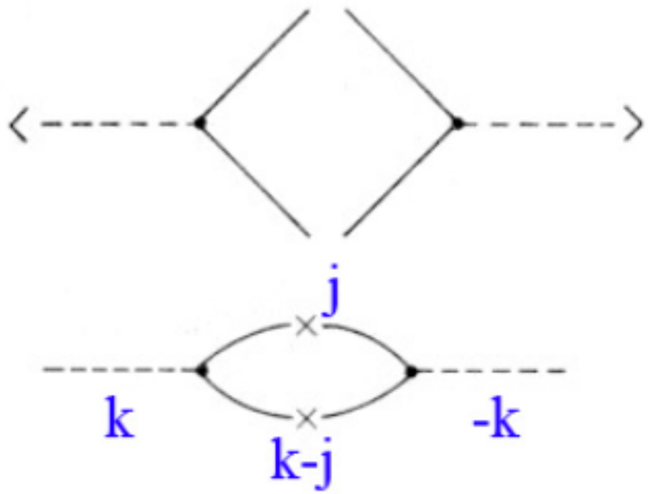
zero-order: $\langle u_\alpha^{(0)}(\mathbf{k})\, u_\beta^{(0)}(-\mathbf{k}) \rangle =$

$=$




second order: $\langle u_\alpha^{(1)}(\mathbf{k})\, u_\beta^{(1)}(-\mathbf{k}) \rangle =$

$= 2$

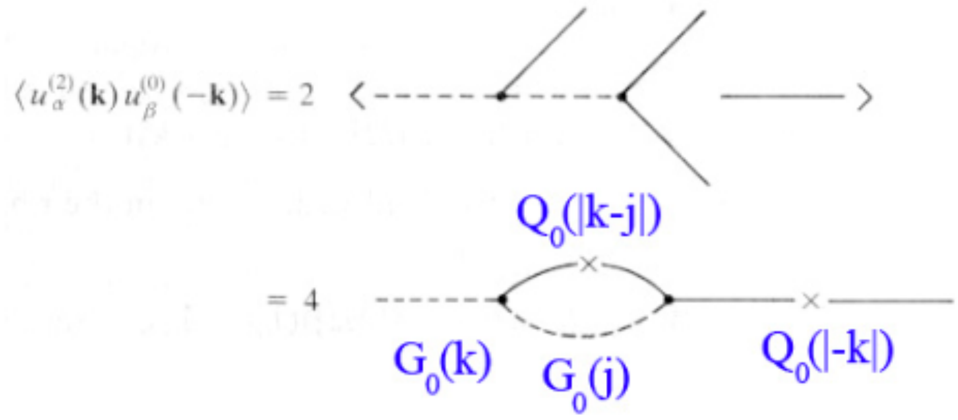



this is middle second-order term:

$$+2G_0(k,\omega)M_{\alpha\delta\gamma}(\mathbf{k})\int \mathrm{d}^3j \int \mathrm{d}\omega'' \int \mathrm{d}\omega''' G_0\left(k,\omega'\right) \times$$

$$\times M_{\beta\rho\sigma}(-\mathbf{k})D_{\delta\sigma}(\mathbf{j})D_{\gamma\rho}(\mathbf{k}-\mathbf{j}) \times Q_0\left(|\mathbf{k}-\mathbf{j}|;\omega-\omega'',\omega'''\right) Q_0\left(j;\omega'',\omega'-\omega'''\right)+$$

# Renormalized Perturbation Theory




this is the last second-order term:

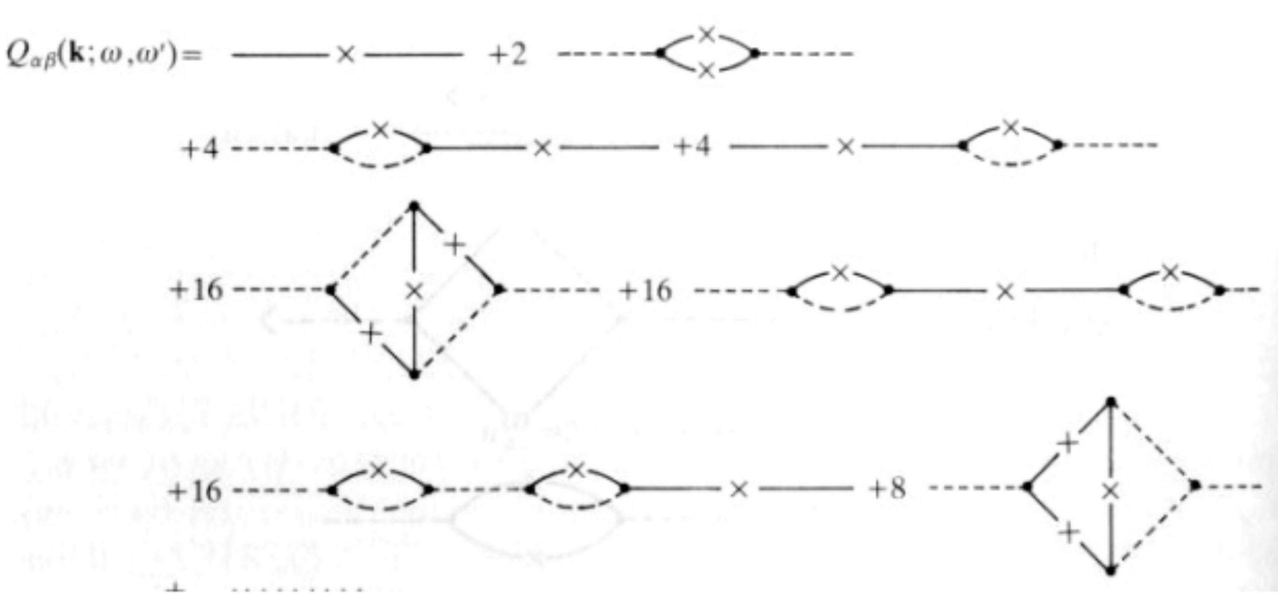
$$+4G_0(k,\omega)M_{\alpha\delta\gamma}(\mathbf{k})\int \mathrm{d}^3 j\int \mathrm{d}\omega''\int \mathrm{d}\omega''' G_0\left(j,\omega''\right)\times$$

$$\times M_{\delta\rho\sigma}(\mathbf{j})D_{\beta\rho}(\mathbf{k})D_{\sigma\gamma}(\mathbf{k}-\mathbf{j})\times Q_0\left(k;\omega',\omega'''\right)Q_0\left(|\mathbf{k}-\mathbf{j}|;\omega-\omega'',\omega''-\omega'''\right)\Big]$$

The third is a mirror image of this one.

## Renormalized Perturbation Theory

fourth-order showing four of the 29 fourth-order diagrams:




Now **resummation** (renormalisation): new diagram elements

| | | |
|---|---|---|
| thick full line | $\leftrightarrow$ $u$ | (exact velocity field) |
| thick broken line | $\leftrightarrow$ $G$ | (renormalized propagator) |
| open circle | $\leftrightarrow$ | (renormalized vertex) |

Write correlation tensor as:

$$Q_{\alpha\beta}(\mathbf{k};\omega,\omega') = Q_{\alpha\beta}(\mathbf{k};\omega,\omega')_A + Q_{\alpha\beta}(\mathbf{k};\omega,\omega')_B$$

Class A diagrams Class B diagrams

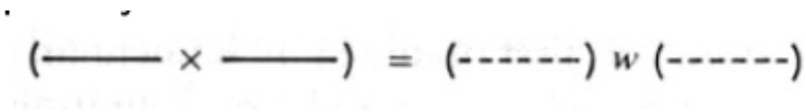
# Renormalized Perturbation Theory

## Class A diagram: the renormalized propagator

Wyld (1961): Class A diagrams are those diagrams which can be split into two pieces by cutting a single $Q_0$ line.

zero-order: $Q_0$ can be expressed in terms of two zero-order propagators acting on the spectrum of the stirring forces $w\left(k; \omega, \omega'\right)$

This looks graphically like



Now second order:

# Renormalized Perturbation Theory

Let's summarize: at zero order, we have $w$ with a $G_0$ on each side. At second order, $w$ has a $G_0$ on one side and a diagram which connects like a $G_0$ on the other. This holds for all orders. Thus we have a generalization

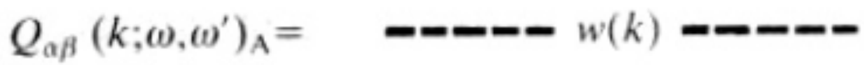
$$Q_0\left(k;\omega,\omega'\right)=G_0(k,\omega)G_0\left(k,\omega'\right)w\left(k;\omega,\omega'\right)$$

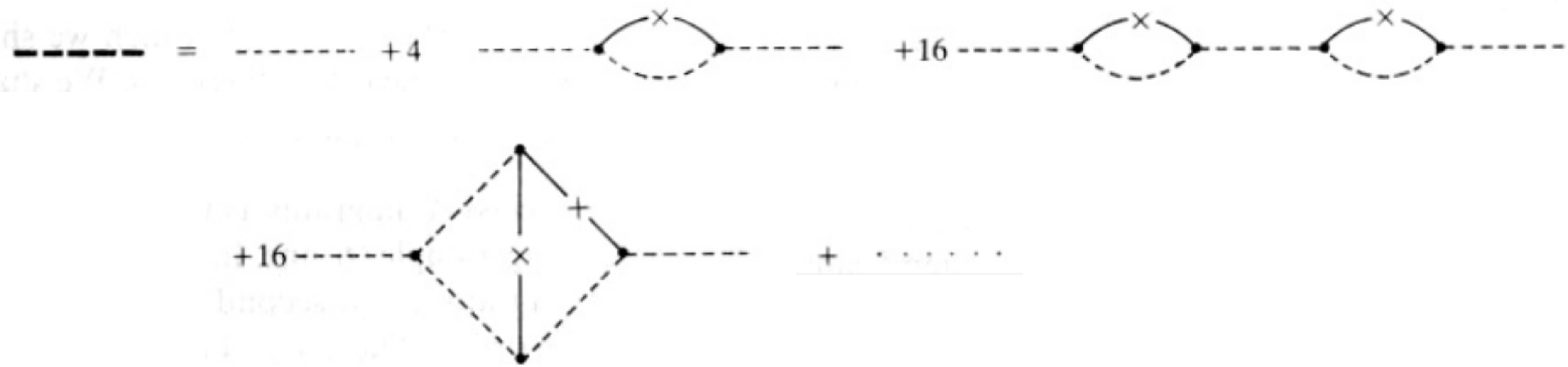
which reads

$$Q\left(k;\omega,\omega'\right)_{\mathrm{A}}=G(k,\omega)G\left(k,\omega'\right)w\left(k;\omega,\omega'\right)$$

where $G(k,\omega)$ is the renormalized propagator.

Graphically, this corresponds to



# Renormalized Perturbation Theory

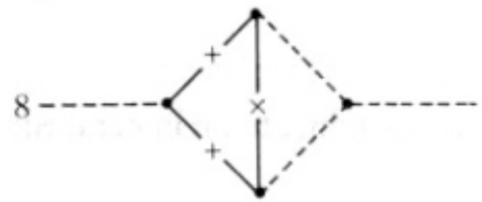
**Class B diagrams: renormalized perturbation series**

Class B diagrams can't be split into two by cutting a single $Q_0$ line.

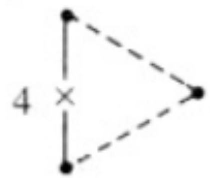
In the class A diagrams, certain diagram parts were propagator like, that is, they connected like $G_0$ : renormalize $G_0$ by adding up all diagrams which connect like $G_0$.

Renormalize vertex: add up all diagrams which connect like a vertex

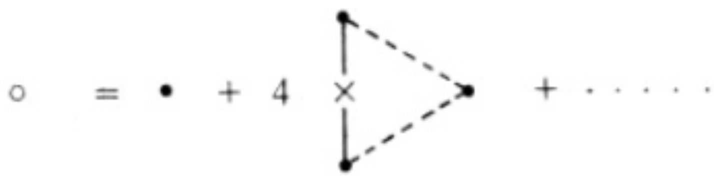
Example: consider fourth-order diagram




The part

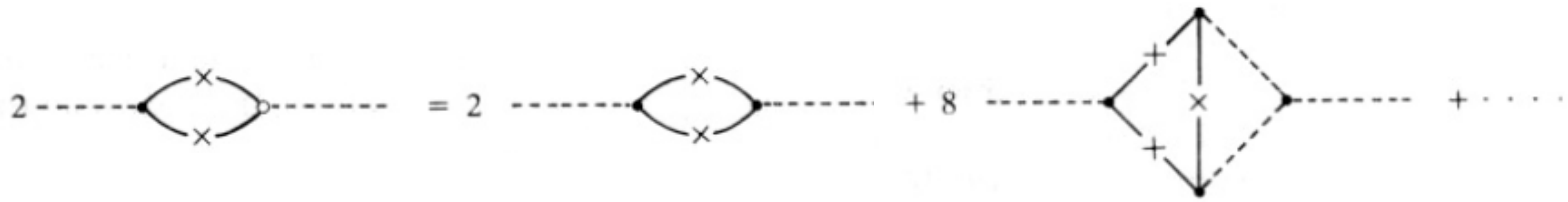



connects like a point vertex $\Longrightarrow$ renormalized vertex



# Renormalized Perturbation Theory

replace vertex by renormalized vertex:




Therefore the key to the class B diagrams is as follows:

1. Find those diagrams which cannot be reduced to a lower order by replacing diagram parts.

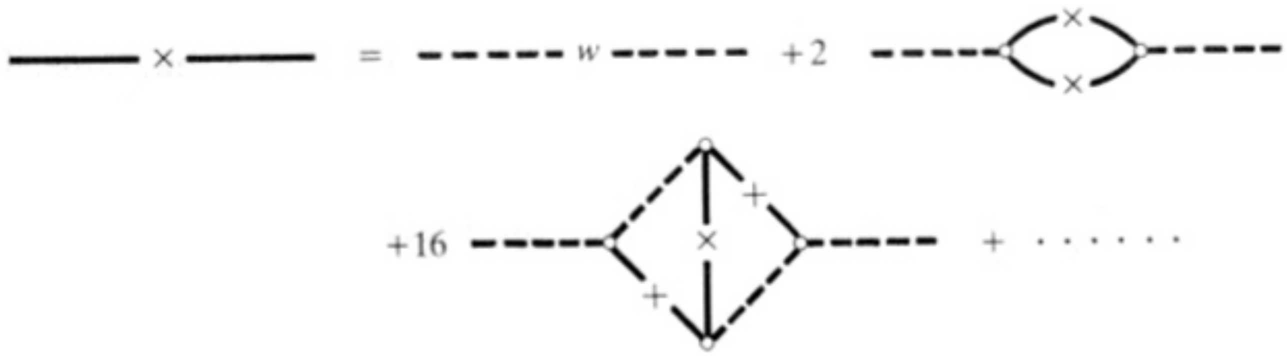
2. Call these the irreducible diagrams.

3. Replace all elements in the irreducible diagrams by their renormalized forms.

4. Write down all these modified diagrams in order, thus generating a *renormalized* perturbation expansion.

# Renormalized Perturbation Theory

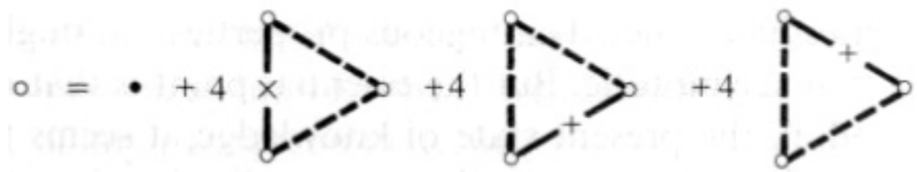
Result for $Q\left(k;\omega,\omega'\right)$




This is an integral equation for $Q(k;\omega,\omega)$

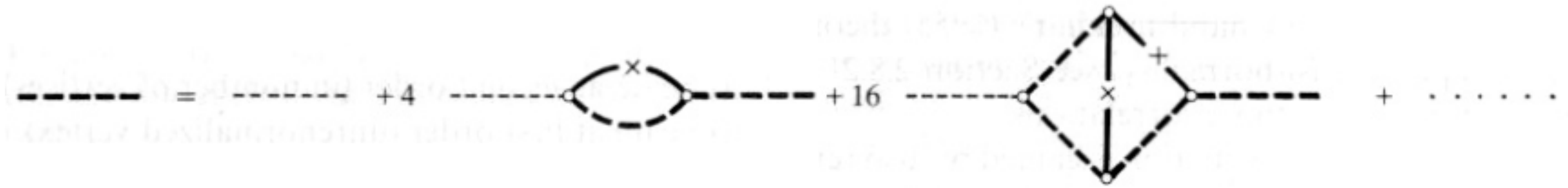
<u>Combine vertex and propagator expansions:</u>

Integral equation for the renormalized vertex



## Renormalized Perturbation Theory

Integral equation for the renormalized propagator $G(k, \omega)$



Pecularity of this diagram:

unrenormalized propagator emerging from the left !!!

Reason for this: symbolic form of Navier-Stokes

$$L_0 u(k) = \lambda M(k) u(j) u(k-j), \quad L_0 = \partial_t + \nu k^2$$

and renormalize r.h.s., then invert $L_0$ which results in $G_0$

**Second-order closures**

We replaced a wildly divergent series with one of unknown properties !

We have hope that it might be assymptotic, but we simple don't know !

Well known examples recovered from this Wyld (1961) formulation:

# Renormalized Perturbation Theory

Example 1:

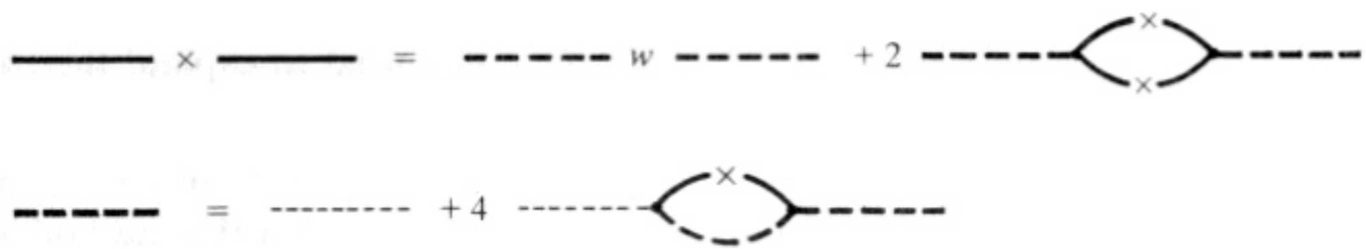
| | | |
|---|---|---|
| correlation tensor: | truncate at second order | (in number vertices) |
| vertex: | truncate at first order | (unrenormalized vertex) |
| propagator: | truncate at zero order | (unrenormalized propagator) |

This is Chandrasekhar's theory (1955) which is the two-time analog of quasi-normality.

Example 2:

| | |
|---|---|
| correlation tensor: | truncate at second order |
| vertex: | truncate at first order |
| propagator: | truncate at second order |

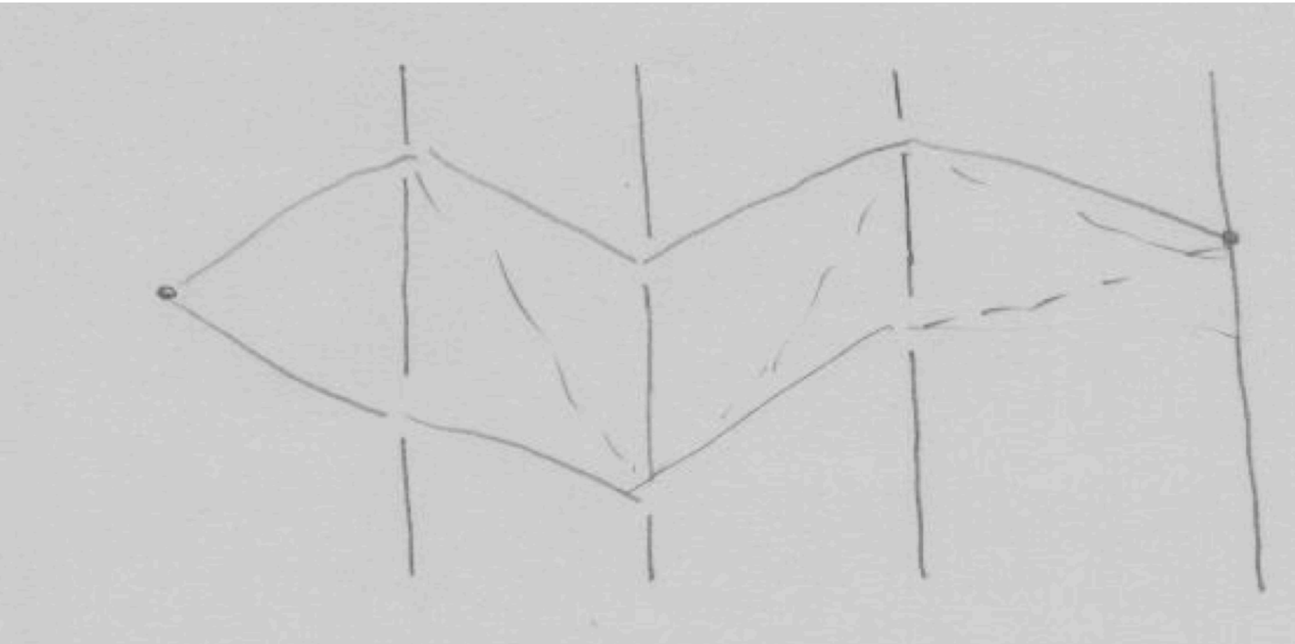
This is the pioneering direct-interaction approximation (DIA) by Kraichnan (1959): second-order closure with line and with no vertex renormalization.



## Intermezzo: Path integral QMI


$$W(x) = \left|\Phi_1 + \Phi_2\right|^2$$

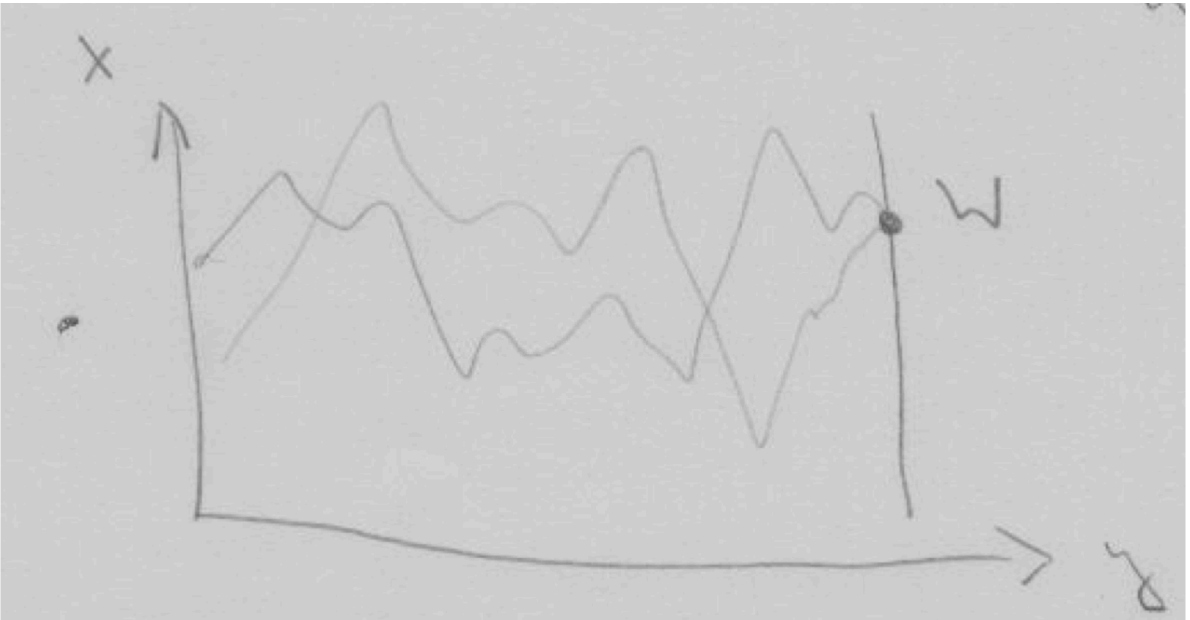
complex amplitudes



$$W(x) = \left|\sum_i \Phi_i\right|^2$$

over all combinations of holes

$$\left.\begin{array}{ll}\text{\#holes} & \to \infty \\ \text{\#apertures} & \to \infty\end{array}\right\} \Longrightarrow \quad \text{sum over all paths}$$




$$W = \left| \sum_{x(y)} \Phi_{x(y)} \right|^2$$

Feynmans basic idea

Important: additional coding of time

Paths are denoted by the set $\{x(t), y(t)\}$

$$W(x) = \left| \sum \text{ over all Amplitudes belonging to the paths } \{x(t), y(t)\} \right|^2$$

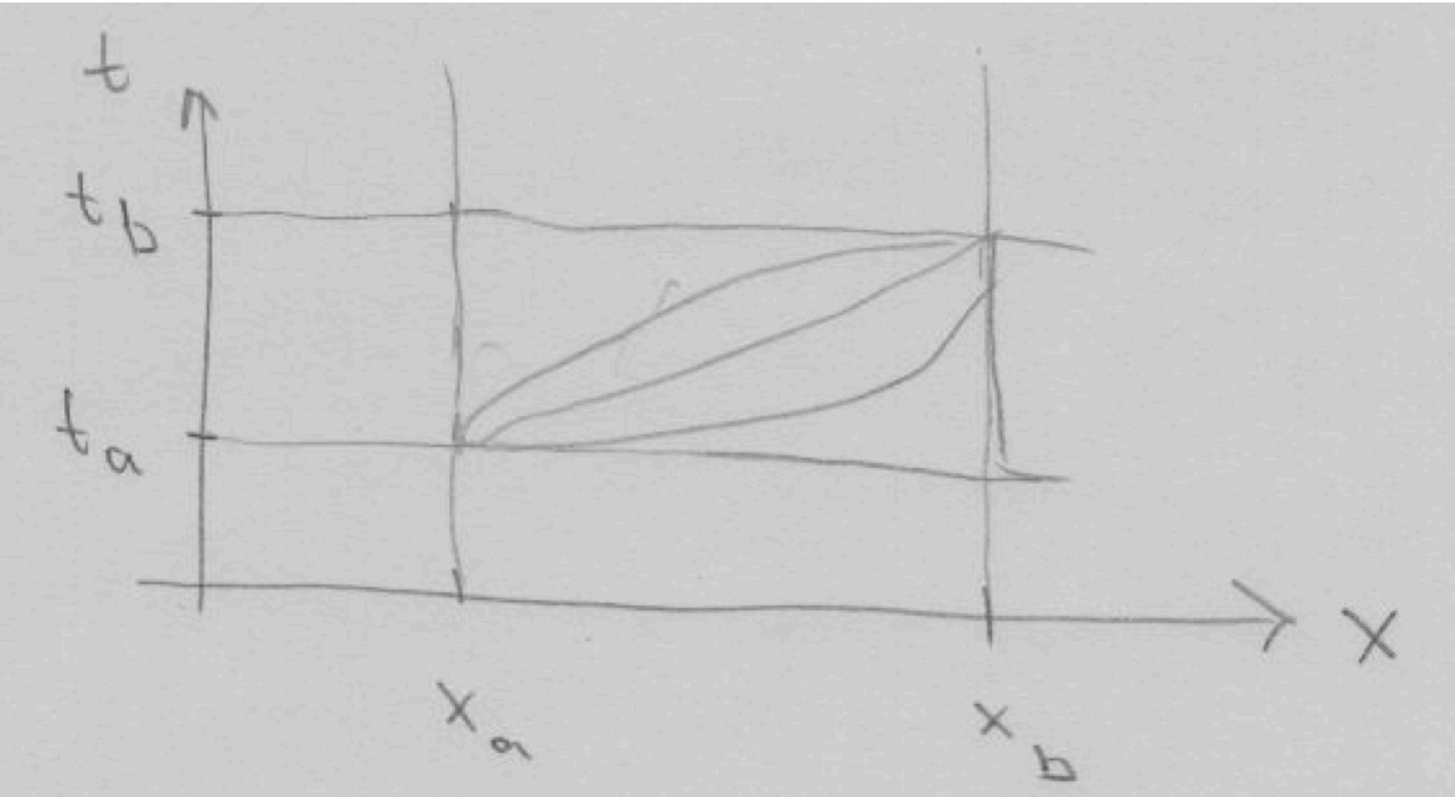
Once we know the procedure to calculate the amplitude for one path

$\Longrightarrow$ we know laws of QM

Consider one-dimensional motion of a particle

start at $t_a$: $x(t_a) = x_a$
final time $t_b$: $x\left(t_b\right) = x_b$

in between all possible paths $x(t)$



## Classical Action

$$S[x(t)] = \int_{t_a}^{t_b} L(x(t), \dot{x}(t))dt$$

Principle of the smallest action

$$\delta S = S[x+\delta x] - S[x] = 0$$

$$\Longrightarrow S[x+\delta x] = \int_{t_a}^{t_b} L(x+\delta x, \dot{x}+\delta\dot{x}, t)dt = \int_{t_a}^{t_b} \left( L(x,\dot{x},t) + \frac{\partial L}{\partial x}\delta x + \frac{\partial L}{\partial \dot{x}}\delta\dot{x} \right) dt$$

$$= S[x] + \int_{t_a}^{t_b} \left( \delta x \frac{\partial L}{\partial x} + \delta\dot{x}\frac{\partial L}{\partial \dot{x}} \right) dt$$

$$\Longrightarrow \delta S = \underbrace{\left. \delta x \frac{\partial L}{\partial x} \right|_{t_a}^{t_b}}_{=0} + \int_{t_a}^{t_b} \delta x \left[ \frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} \right]$$

$\delta x = 0$ at $x_a, x_b$

$$\boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0}$$

Lagrange

QM:

$W(b,a) = |K(b,a)|^2 =$ probability to move from $x_a$ at time $t_a$ to $x_b$ at time $t_b$

$$K(b,a) = \underbrace{\sum}_{\substack{\text{Sum over all paths} \\ \text{from } a \text{ to } b}} \Phi[x(t)]$$

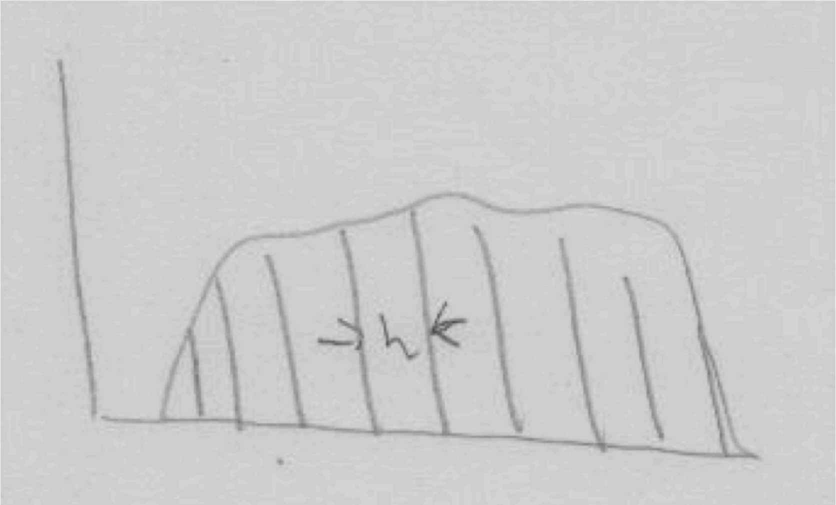
$+$

$$\Phi[x(t)] = \text{ const } e^{(i/\hbar)S(x,t)}$$

classical limit $\frac{S}{\hbar} \gg 1 \Longrightarrow e^{iS[x(t)]}$ oszillates strongly, averages out

Only contribution of extremum is important !

## Analogy with Riemann integral




$$A \sim \sum_i f(x_i)$$

such that limit exists

$$A = \lim_{h\to 0} h \sum_i f(x_i)$$

Quit analog for the path: Choose subset of paths time discretized in $\epsilon$ :

$$N\epsilon = t_b - t_a \quad ; \quad \epsilon = t_{i+1} - t_i$$

$$t_0 = t_a \quad ; \quad t_N = t_b$$

$$x_0 = x_a \quad ; \quad x_N = x_b$$

For every time $t_i$ $(i = 0,\ldots,N)$ choose $x_i$.

Connect points with straight line (in space time)

$$\Longrightarrow \quad K(b,a) \sim \int \cdots \int \Phi[x(t)] dx_1 \ldots dx_{N-1}$$

limiting process: $\epsilon \to 0$, but what is the limit ?

difficult problem, in general no solution, but for all practical problems there exists solution, e.g. let

$$L = \frac{m}{2}\dot{x}^2 - V(x,t)$$

$\Longrightarrow$ normalisation is given by $A^{-N}$ with $A = \left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{1/2}$

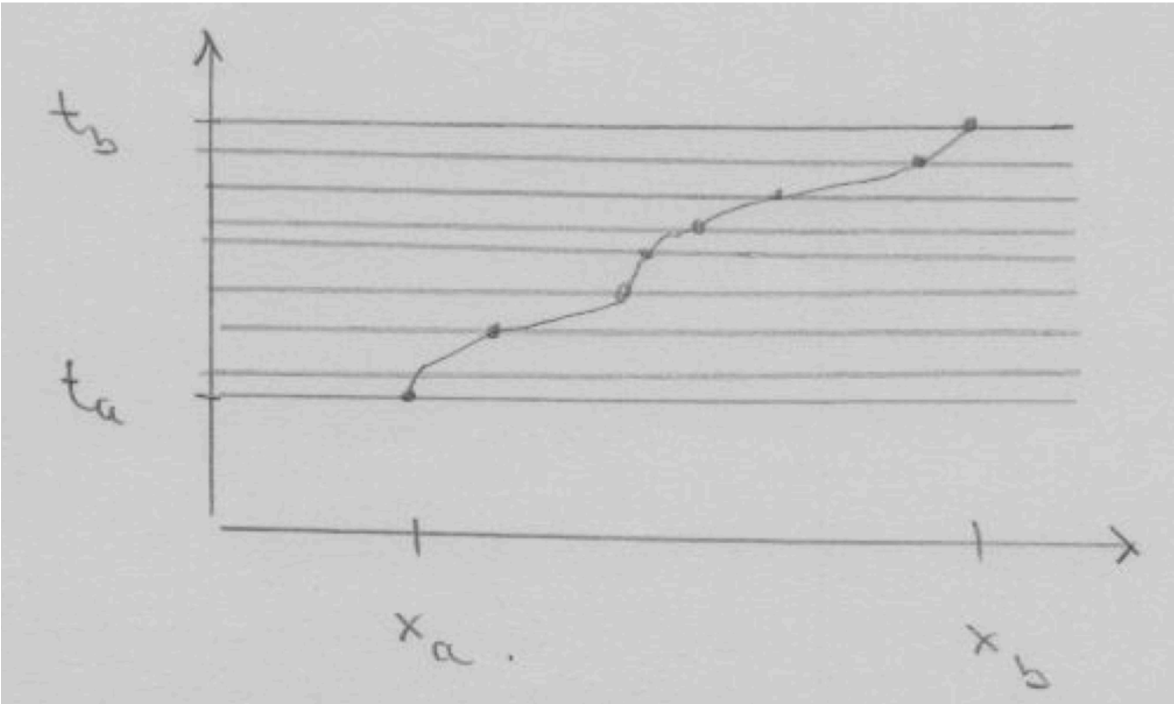
(We proof that soon ...)

thus

$$K(b,a) = \lim_{\varepsilon \to 0} \frac{1}{A} \int \cdots \int e^{\frac{i}{\hbar} S[b,a]} \frac{dx_1}{A} \frac{dx_2}{A} \frac{dx_3}{A} \cdots \frac{dx_{N-1}}{A}$$

$$S[b,a] = \int_{t_a}^{t_b} L(x, \dot{x}, t) dt$$

with piecewise linear trajectories




Instead of piecewise linear trajectories we could have used the classical trajectories.

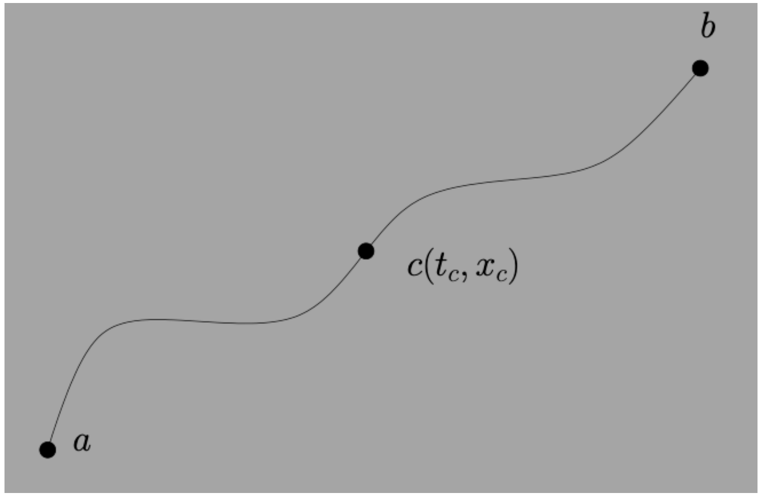
There are many ways to define this integral

$\Longrightarrow$ general notation

$$K(b,a) = \int_a^b \mathscr{D}x(t)\; e^{\frac{i}{\hbar}S[b,a]}$$

path integral

important rules:




$$S[b,a] = S[b,c] + S[c,a]$$

$$\Longrightarrow \quad K(b,a) = \int_{x_c} dx_c \int_a^c \int_c^b e^{\frac{i}{\hbar}S[b,c]+\frac{i}{\hbar}S[c,a]}\mathscr{D}x(t) = \int_{x_c} K(b,c)K(c,a)\mathrm{d}x_c$$

The wavefunction

$K\left(x_2, t_2; x_1, t_1\right)$ amplitude at 2 which starts at 1
$\psi(x, t)$ amplitude at $(x, t)$

Just a question of notation! if info $\left(x_1, t\right)$ not important, then we write $\psi(x, t) =$ wave function.

Especially we have:

$$\psi\left(x_2, t_2\right) = \int_{-\infty}^{\infty} K\left(x_2, t_2; x_1, t_1\right) \psi\left(x_1, t_1\right) \mathrm{d}x_1$$

From this equation we can derive the Schrödinger equation:

$$\psi(x, t+\epsilon) = \int_{-\infty}^{\infty} \frac{\mathrm{d}y}{A} \exp\left(\frac{\mathrm{i}}{\hbar}\int_t^{t+\epsilon} \mathrm{d}t L(\tilde{x}, \dot{\tilde{x}})\right)\psi(y, t)$$

$$= \int_{-\infty}^{\infty} \frac{\mathrm{d}y}{A} \exp\left(\frac{\mathrm{i}}{\hbar}\epsilon L\left(\frac{x+y}{2}, \frac{x-y}{\epsilon}\right)\right)\psi(y, t)$$

consider the case $L = \frac{m\dot{x}^2}{2} - V(x,t)$

$$\psi(x, t+\epsilon) = \int_{-\infty}^{\infty} \frac{\mathrm{d}y}{A} \underbrace{\exp\left(\frac{\mathrm{i}}{\hbar}\frac{m(x-y)^2}{2\epsilon}\right)}_{\substack{\text{strongly oscillating,} \\ \text{contributions only from} \\ \text{the neighborhood of } x}} \exp\left(-\frac{\mathrm{i}}{\hbar}\epsilon V\left(\frac{x+y}{2}, t\right)\right)\psi(y,t)$$

$\implies$ substitution $y = x + \eta$

$$\psi(x, t+\epsilon) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\eta}{A} \exp\left(\frac{\mathrm{i}}{\hbar}\frac{m\eta^2}{2\epsilon}\right) \exp\left(-\epsilon\frac{\mathrm{i}}{\hbar}V\left(x+\frac{\eta}{2}, t\right)\right)\psi(x+\eta,t)$$

phase of exponential function changes in first order for $\eta \sim \sqrt{\frac{\epsilon\hbar}{m}}$

power series: 1 . order in $\epsilon \implies$ 2 . order in $\eta$

$$\Longrightarrow \quad \epsilon V\left(x+\frac{\eta}{2}, t\right) \to \epsilon V(x,t) + \text{error of higher order}$$

$$\Longrightarrow \quad \psi(x,t) + \epsilon\frac{\partial\psi}{\partial t} = \int_{-\infty}^{\infty}\frac{\mathrm{d}\eta}{A}\exp\left(\frac{\mathrm{i}}{\hbar}\frac{m\eta^2}{2\epsilon}\right)\left(1-\frac{\mathrm{i}}{\hbar}\epsilon V(x,t)\right)\left(\psi(x,t)+\eta\frac{\partial\psi}{\partial x}+\frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right)$$

<u>order $\epsilon^0$</u>

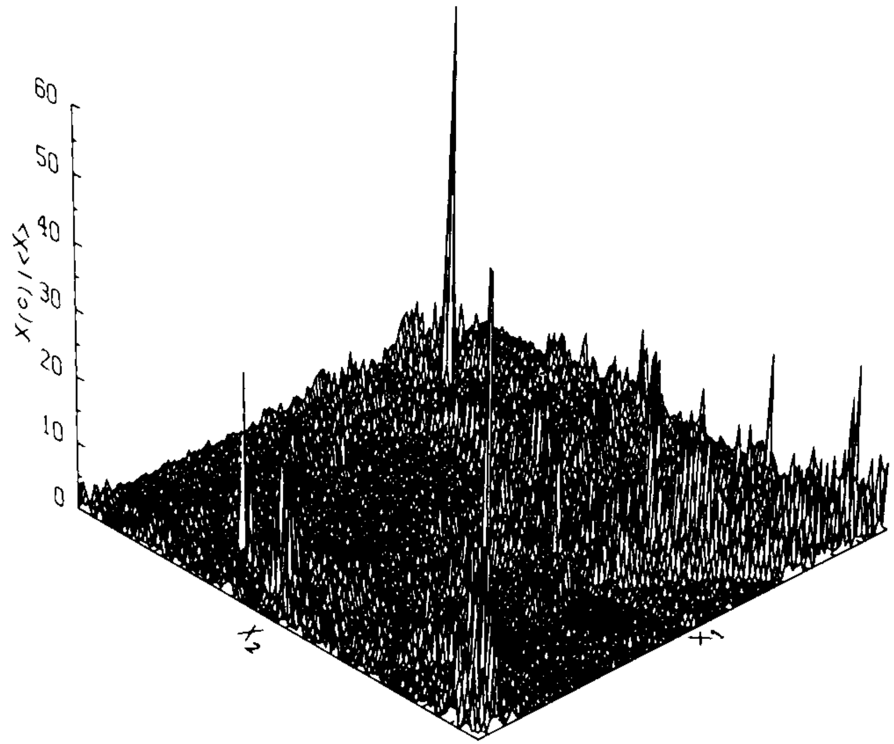
$$\Longrightarrow \quad 1 = \int_{-\infty}^{\infty}\frac{\mathrm{d}\eta}{A}\exp\left(\frac{i}{\hbar}\frac{m\eta^2}{2\epsilon}\right) = \frac{1}{A}\left(\frac{2\pi\mathrm{i}\hbar\epsilon}{m}\right)^{\frac{1}{2}} \qquad \Longrightarrow A = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{1}{2}}$$

two integrals:

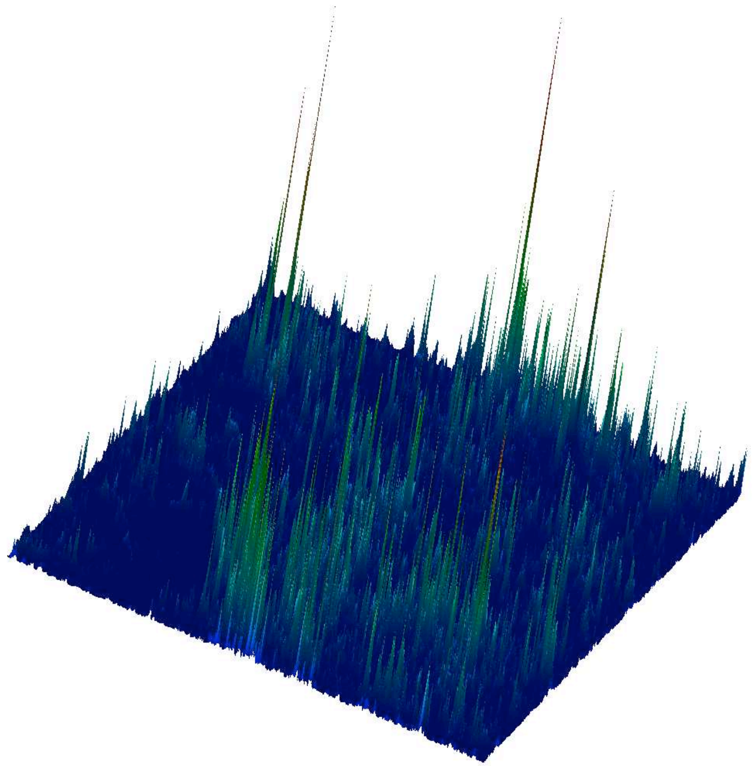
$$\int_{-\infty}^{\infty}\frac{1}{A}e^{\mathrm{i}m\eta^2/2\hbar\epsilon}\eta\,\mathrm{d}\eta = 0 \;,\; \int_{-\infty}^{\infty}\frac{1}{A}e^{\mathrm{i}m\eta^2/2\hbar\epsilon}\eta^2\,\mathrm{d}\eta = \frac{\mathrm{i}\hbar\epsilon}{m} \Longrightarrow \psi + \epsilon\frac{\partial\psi}{\partial t} = \psi - \frac{\mathrm{i}\epsilon}{\hbar}V\psi - \frac{\hbar\epsilon}{2\mathrm{i}m}\frac{\partial^2\psi}{\partial x^2}$$

$$\Longrightarrow \quad \boxed{-\frac{\hbar}{\mathrm{i}}\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t)\psi}$$

# What is wrong with K41?

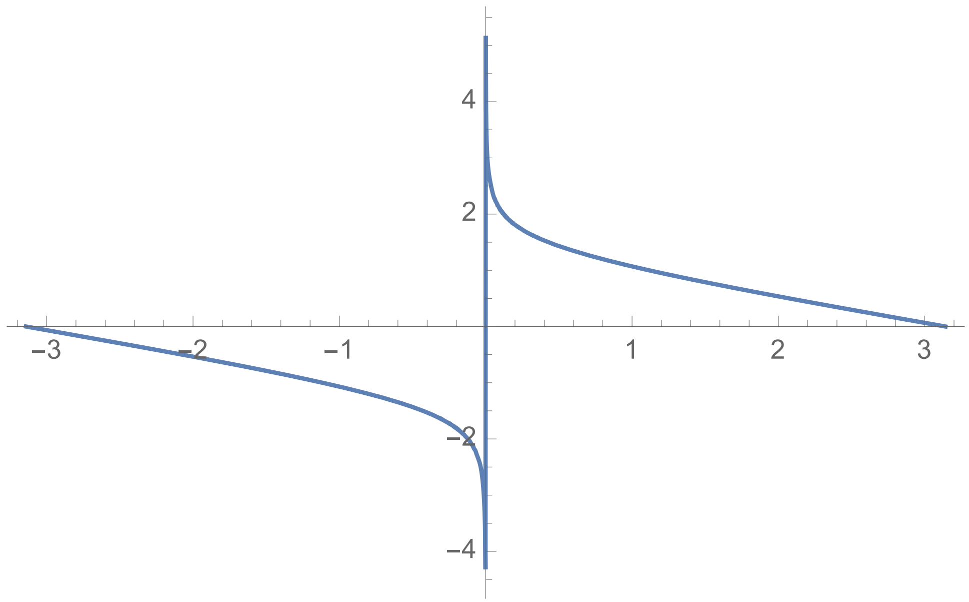


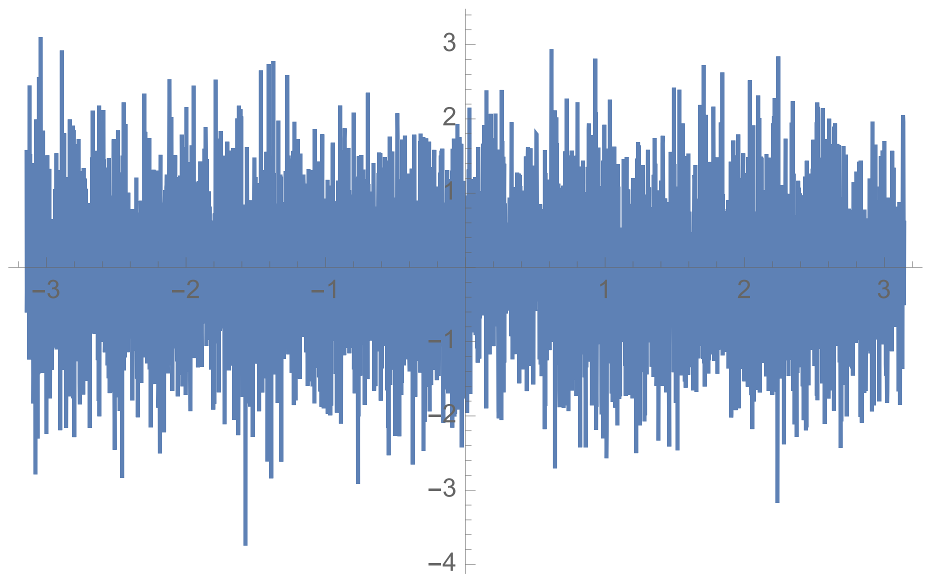

Prasad, Meneveau, Sreenivasan (1989)



DNS $1024^3$: Homann, Grauer (2006)

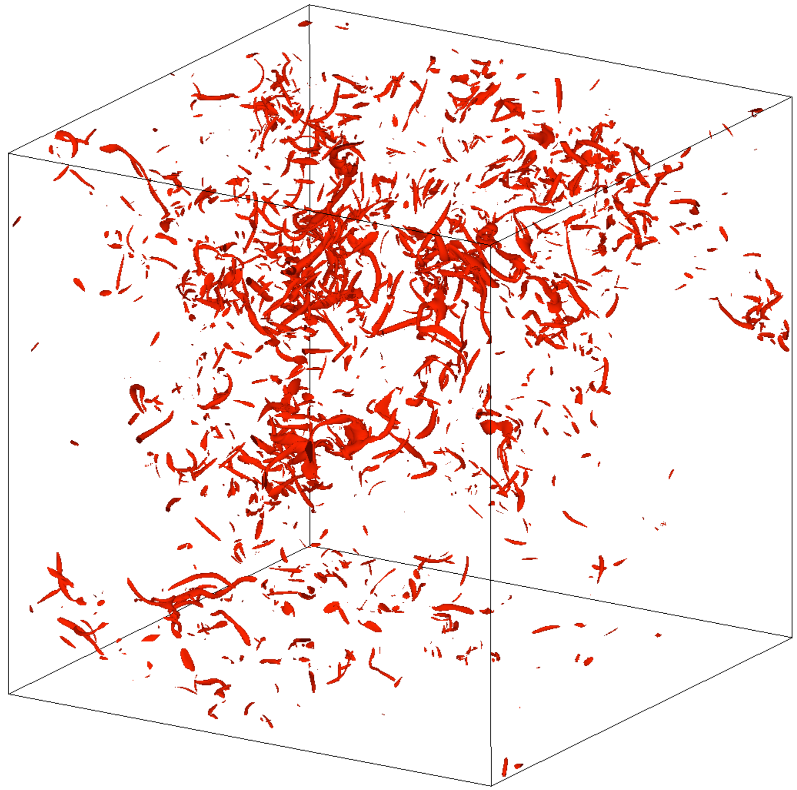
# What is wrong with K41?




both functions have the same energy spectrum !!!

# What is wrong with K41?



vortex tubes

*structure means:*

order

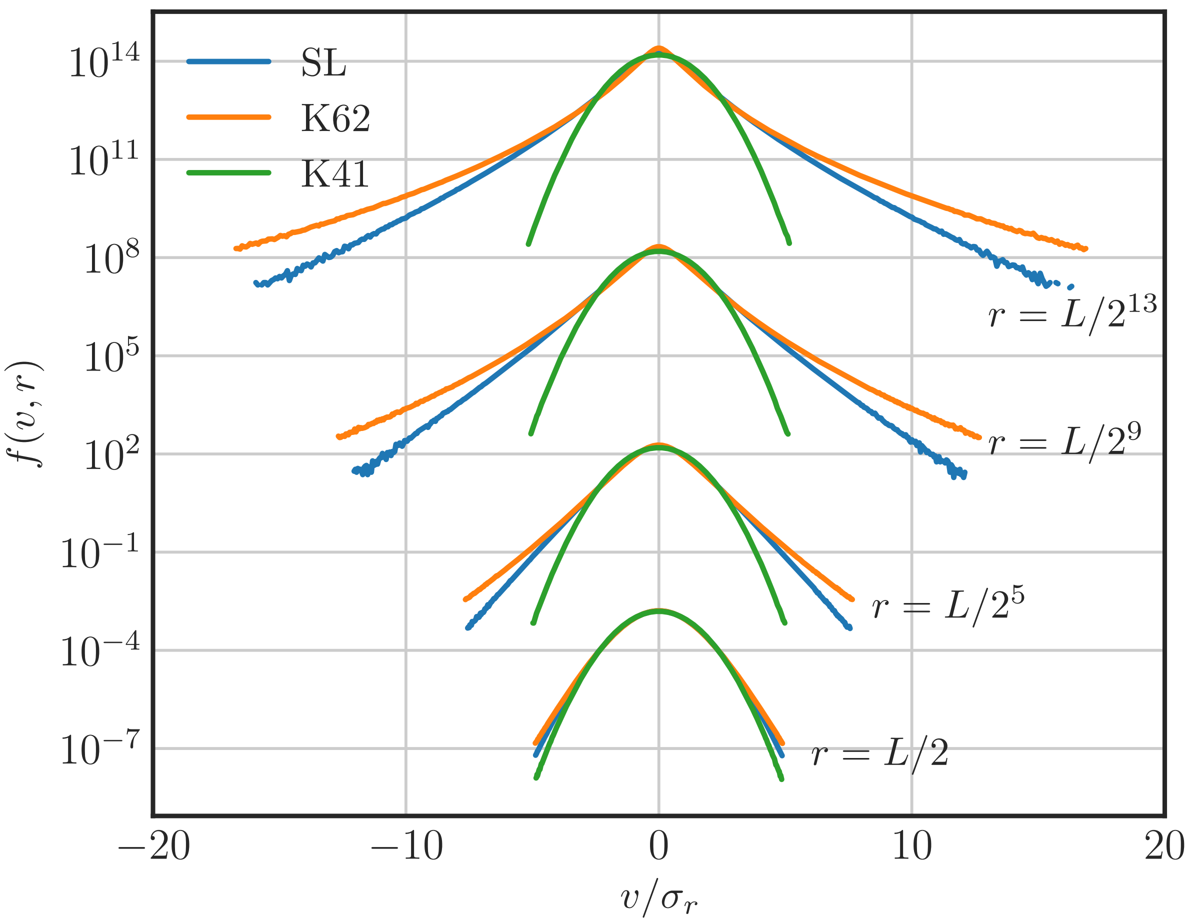
correlation

far from Gaussian

# Distributions of increments

K41

$$f(v,r) = \frac{1}{\sqrt{2\pi}\langle\varepsilon\rangle^{1/3} r^{1/3}} \exp\left[-\frac{v^2}{2\langle\varepsilon\rangle^{2/3} r^{2/3}}\right]$$




*real* turbulence: SL, K62

# Turbulence

is the tendency to form
singular structures.

*How can we use that ?*

- until now: Kolmogorov 1941 theory; RPT (DIA), RG

- purely phenomelogical
  we just used quadratic nonlinearity with gradient and energy conservation
- no intermittency, thus close to Gaussian distributions

$\Longrightarrow$ **Instantons**

“After trying for few years to do something with the Wyld approach I conclude that this is a dead end. The best bet here would be the renormalization group, which magically works in statistical physics. Those critical phenomena were close to Gaussian.”

“The observed variety of vorticity structures with their long range interactions does not look like the block spins of critical phenomena. There is no such luck in turbulence. The nonlinear effects are much stronger!”

“No! These old tricks are not going to work, we have to invent the new ones.”

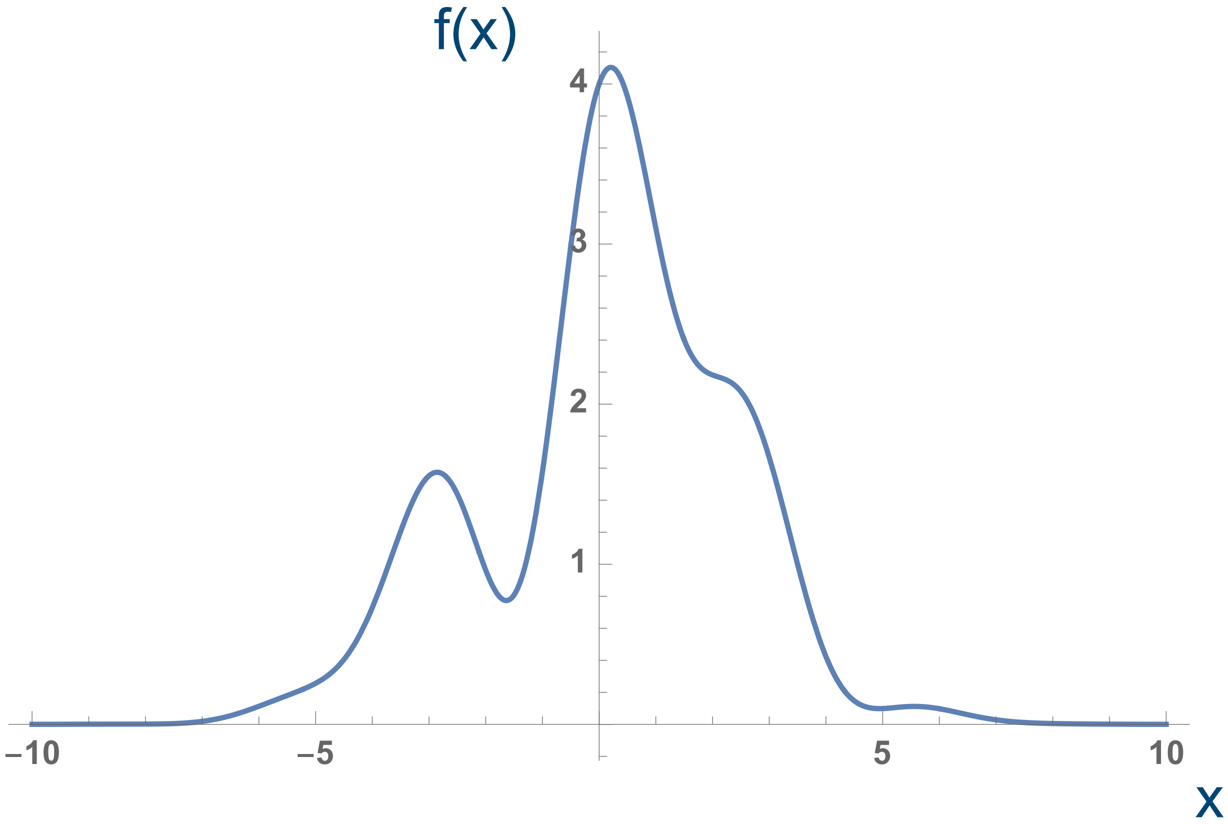
A. A. Migdal (1993)
arXiv:hep-th/9306152

→ **need for non-perturbative methods**

# Path integral

<u>1D:</u>

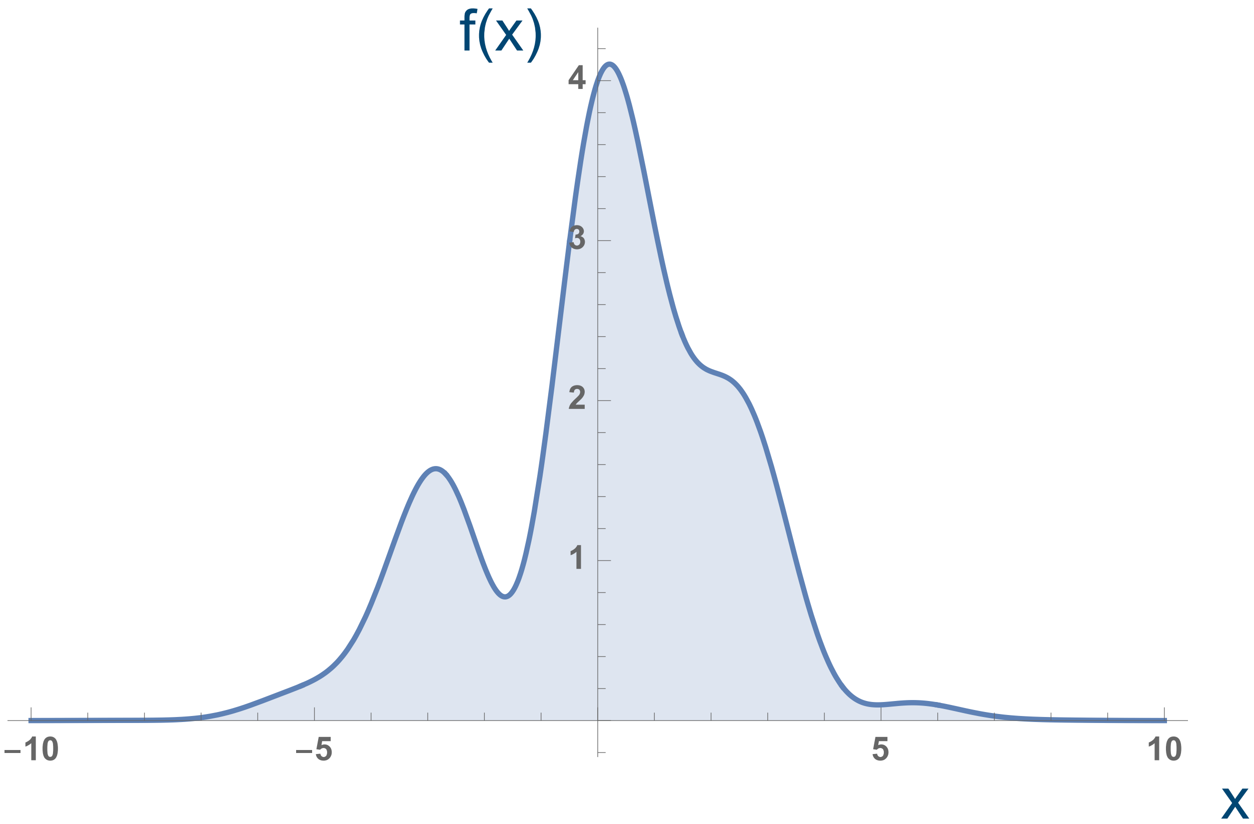
arbitrary function f(x)



# Path integral

<u>1D:</u>

arbitrary function f(x)



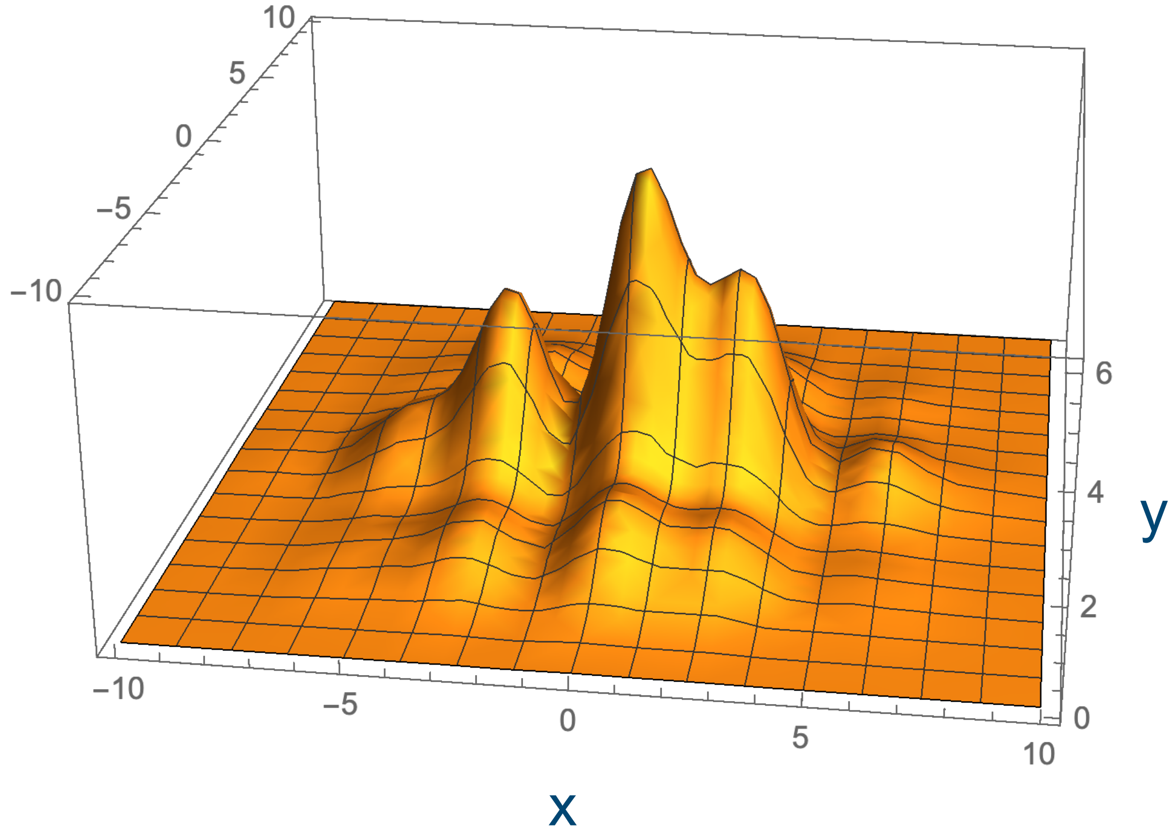

integral:

blue area

## Path integral

2D:

arbitrary function f(x,y)




integral:

volume below

## Path integral

3D: arbitrary function f(x,y,z)

integral: 3+1 dim volume

4D: quite similar

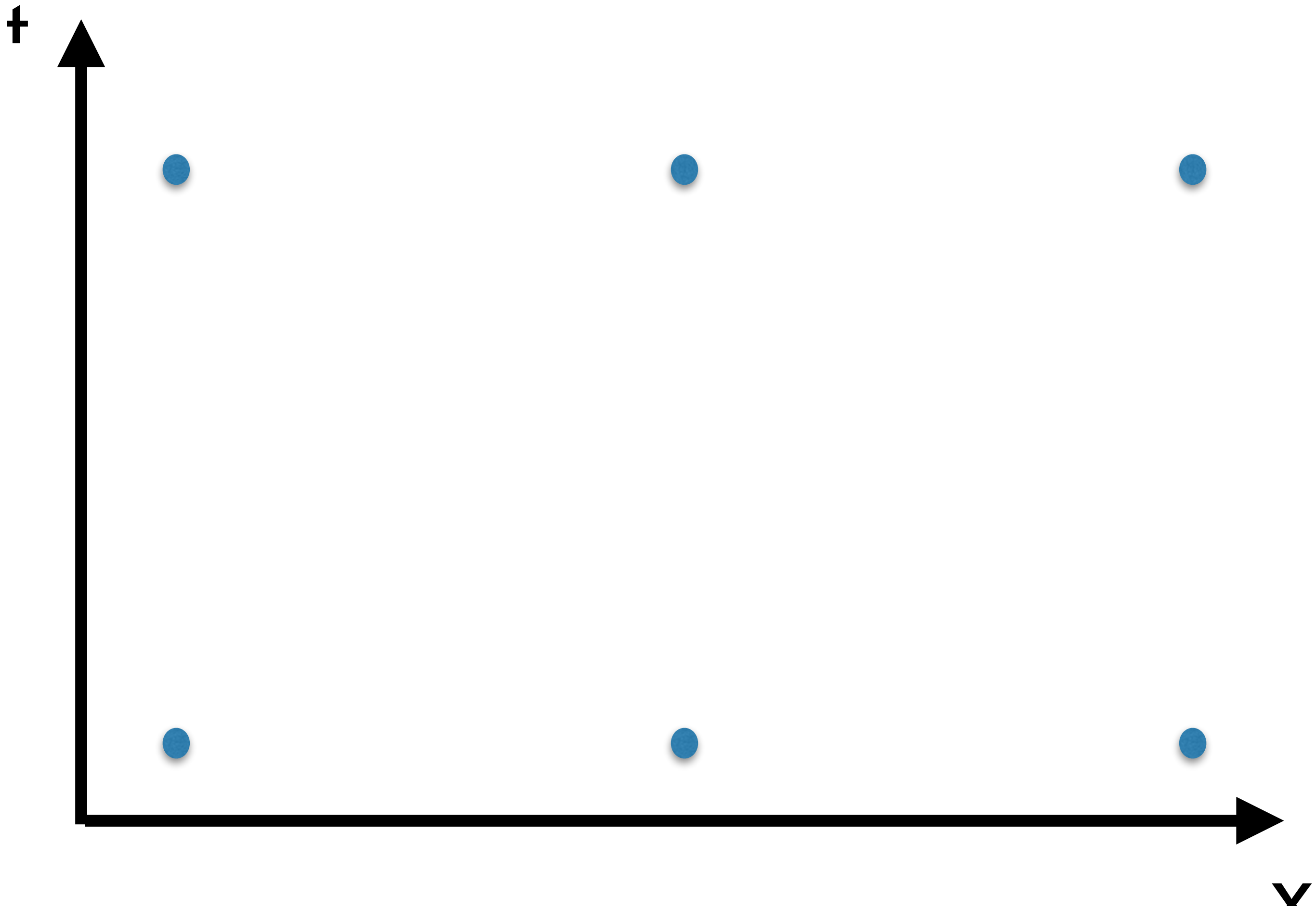
•
•
•

•
•
•

nD: quite similar

## Path integral

Geschwindigkeitsfeld u(x,t)

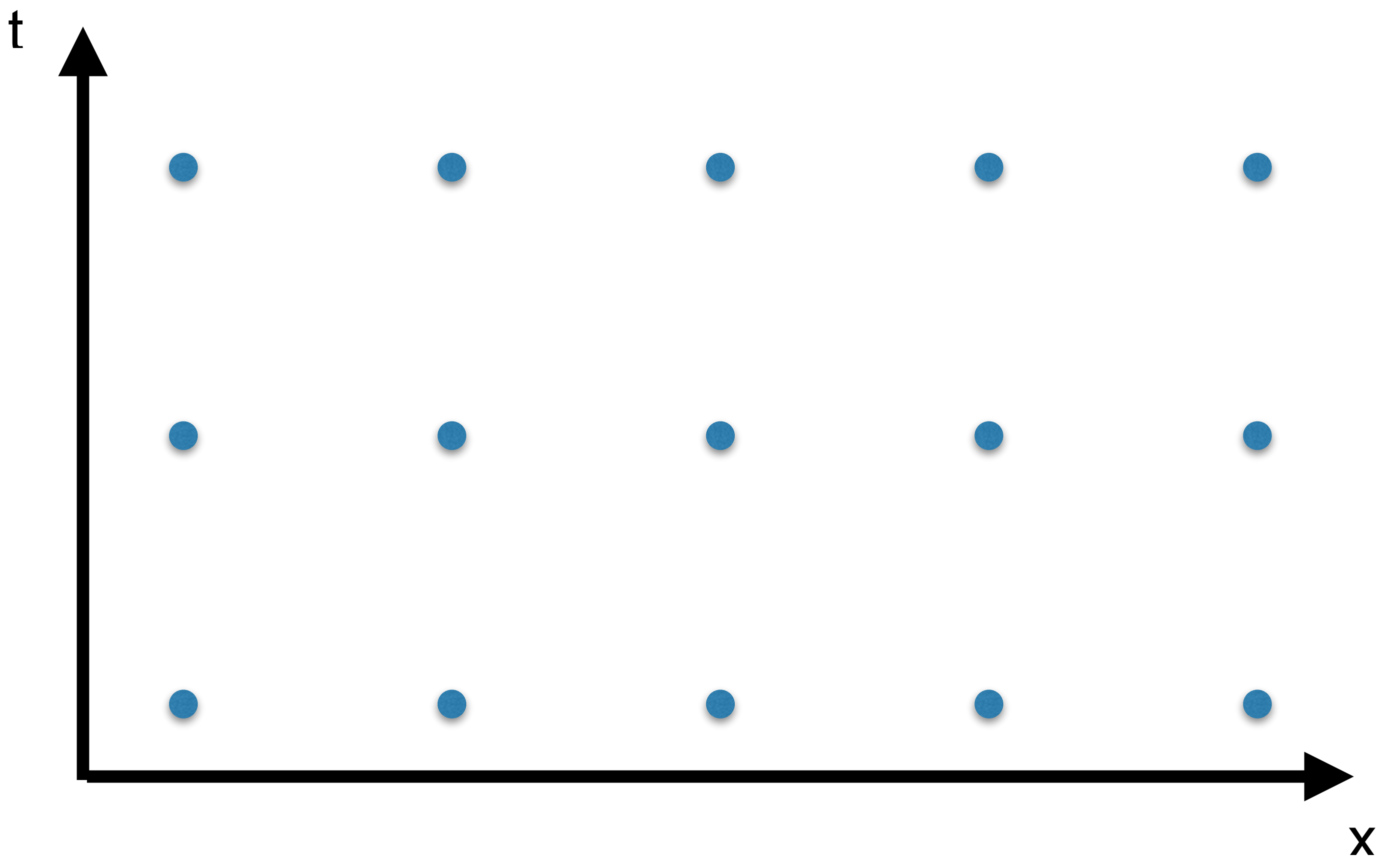



6d Integral

$$\int du_{11} \ldots du_{32} \;\ldots$$

## Path integral

Geschwindigkeitsfeld u(x,t)

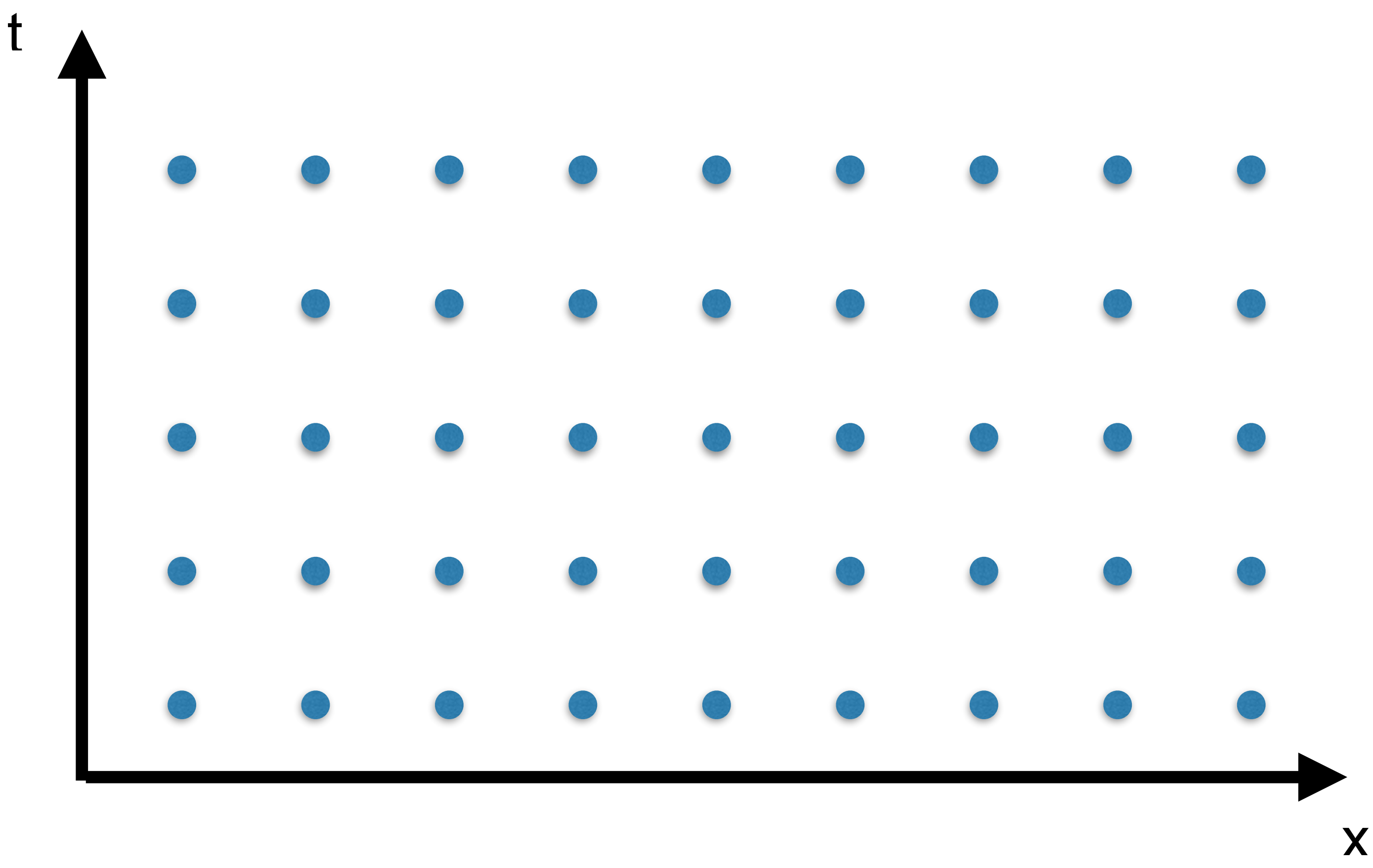



15d Integral

$$\int du_{11} \ldots du_{53} \;\ldots$$

## Path integral

Geschwindigkeitsfeld u(x,t)

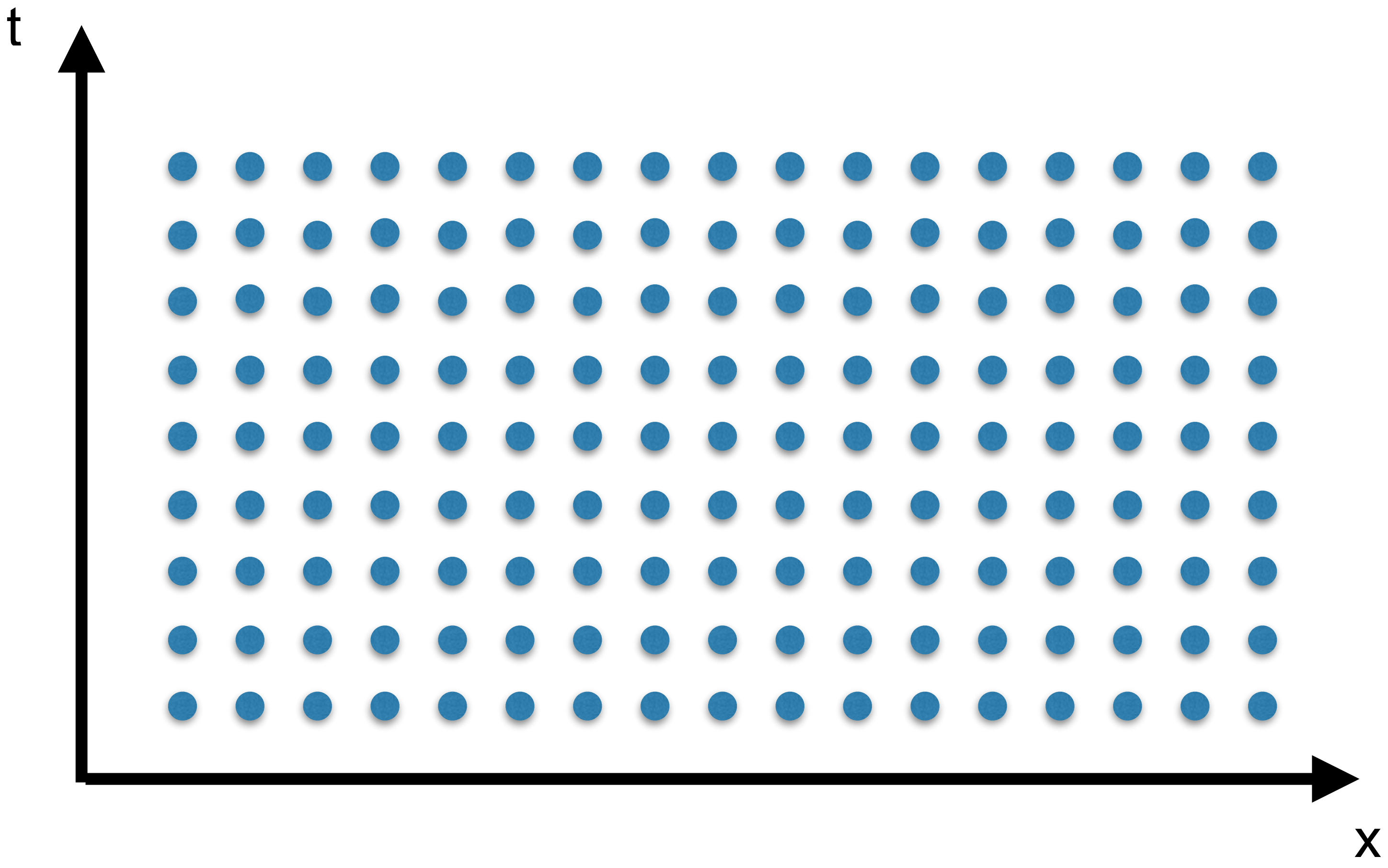



45d Integral

$$\int du_{11} \ldots du_{95} \ \ldots$$

## Path integral

Geschwindigkeitsfeld u(x,t)

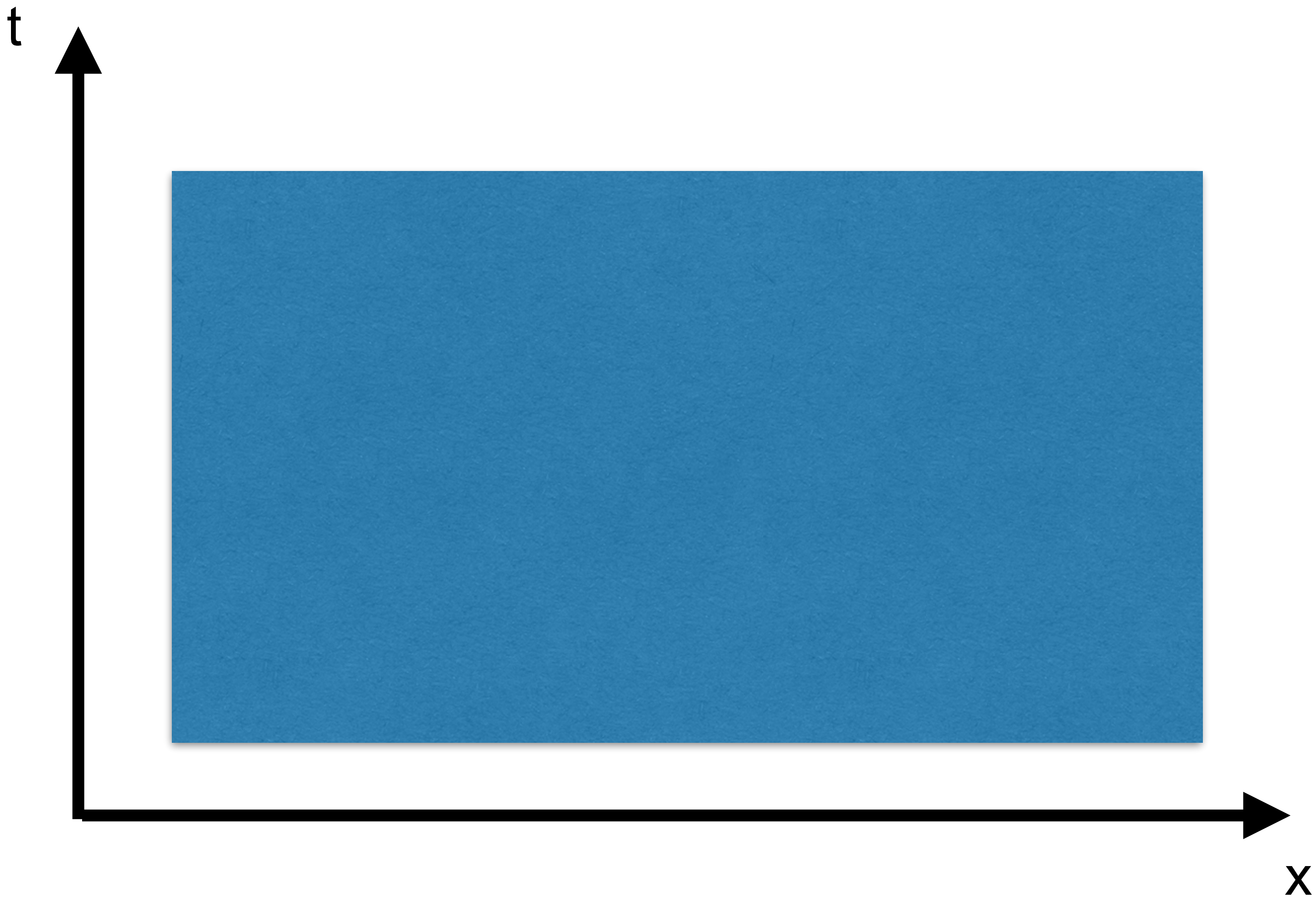



153d Integral

$$\int du_{11} \ldots du_{17,9} \;\ldots$$

# Path integral

Geschwindigkeitsfeld u(x,t)




infinite d Integral

$$\int du_{11} \ldots du_{\infty,\infty} \;\; \ldots$$

Feynman
path integral

$$\int \mathscr{D}u(x,t) \;\; \ldots$$

## Onsager/Machlup, Janssen/de Dominicis Functional

L. Onsager, S. Machlup
*Fluctuations and irreversible processes*
Phys. Rev. 91 1953 1505–12

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 phénomènes critiques
J. Phys. C **1** (1976) 247

## Onsager/Machlup, Janssen/de Dominicis Functional

$$\partial_t u + N[u, x] = \eta(x, t) \qquad \text{(stochastic diff. eqn.)}$$

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 $\eta$

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

## Onsager/Machlup, Janssen/de Dominicis Functional

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

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

## 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

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

we will use notation from paper

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

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

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

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 tim

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 $\mu$:

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

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

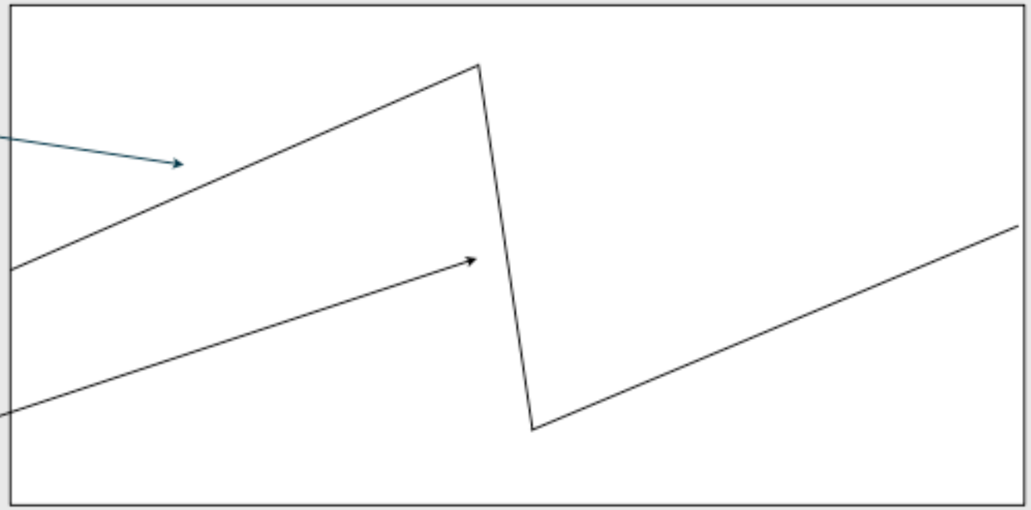
$$\mathcal{P}(A) \simeq e^{-S(A)}$$

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 $\mathcal{P}(A) \simeq e^{-\alpha|A|^{\gamma}}$

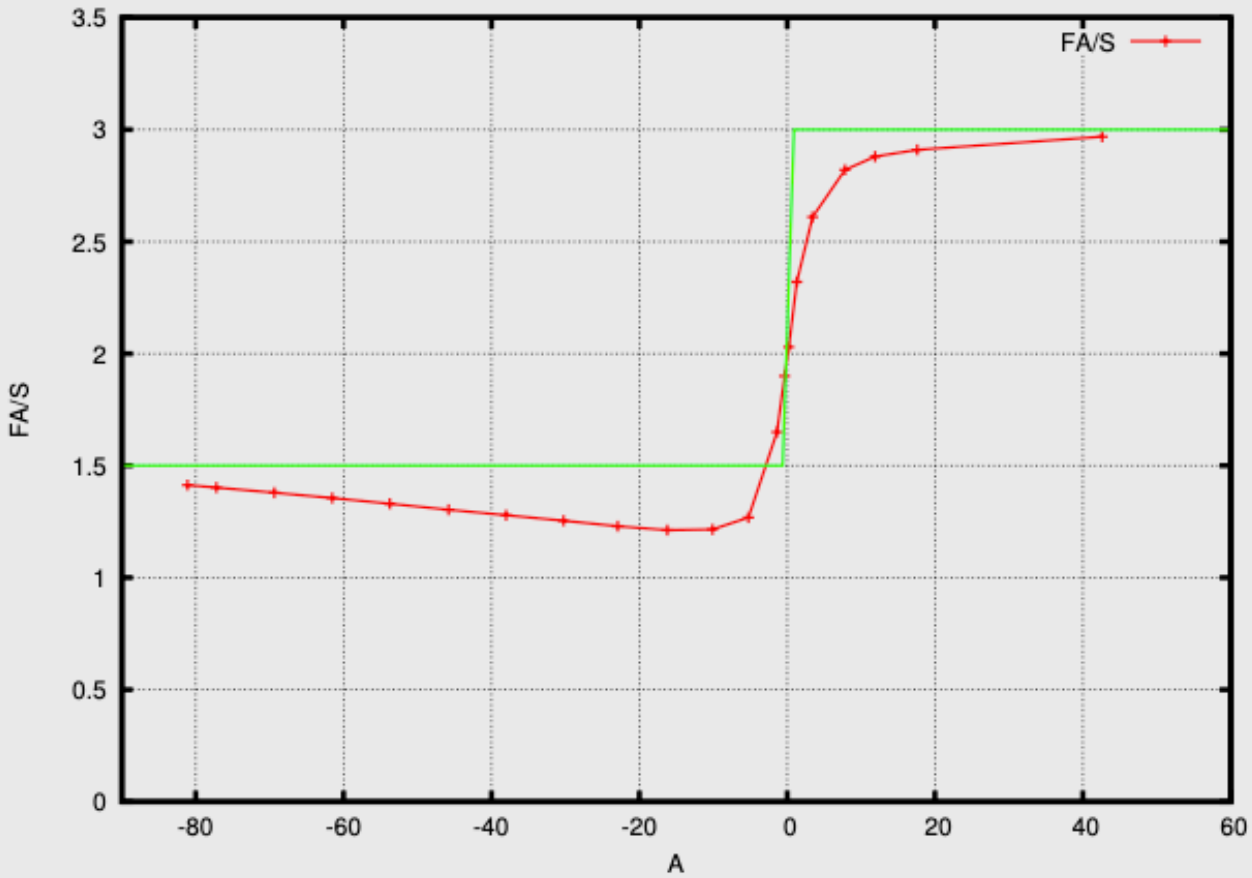
right tail: $\gamma = 3$
Gurarie, Migdal (1996)
easy

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



x

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



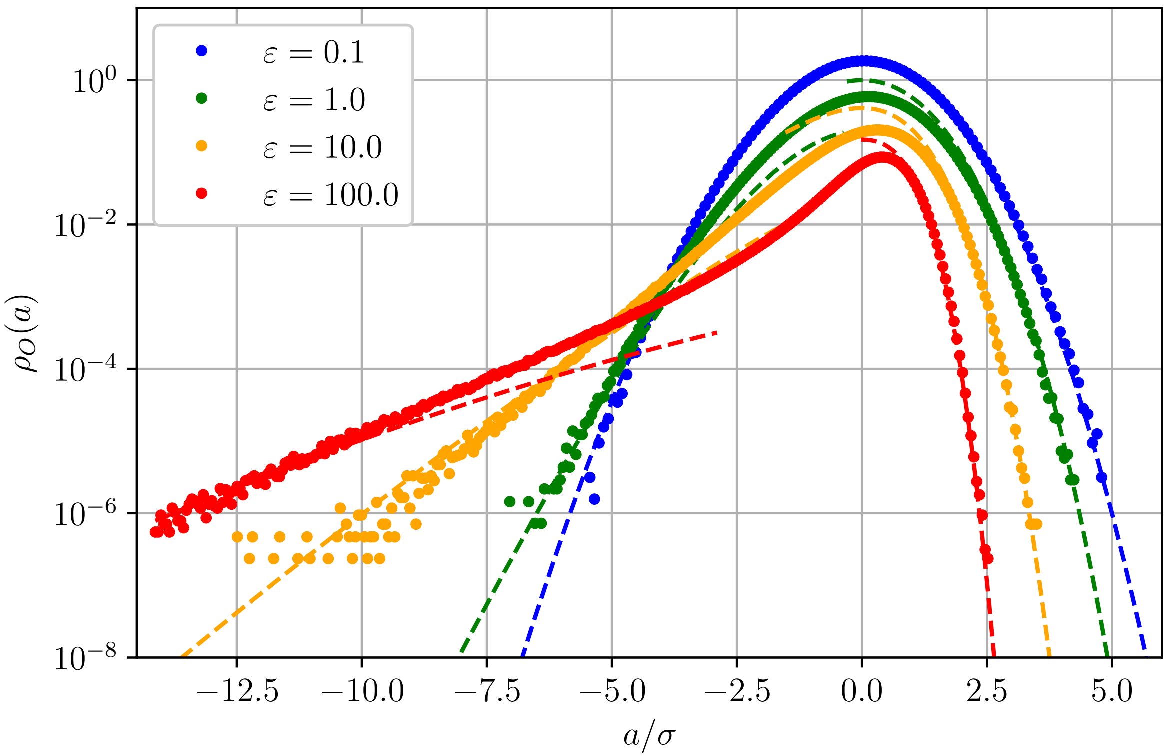

X

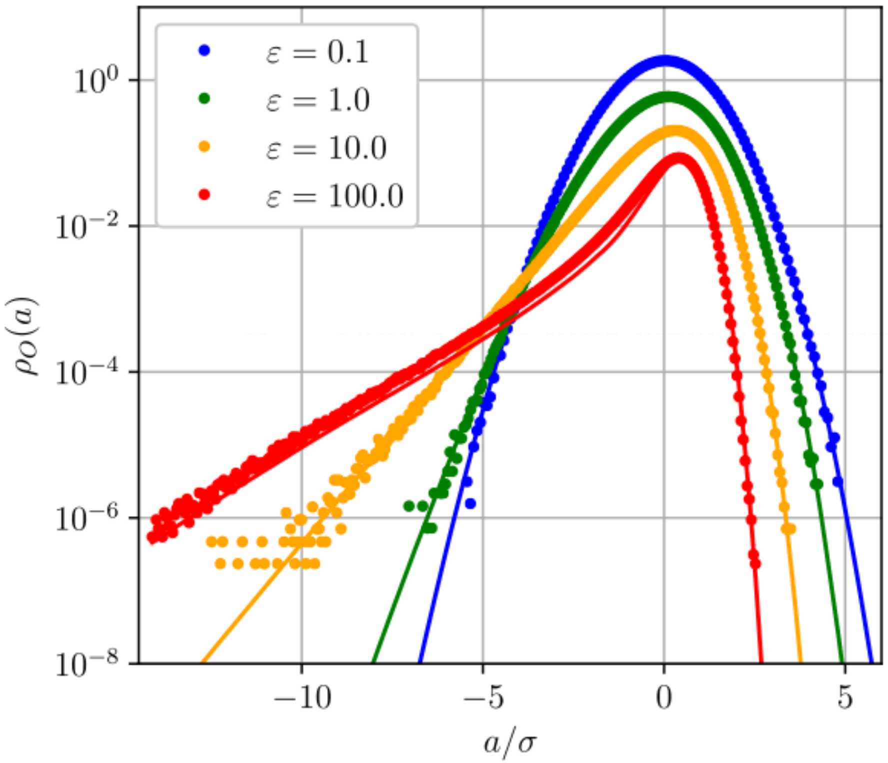
# Fluctuations

- standard way:
  linearize around instanton, calculate action to quadratic order
  Eigenfunctions + Eigenvalues —> fluctuation determinant
  - eigenvalues of a matrix of size
    - in 1D: (2048x4096)x(2048x4096)
    - in 3D: (2048x2048x2048x4096)x(2048x2048x2048x4096)
    - the matrix is sparse
    - need only few eigenvalues (~ 1000) near zero
    - Tensor Network
- Gel'fand-Yaglom
  transform into initial value problem:
  - in 1D: 2048 initial value problems of size (2048x4096)
  - in 2D: 2048x2048 initial value problems of size (2048x2048x4096)

  Why does this help? It is fully parallel !

# Fluctuations




Timo Schorlepp, Tobias Grafke, Rainer Grauer
Gel'fand-Yaglom type equations for calculating fluctuations around Instantons in stochastic systems
Journal of Physics A: Mathematical and Theoretical 54 (2021) 235003

## Instanton based importance sampling for rare events in stochastic PDEs

Start with Onsager-Machlup

$$S_{\mathscr{L}}[u,\dot{u}] = \frac{1}{2}\int dt \left\langle \dot{u} + N[u], \chi^{-1}(\dot{u} + N[u]) \right\rangle$$

$$= \frac{1}{2}\int dtdxdx' \left[u_t + uu_x - \nu u_{xx}\right] \chi^{-1}(x - x') \left[u_t + uu_{x'} + \nu u_{x'x'}\right]$$

decompose the field into instanton and fluctuation

$$u = u^{I(a)} + \delta u$$

$$\Longrightarrow S_{\mathscr{L}} = \frac{1}{2}\int dtdxdx' \left[P^{I(a)} + \delta u_t + \delta u \delta u_x - \nu \delta u_{xx} + \left(u^{I(a)}\delta u\right)_x\right] \chi^{-1}(x - x')[\dots]$$

$$= S^{I(a)} + \tilde{S}^a - \frac{1}{2}\int dtdxp_x^{I(a)}(\delta u)^2$$

with

$$\tilde{S}^a = \frac{1}{2}\int dtdxdx' \left[\delta u_t + \delta u \delta u_x - \nu \delta u_{xx} + \left(u^{I(a)}\delta u\right)_x\right] \chi^{-1}(x - x')[\dots]$$

Note that all linear variations vanish by definition of the instanton. Thus we define

$$\Delta S^a = S_{\mathscr{L}} - \tilde{S}^a = S^{I(a)} - \frac{1}{2}\int dtdxp_x^{I(a)}(\delta u)^2 \qquad **$$

To derive the stochastic equation corresponding to the action $\widetilde{S}^a$, we reverse the derivation of the path integral formulation

$$\delta u_t + \delta u \delta u_x - \nu \delta u_{xx} = \eta - \left(u^{I(a)}\delta u\right)_x$$

Next, change the path measure for this process in order to connect the statistics to the original one. To do that, we first consider the identity

$$\begin{aligned} P_{S_{\mathscr{L}}}(s) &:= \delta\left(u_x(0,0) - s\right) e^{-S_{\mathscr{L}}} \\ &= \delta\left(u_x(0,0) - s\right) e^{-\left(\tilde{S}^a + \Delta S^a\right)} \\ &= \delta\left(\delta u_x(0,0) + a - s\right) e^{-\tilde{S}^a} e^{-\Delta S^a} \qquad * \end{aligned}$$

where $P_{S_{\mathscr{L}}}(s)$ denotes the path measure of the distribution of gradients, $s = u_x(x,t)$ at $(x,t) = (0,0)$ in the original Burgers equation as one would obtain it by performing DNS.

On the other hand, if we sample events for the gradient of the fluctuations, $\delta u$, around the instanton $I^{(a)}$, i.e. when $u_x = a$ through the new stochastic equation * we would get a PDF generated by the measure $e^{-S^a}$. The last equality in * tells us that in order to get the unbiased original PDF we need to reweight with a factor $e^{-\Delta S^a}$.

If we would proceed in choosing one value $u_x = a$ to calculate the instanton with $u_x^{I(a)}(x = 0, t = 0) = a$, we will be able to sample the statistics near this value very efficiently. However, values $u_x = s$ far away from $a$ will be sampled with poor performance. Thus a major step is to choose $s = a$, which means that for every point $u_x = a$ in the PDF we first calculate the instanton and then using ** to obtain the PDF at $u_x = a$. Thus the actual form of the Girsanov transformation used in our instanton reweighting approach reads

$$P_{S_{\mathscr{L}}}(s) := \delta\left(u_x(0,0) - s\right) e^{-S_{\mathscr{L}}} = \delta\left(\delta u_x(0,0)\right) e^{-\left(\bar{S}^a + \Delta S^a\right)}$$

## Algorithm

1. Solve instanton equation $\longrightarrow u^{I(a)}, p^{I(a)}$

2. Calculate instanton action $S^{I(a)} = \frac{1}{2}\int_{-\infty}^{0} dt \int dx dx' p(x,t)\chi\,(x - x')\,p\,(x', t)$

3. For a chosen number of realizations $N$:

   a) Calculate the fluctuations around the instanton whilst calculating the space integral $\frac{1}{2}\int dx p_x^{I(a)}(\delta u)^2$ at every time step, such that the sum over all time steps gives the space time integral from

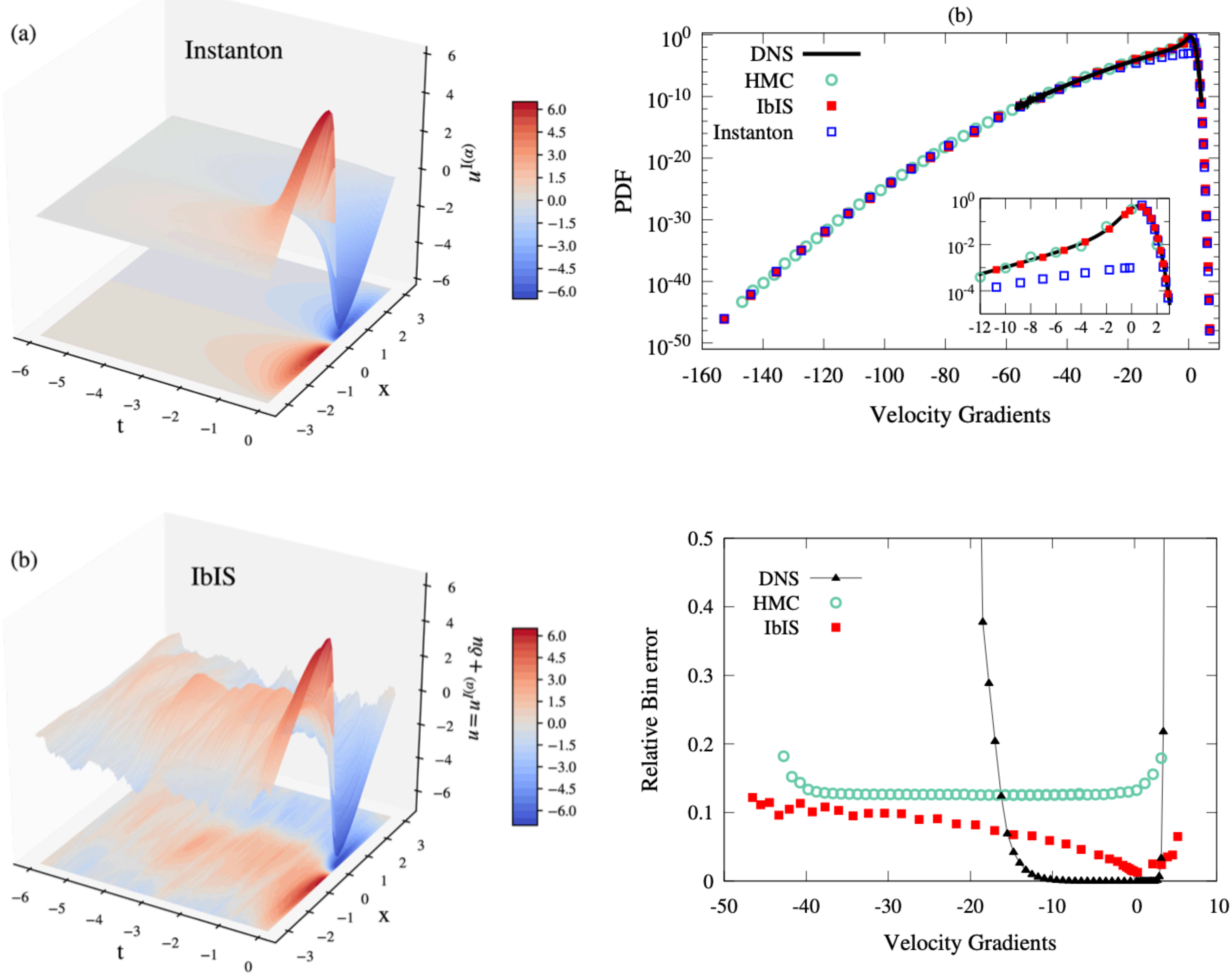
$$\Delta S^a = S_{\mathscr{L}} - \tilde{S}^a = S^{I(a)} - \frac{1}{2}\int dt dx p_x^{I(a)}(\delta u)^2$$

   that is required in order to calculate the reweighting factor.

   b) Add the instanton and the fluctuation $u = u^{I(a)} + \delta u$ and subsequently calculate the gradient $u_x$ at the space-time point $(x, t) = (0,0)$.

   c) Create the histogram of $u_x$ around $a$, where the bin size corresponds to the spacing of the gradients $a$, and the current realization of $u_x(0,0)$ is weighted by the factor $e^{-\Delta S^{\alpha}}$.

4. Take the mean value of all the histograms to obtain the value of the PDF at $u_x = a$.



(a)
Instanton
$u^{I(\alpha)}$
t
x
(b)
PDF
DNS
HMC
IbIS
Instanton
Velocity Gradients
(b)
IbIS
$u = u^{I(\alpha)} + \delta u$
t
x
Relative Bin error
DNS
HMC
IbIS
Velocity Gradients

| $\nu$ | # meshpoints | # timesteps | time interval | # realizations | method | computing time (cpu hrs) |
|---|---|---|---|---|---|---|
| 0.5 | 64 | 576 | 6 | $1 \times 10^9$ | DNS | $1 \times 10^3$ |
| 0.5 | 64 | 576 | 6 | $6 \times 10^5$ | HMC | $1 \times 10^3$ |
| 0.5 | 64 | 576 | 6 | $170 \times 10^5$ | IbIS | 24 |
| 0.2 | 256 | 1152 | 4 | $2 \times 10^8$ | DNS | $2.7 \times 10^3$ |
| 0.2 | 256 | 1152 | 4 | $4 \times 10^5$ | HMC | $1.2 \times 10^4$ |
| 0.2 | 256 | 1152 | 4 | $180 \times 10^5$ | IbIS | 250 |

TABLE I: The parameters used for the numerical simulations. $\nu$ is the viscosity, # meshpoints is the number of grid points $N_x$ in space, # timesteps is the number of points $N_t$ in time, while time interval denotes the physical temporal length. By # realizations we denote the number of produced space-time configurations. In the case of the IbIS method the notation $170 \times 10^5$ implies that we produced $10^5$ space-time configurations for each of the 170 instantons with a given $u_x(0,0) = a$. Accordingly for the HMC we produced $10^5$ configurations for each of the six values of $c_1$: (1.9, 1.6, 1.2, -1, -10, -20) for $\nu = 0.5$, and of the four $c_1$: (0.9, 0.8, 0.6, 0.5) for $\nu = 0.2$, which were finally combined. The computing time in cpu hours is the total budget required to produce the corresponding # realizations, that were used in Fig. 3. Notice that the IbIS method is substantially cheaper than the HMC in providing similar quality of extreme events.

# Markov in scale

Now we start with the multi-increment PDF:

$$f_n\left(v_n, r_n; \ldots; v_1, r_1; \mathbf{x}, t\right) = \prod_{i=1}^{n} \left\langle \delta\left(v_i - \delta_{r_i} v(\mathbf{x}, t)\right)\right\rangle$$

and the conditional probability

$$p\left(v_n, r_n \mid v_{n-1}, r_{n-1}; \ldots; v_1, r_1\right) = \frac{f_n\left(v_n, r_n; \ldots; v_1, r_1\right)}{f_{n-1}\left(v_{n-1}, r_{n-1}; \ldots; v_1, r_1\right)}$$

Friedrich and Peinke 1997 observed that real turbulent flows possess an approximate Markov property in scale:

$$f_n\left(v_n, r_n; v_{n-1}, r_{n-1}; \ldots; v_1, r_1\right) = p\left(v_n, r_n \mid v_{n-1}, r_{n-1}\right) \ldots p\left(v_2, r_2 \mid v_1, r_1\right) f_1\left(v_1, r_1\right)$$

$\Longrightarrow$ Kramers-Moyal expansion

## Fluctuations

- Markov in scale

Friedrich and Peinke (1997): evolution in scale of the conditional probability $p(v,r|v',r')$ of velocity increments at scales $r$ and $r'$, $r > r'$:

$$\frac{\partial}{\partial r} p(v,r|v',r') = -\sum_{i=1}^{\infty} \left[ (-1)^i \frac{\partial^i}{\partial v^i} D^{(i)}(v,r) \right] p(v,r|v',r')$$

Integration over $v'$ yields the increment pdf $f(v,r)$:

$$\boxed{\frac{\partial}{\partial r} f(v,r) = -\sum_{i=1}^{\infty} \left[ (-1)^i \frac{\partial^i}{\partial v^i} D^{(i)}(v,r) \right] f(v,r)}$$

# Markov in scale

## Relation to phenomenological models of turbulence

moments of the velocity increments

$$\frac{\partial}{\partial r}\langle v^p \rangle = -\sum_{i=1}^{p} \int_{-\infty}^{\infty} dv \, \frac{p!}{(p-i)!} v^{p-i} D^{(i)}(v,r) f(v,r)$$

Assume scaling

$$\langle v^p \rangle \sim |r|^{\zeta_p}$$

$$\boxed{\Longrightarrow D^n(v,r) = \frac{1}{n!} \frac{v^n}{r} \sum_{i=1}^{n} (-1)^{n+1-i} \binom{n}{i} \zeta_i}$$

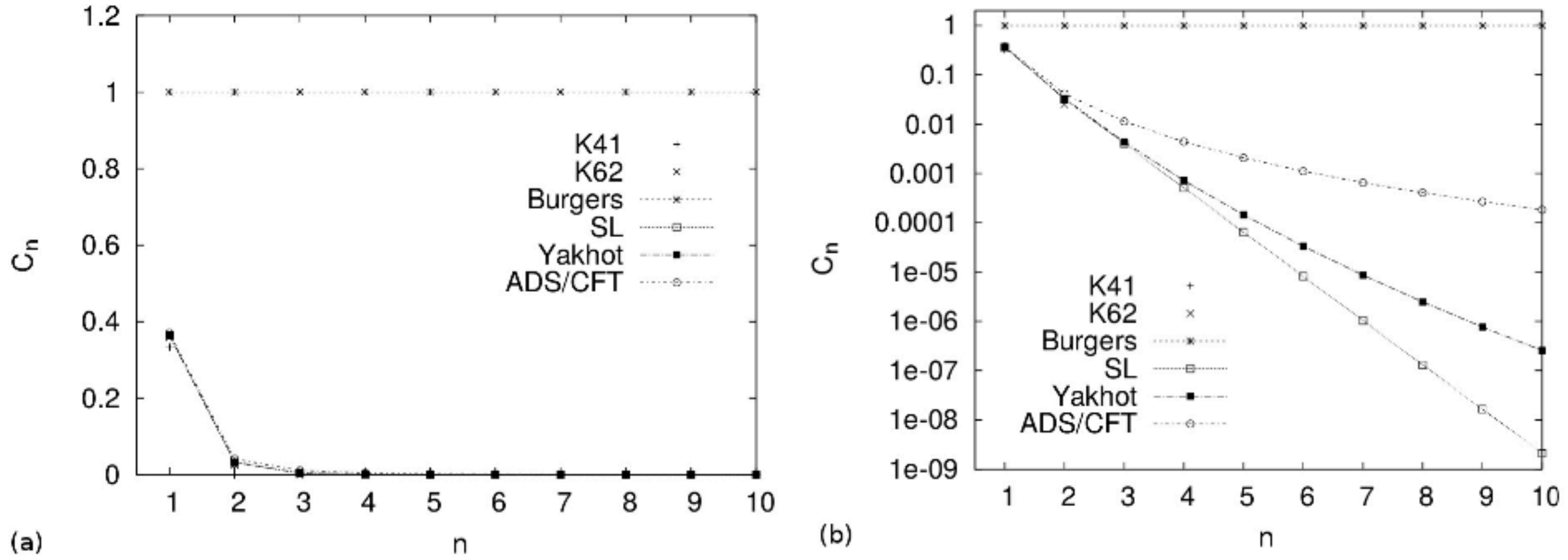
# Markov in scale

## reduced Kramers-Moyal coefficients

$$D^{(n)}(v,r) = C_n \frac{(-1)^n}{n!} \frac{v^n}{r}$$

| model | $\zeta_n$ | reduced Kramers-Moyal coefficients |
|---|---|---|
| K41 | $n/3$ | $C_1 = 1/3$ , no higher orders |
| K62[a)] | $n/3 - \mu n(n-3)/18$ | $C_1 = (3+\mu)/9$, $C_2 = \mu/9$, no higher orders |
| Burgers-ramps | $n$ | $C_1 = 1$, no higher orders |
| Burgers-shocks | 1 | $C_n = 1$ |
| She-Leveque[(d)] | $\frac{n}{9} + 2\left(1 - \left(\frac{2}{3}\right)^{n/3}\right)$ | $C_n = \frac{1}{9}\left(n\,{}_1F_0(1-n;;1) + 18\left(1 - \sqrt[3]{\frac{2}{3}}\right)^n\right)$ |
| Yakhot[b)] | $\zeta_{2n} = \frac{2(1+3\beta)n}{3(1+2\beta n)}$ | $C_n = \frac{\Gamma[n+1]}{\Gamma[n+1+\frac{1}{\beta}]}\left(\Gamma[1+\frac{1}{\beta}] + \frac{1}{3\beta^2}\Gamma[\frac{1}{\beta}]\right)$ |
| ADS/CFT[c)] | $\frac{\left((1+\gamma^2)^2+4\gamma^2(\frac{n}{3}-1)\right)^{\frac{1}{2}}+\gamma^2-1}{2\gamma^2}$ | no analytic expression |

# Markov in scale




Markov in scale is usefull

Perturbation Method: not Gaussian but Markov in scale

## Renormalization Group

The Forster-Nelson-Stephen (FNS, 1976/77) theory:

maximum wavenumber $\lambda$ (ultraviolet cutoff)

Fourier decomposition:

$$u_x(\mathbf{x},t) = \left(\frac{1}{2\pi}\right)^{d+1} \int_{k\leqslant\Lambda} \mathrm{d}^d k \int \mathrm{d}\omega u_\alpha(\mathbf{k},\omega)\exp(\mathrm{i}\mathbf{k}\cdot\mathbf{x} + \mathrm{i}\omega t)$$

and equation of motion:

$$\left(\mathrm{i}\omega + v_0 k^2\right) u_\alpha(\mathbf{k},\omega) = D_{\alpha\beta}(\mathbf{k}) f_\beta(\mathbf{k},\omega) + \lambda_0 M_{\alpha\beta\gamma}(\mathbf{k}) \int_{j\leqslant\Lambda} \mathrm{d}^3 j \int \mathrm{d}\Omega u_\beta(\mathbf{j},\Omega) u_\gamma(\mathbf{k}-\mathbf{j},\omega-\Omega)$$

$\nu_0$ unrenormalized viscosity,
$\lambda_0$ unrenormalized expansion parameter

Forcing:

$$\left\langle f_\alpha(\mathbf{k},\omega) f_\beta(\mathbf{k}',\omega')\right\rangle = 2W(k)(2\pi)^{d+1} D_{\alpha\beta}(\mathbf{k})\delta(\mathbf{k}+\mathbf{k}')\,\delta(\omega+\omega')$$

with power law $W(k) = W_0 k^{-y}$ .

# Renormalization Group

Dividing in low and high frequency parts:

$$u_\alpha(\mathbf{k},\omega) = \begin{cases} u_\alpha^<(\mathbf{k},\omega) & 0 < k < \Lambda\exp(-l) \\ u_\alpha^>(\mathbf{k},\omega) & \Lambda\exp(-l) < k < \Lambda \end{cases} \qquad f_\alpha(\mathbf{k},\omega) = \begin{cases} f_\alpha^<(\mathbf{k},\omega) & 0 < k < \Lambda\exp(-l) \\ f_\alpha^>(\mathbf{k},\omega) & \Lambda\exp(-l) < k < \Lambda \end{cases}$$

where $l$ is chosen such that $0 < \exp(-l) < 1$

Decomposition of Navier-Stokes:

$$\left(\mathrm{i}\omega + v_0 k^2\right) u_\alpha^<(\mathbf{k},\omega) = f_\alpha^<(\mathbf{k},\omega) + i_0 M_{\alpha\beta\gamma}^<(\mathbf{k}) \int_{j\leqslant\Lambda} \mathrm{d}^3 j \int \mathrm{d}\Omega \left\{ u_\beta^<(\mathbf{j},\Omega) u_\gamma^<(\mathbf{k}-\mathbf{j},\omega-\Omega) + \right.$$

$$\left. +2u_\beta^<(\mathbf{j},\Omega) u_\gamma^>(\mathbf{k}-\mathbf{j},\omega-\Omega) + u_\beta^>(\mathbf{j},\Omega) u_\gamma^>(\mathbf{k}-\mathbf{j},\omega-\Omega) \right\}$$

$$\left(\mathrm{i}\omega + v_0 k^2\right) u_\alpha^>(\mathbf{k},\omega) = f_\alpha^>(\mathbf{k},\omega) + \lambda_0 M_{\alpha\beta\gamma}^>(\mathbf{k}) \int_{j\leqslant\Lambda} \mathrm{d}^3 j \int \mathrm{d}\Omega \left\{ u_\beta^<(\mathbf{j},\Omega) u_\gamma^<(\mathbf{k}-\mathbf{j},\omega-\Omega) + \right.$$

$$\left. +2u_\beta^<(\mathbf{j},\Omega) u_\gamma^>(\mathbf{k}-\mathbf{j},\omega-\Omega) + u_\beta^>(\mathbf{j},\Omega) u_\gamma^>(\mathbf{k}-\mathbf{j},\omega-\Omega) \right\}$$

Aim is now to to eliminate $u^>$ in terms of $u^<$

**The perturbation series**

very similar as last week

$$u_0^>(k) = G_0(k) f^>(k)$$

perturbation expansion:

$$u^>(\hat{k}) = u_0^>(\hat{k}) + \lambda_0 u_1^>(\hat{k}) + \lambda_0^2 u_2^>(\hat{k}) \cdots + \lambda_0^n u_n(\hat{k}) \cdots$$

Result up to second order:

$$n = 0: \quad u_0^>(\hat{k}) = G_0(\hat{k}) f^>(\hat{k})$$

$$n = 1: \quad u_1^>(\hat{k}) = G_0(\hat{k}) M^>(\hat{k}) \sum_{\hat{j}} \left\{ u^<(\hat{j}) u^<(\hat{k} - \hat{j}) + 2u^<(\hat{j}) u_0^>(\hat{k} - \hat{j}) + u_0^>(\hat{j}) u_0^>(\hat{k} - \hat{j}) \right\}$$

$$n = 2: \quad u_2^>(\hat{k}) = G_0(\hat{k}) M^>(\hat{k}) \sum_{\hat{j}} \left\{ 2u^<(\hat{j}) u_1^>(\hat{k} - \hat{j}) + 2u_0^>(\hat{j}) u_1^>(\hat{k} - \hat{j}) \right\}$$

Now substitute everywhere $u_0^>$:

$$u^<(\hat{k}) = G_0(\hat{k})f^<(\hat{k}) + \lambda_0 G_0(\hat{k})M^<(\hat{k})\sum_{\hat{i}} u^<(\hat{j})u^<(\hat{k}-\hat{j}) + \lambda_0 G_0(\hat{k})M^<(\hat{k})\sum_{\hat{j}}\Big\{2u^<(\hat{j})u^>(\hat{k}-\hat{j})+$$

$$+2\lambda_0 u^<(\hat{j})u_1^>(\hat{k}-\hat{j}) + 2\lambda_0^2 u^<(\hat{j})u_2^>(\hat{k}-\hat{j})\Big\} + \lambda_0 G_0(\hat{k})M^<(\hat{k})\sum_{\hat{j}}\Big\{u_0^>(\hat{j})u_0^>(\hat{k}-\hat{j}) + 2\lambda_0 u_0^>(\hat{j})u_1^>(\hat{k}-\hat{j})+$$

$$+\lambda_0^2 u_1^>(\hat{j})u_1^>(\hat{k}-\hat{j}) + 2\lambda_0^2 u_2^>(\hat{j})u_0^>(\hat{k}-\hat{j})\Big\} + O\left(\lambda_0^4\right)$$

Average out effect of high frequencies according to the rules:

1. The low-frequency components are statistically independent of the high-frequency components and are invariant under the averaging process: $\langle f^< \rangle = f^<$ and $\langle u^< \rangle = u^<$.

2. Averages involving $u_0^>$ can be evaluated from $f^>$ and $G_0$.

3. The stirring forces are statistically homogeneous and thus $M^<(k)\langle u_0^>(j)u_0^>(k-j)\rangle = 0$ as $M^<(0) = 0$.

4. The stirring forces have zero mean, thus $\langle u_0^> \rangle = 0$ as $\langle f^> \rangle = 0$.

5. The probability distribution of the stirring forces is Gaussian. Therefore $\langle f^> f^> f^> \rangle = 0$ and hence $\langle u^> u^> u^> \rangle = 0$.

Thus we have:

$$u^<(\hat{k}) = G_0(\hat{k})f^<(\hat{k}) + \lambda_0 G_0(\hat{k})M^<(\hat{k})\sum^{<}(\hat{j})u^<(\hat{k}-\hat{j})+$$

$$+2\lambda_0^2 G_0(\hat{k})M^<(\hat{k})\sum_{\hat{j}}\sum_{\hat{p}} G_0(\hat{k}-\hat{j})M^>(\hat{k}-\hat{j})u^<(\hat{j})u^<(\hat{p})u^<(\hat{k}-\hat{j}-\hat{p})+$$

$$+\left\{8\lambda_0^2 G_0(\hat{k})M^<(\hat{k})\sum_{\hat{j}} G_0(\hat{k}-\hat{j})M^>(\hat{k}-\hat{j})\left|G_0(\hat{j})\right|^2 \times D(\hat{j})(2\pi)^{d+1}W(\hat{j})\right\}u^<(\hat{k}) + O\left(\lambda_0^3\right)$$

This can be written with increased viscosity $\nu_0 + \Delta\nu_0(k)$. Multiply with $i\omega + \nu_0 k^2$ to get rid of $G_0$ :

$$\left\{\mathrm{i}\omega + \nu_0 k^2 + \Delta\nu_0(k)k^2\right\} u_\alpha^<(\mathbf{k},\omega)$$

$$= f_\alpha^<(\mathbf{k},\omega) + \lambda_0 M_{\alpha\beta\gamma}^<(\mathbf{k})\int_{j\leqslant\Lambda}\mathrm{d}^3 j\int \mathrm{d}\Omega\, u_\beta^<(\mathbf{j},\Omega)u_\gamma^<(\mathbf{k}-\mathbf{j},\omega-\Omega)+$$

$$+2\lambda_0^2 M_{\alpha\beta\gamma}^<(\mathbf{k})\int \mathrm{d}^3\hat{j}\int \mathrm{d}^3\hat{p}\, M_{\beta\rho\sigma}^>(\hat{k}-\hat{j})G_0(\hat{k}-\hat{j})\times u_\gamma^<(\hat{k}-\hat{j})u_\rho^<(\hat{p})u_\sigma^<(\hat{k}-\hat{j}-\hat{p})$$

# Renormalization Group

This looks similar to original Navier-Stokes, but with additional viscosity and triple terms. Consider $k \longrightarrow 0$, than one can neglect triple term (irrelevant). This is basis of iteration:

$$\left\{ \mathrm{i}\omega + v_0 k^2 + \Delta v_0(k) k^2 \right\} u_\alpha^<(\mathbf{k}, \omega) = f_\alpha^<(\mathbf{k}, \omega) + \lambda_0 M_{\alpha\beta\gamma}^<(\mathbf{k}) \int_{j \leqslant \Lambda} \mathrm{d}^3 j \int \mathrm{d}\Omega u_\beta^<(\mathbf{j}, \Omega) u_\gamma^<(\mathbf{k} - \mathbf{j}, \omega - \Omega)$$

with effective viscosity

$$\Delta v_0(k) = 8 \lambda_0^2 k^{-2} M_{\rho\beta\gamma}^<(\mathbf{k}) \int_> \mathrm{d}^3 j \int \mathrm{d}\Omega G_0(|\mathbf{k} - \mathbf{j}|, \omega - \Omega) \times \left| G_0(j, \Omega) \right|^2 M_{\gamma\sigma\rho}^<(\mathbf{k} - \mathbf{j}) D_{\beta\sigma}(\mathbf{j}) W(j)$$

Integrate over angles in wavenumber space and use area $S_d$ of the unit sphere

$$S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$$

calculate $\longrightarrow$ $\Delta v_0(0) = \dfrac{K(d)\lambda_0^2 W_0}{v_0^2 \Lambda^\epsilon} \dfrac{\exp\{\epsilon l\} - 1}{\epsilon}$

where

$$\epsilon = 4 + y - d$$

and

$$K(d) = \frac{A(d)S_d}{(2\pi)^d}, \quad A(d) = \frac{d^2 - d - \epsilon}{2d(d+2)}$$

Total viscosity $\nu_1$ after elimination of modes in the band $\Lambda \exp(-l) < k < \Lambda$ is given by:

$$v_1 = v_0 + \Delta v_0(0) = v_0 \left\{ 1 + \frac{K(d)\lambda_0^2 W_0}{v_0^2 \Lambda^\epsilon} \frac{\exp\{\epsilon l\} - 1)}{\epsilon} \right\} = v_0 \left\{ 1 + K(d)\bar{\lambda}_0^2 \frac{\exp\{\epsilon l\} - 1}{\epsilon} \right\}$$

with modified strength parameter

$$\bar{\lambda}_0 = \frac{\lambda_0 W_0^{1/2}}{v_0^{3/2} \Lambda^{\epsilon/2}}$$

and new propagator

$$G_1(k, \omega) = \frac{1}{i\omega + \nu_1 k^2}$$

Now try to make the new equation look as much as possible as the original one by scaling both dependent and independent variables.
After filtering, wavenumber range is restricted to $0 < k < \Lambda \exp(-l)$. If we divide by $\exp(-l)$,

$$\tilde{k} = k \exp(l)$$

then $\tilde{k}$ is defined on the original interval $0 < k < \Lambda$.

Now allow scaling of other quantities:

$$\hat{\omega} = \omega \exp\{\mathrm{a}(l)\}$$
$$\tilde{u}_\alpha(\tilde{k}, \tilde{\omega}) = u_\alpha^<(\mathbf{k}, \omega)\exp\{-c(l)\}$$

With $\nu_1 = \nu_1 + \Delta\nu_0$ we have:

$$\left\{ \mathrm{i}\tilde{\omega} + \nu(l)\tilde{k}^2 \right\} \tilde{u}_\alpha(\tilde{\mathbf{k}}, \tilde{\omega}) = \tilde{f}_\alpha(\tilde{\mathbf{k}}, \tilde{\omega}) + \lambda(l) M_{\alpha\beta\gamma}(\tilde{\mathbf{k}}) \times \int_{\tilde{j} \leqslant \Lambda} \mathrm{d}^3 j \int \mathrm{d}\Omega \tilde{u}_\beta(\tilde{\mathbf{j}}, \tilde{\Omega}) \tilde{u}_\gamma(\tilde{k} - \tilde{j}, \tilde{\omega} - \tilde{\Omega})$$

Then stirring force, viscosity and strength parameter must then satisfy:

$$\tilde{f}_\alpha(\tilde{\mathbf{k}}, \tilde{\omega}) = f_\alpha^<(\mathbf{k}, \omega)\exp(a - c)\ ,\ \ \nu(l) = \nu_1 \exp(a - 2l)\ ,\ \ \lambda(l) = \lambda_0 \exp\{c - (d+1)l\}$$

where $d$ is the spatial dimension.

# Renormalization Group

Although stirring forces are rescaled, the rate at which they do work must be uneffected. This gives a relation for the scaling functions.

Correlation of the stirring forces:

$$\left\langle f_\alpha(\mathbf{k},\omega) f_\beta(\mathbf{k}',\omega')\right\rangle = 2(2\pi)^{d+1} W_0 D_{\alpha\beta}(\mathbf{k}) k^{-y} \times \delta\left(\mathbf{k}+k'\right)\delta\left(\omega+\omega'\right)$$

Scaling transformations lead to

$$\left\langle \tilde{f}_\alpha(\tilde{\mathbf{k}},\tilde{\omega}) \tilde{f}_\beta\left(\tilde{\mathbf{k}}',\tilde{\omega}'\right)\right\rangle = 2(2\pi)^{d+1} W_0 D_{\alpha\beta}(\tilde{\mathbf{k}}) \tilde{k}^{-y} \times \delta\left(\tilde{\mathbf{k}}+\tilde{k}'\right)\delta\left(\tilde{\omega}+\tilde{\omega}'\right)$$

only if $\quad 2c = 3a + (y+d)l$

FNS (1977) iteration based on infinitesimal wavenumber bands: recursion relations go to differential equations with $l$ as continuous variable:

$$\frac{\mathrm{d}\nu}{\mathrm{d}l} = \nu(l)\left\{z - 2 + \mathrm{K}(d)\bar{\lambda}^2\right\}, \quad \frac{\mathrm{d}W_0}{\mathrm{d}l} = 0, \quad \frac{\mathrm{d}\lambda}{\mathrm{d}l} = \lambda(l)\left(\frac{3z}{2} - 1 - \frac{d-y}{2}\right) \qquad \text{where} \qquad z = \frac{da}{dt}$$

Using the modified strength parameter $\bar{\lambda}^2 = \dfrac{\lambda^2 W_0}{\nu^3 \Lambda^\epsilon}$

we have the relation

$$\frac{d\bar{\lambda}}{dl} = \frac{\bar{\lambda}}{2}\left(\epsilon - 3K(d)\bar{\lambda}^2\right)$$

# Renormalization Group

## Behaviour near the fixed point

Consider limit k $\longrightarrow 0$ : not a theory of turbulence !
Nature of solutions depends on the value of $\epsilon$. We distinguish three cases:

$\epsilon < 0$: $\bar{\lambda}(l)$ tends exponentially to zero as $l \to \infty$

$\epsilon = 0$: $\bar{\lambda}(l)$ tends to zero as $1/l$, and there are logarithmic corrections to $v(l)$

$\epsilon > 0$: $\bar{\lambda}$ tends to the fixed point $\bar{\lambda}*$

The last is the interesting with the fixed point $\bar{\lambda}* = \left\langle \frac{\epsilon}{3K(d)} \right\rangle^{1/2}$

Renormalized viscosity becomes independent of $l$ if $z = 2 - \epsilon/3 \Longrightarrow a = (2 - \epsilon/3)l$

$\epsilon = 0$: upper critical dimension

$\epsilon > 0$: $\Longrightarrow y > d - 4$

We can derive an upper bound on the $y$ by searching for a condition, such that the triple moments $u^{<}u^{<}u^{<}$are irrelevant. Associate a scaling function $g$ with the triple moments than it must follow:

$$g(l) = g_0 \exp\langle -(d-y)l \rangle$$

# Renormalization Group

**Energy spectrum:**

$$E(k) \sim k^{\alpha}, \quad \alpha = -5/3 + 2/3(d-y)$$

$$\bar{\lambda}^* = \left(\frac{\epsilon}{3K(d)}\right)$$
$$z = 2 - \epsilon/3$$
$$a = (2 - \epsilon/3)l$$
$$2c = 3a + (y+d)l$$
$$2c = 6l - \epsilon l + (y-d)l$$
$$\epsilon = 4 + y - d$$
$$c = (1+d)l$$
$$-2c + (d-1)l = \alpha l - dl - a - a$$
$$-2l - 2dl + dl - l = \alpha l - 4dl - 4l + 2/3\epsilon l$$
$$1 = \alpha + 2/3\epsilon = \alpha + 8/3 + 2/3(y-d)$$
$$\alpha = -5/3 + 2/3(d-y)$$

**Simple Scaling Ansatz**

force power spectrum in Fourier space:

$$k^{-y+d-1}$$

and in real space for structure function:

$$l^{y+1-d-1} = l^{y-d}$$

now balance nonlinearity and forcing:

$$(y-d) = 3\zeta_1 - 1$$

$$\implies 2\zeta_1 = \frac{2}{3} + 2(y-d)/3$$

$$\implies E(k) \sim k^{-5/3+2(d-y)/3}$$

## Optimization Techniques for Instantons

Spontaneous symmetry breaking for extreme vorticity and strain in the three-dimensional Navier-Stokes equations
T. Schorlepp, T. Grafke, S. May, R. Grauer, Phil. Trans. R. Soc. A 380 (2022) 20210051.

general $d$-dimensional system of stochastic partial differential equations (SPDEs)

$$\partial_t u(x,t) + N(u(\,\cdot\,,t))(x) = \eta(x,t), \qquad \left\langle \eta(x,t)\eta^\top(x',t') \right\rangle = \varepsilon\chi\,(x-x')\,\delta\,(t-t')$$

vector field $u : \Omega \times [-T,0] \to \mathbb{R}^d$ on time interval $[-T,0]$ with $T > 0$ and initial condition

$$u(x,-T) = u_0(x)$$

Gaussian $d$-dimensional forcing $\eta$ with zero mean, white in time, and stationary spatial covariance matrix $\chi : \Omega \to \mathbb{R}^{d\times d}$ acting on large scales
$\varepsilon \in \mathbb{R}$ small positive number

Path integral for the PDF $\rho_O$ of a general, $\mathbb{R}^{d'}$-valued observable $O[u(\cdot,0)]$ at $a \in \mathbb{R}^{d'}$

$$\rho_O(a) = \int \mathcal{D}u\, \delta\left(u(\,\cdot\,, -T) - u_0\right) \delta(O[u(\cdot,0)] - a) J[u] \exp\left\{-\varepsilon^{-1} S[u]\right\}$$

Jacobi determinant $J[u]$ from the coordinate change $\eta \to u$

$S$ denotes Onsager-Machlup (or Freidlin-Wentzell) action

$$S[u] = \frac{1}{2}\int_{-T}^{0} \mathrm{d}t \mathscr{L}\left(u, \partial_t u\right) = \frac{1}{2}\int_{-T}^{0} \mathrm{d}t \left(\partial_t u + N(u), \chi^{-1} * \left[\partial_t u + N(u)\right]\right)_{L^2(\Omega, \mathbb{R}^d)} \geq 0$$

Instanton or large deviation limit: minimum of the action

$$\begin{cases} \min_u S[u] \\ \text{subject to } u(\,\cdot\,, -T) = u_0 \\ O[u(\cdot,0)] = a \end{cases}$$

constrained minimization problem

evaluating the action $S_\mathrm{I} := S\left[u_\mathrm{I}\right]$ at the minimum $u_I$, yields the log-asymptotics of the PDF

$$\rho_O(a) \sim \exp\left\{-\varepsilon^{-1} S_\mathrm{I}(a)\right\} \text{ for } \varepsilon \to 0$$

## Reformulation as an optimal control problem

introduce conjugate momentum $p := \nabla_{\partial_t u}\mathscr{L} = \chi^{-1} * \left[\partial_t u + N(u)\right]$

treat $p$ as the only independent variable in the minimisation problem

$$\begin{cases} \min_p S[p] = \min_p \frac{1}{2}\int_{-T}^{0} \mathrm{d}t (p, \chi * p)_{L^2(\Omega, \mathbb{R}^d)} \\ \text{s.t. } O[u[p](\cdot, 0)] = a \end{cases}$$

Optimal control: $p$ is the (distributed) control of the system

minimization is carried out over all $p$ for which the dependent state variable $u = u[p]$, that solves the $p$-dependent PDE

$$\begin{cases} \partial_t u + N(u) = \chi * p \\ u(\,\cdot\,, -T) = u_0 \end{cases} \qquad \text{with final time constraint} \quad O[u[p](\cdot, 0)] = a$$

Note that only $\chi * p$ enters the target functional and the PDE constraint

$\Longrightarrow$ memory savings !!!

## Conversion to unconstrained problems: Method of Lagrange multipliers

Introduce Lagrange multiplier $\mathscr{F} \in \mathbb{R}^{d'} \implies$ new objective

$$L[p, \mathscr{F}] = S[p] + (\mathscr{F}, O[u[p](\cdot,0)] - a)_{d'}$$

Note that a minimum of $S$ will always be at a saddle point of $L$, since the constraint is added linearly.

Keeping $\mathscr{F}$ fixed corresponds to the Chernykh and Stepanov (CS) method:

Input:

Fixed Lagrange multiplier $\mathscr{F} \in \mathbb{R}^{d'}$

Initial control $p^{(0)}$ (e.g. $p^{(0)} \equiv 0$, or random initialization, or result from previously solved problem)

Error tolerance $\delta$.

Output:

Control $p^{(*)}$

Action $S\left[p^{(*)}\right]$

Observable value $a^{(*)}$ for $p^{(*)}$

Starting from $p^{(0)}$, approximately determine a minimum $p^{(*)}$ of $L[p, \mathscr{F}]$ with

$$\left\| \frac{\delta L}{\delta p} \left[p^{(*)}, \mathscr{F}\right] \right\|_{L^2(\Omega \times [-T,0], \mathbb{R}^d)} < \delta$$

where $L$ is the target functional

$$L[p, \mathscr{F}] = S[p] + (\mathscr{F}, O[u[p](\cdot,0)] - a)_{d'}$$

and possible minimization algorithms are described soon. In the original CS method this is realized by a simple iterative forward-backward step with some "mild" update of the "force".

Evaluate $S\left[p^{(*)}\right]$ and $a^{(*)} = O\left[u\left[p^{(*)}\right](\cdot,0)\right]$

If this approach is feasible, it is numerically cheaper than solving a series of unconstrained problems in order to find the minimizer for given values of $a$.

In general, however, there are several problems with this approach, as the map $\mathscr{F} \mapsto a$ can become multivalued or diverge.

In particular, this is relevant whenever the PDF that we want to estimate displays heavy tails in the sense that $\rho_O$ decays slower than $\exp\{-c\|a\|\}$, or more generally if the map $a \mapsto S_{\mathrm{I}}(a)$ fails to be convex. There, nonlinear transformations of the observable that convexify the action are proposed as a solution to this problem.

## Conversion to unconstrained problems: Penalty method

Introduce penalty parameter $\mu > 0$, new objective

$$R[p,\mu] = S[p] + \frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'} \qquad \text{and let } \mu \to \infty$$

good: functional $R[p,\mu]$ is bounded from below by $0$

Care is needed for the choice of the sequence of $\mu$-values and the termination criterium

**Input:**

Target observable value $a \in \mathbb{R}^{d'}$

Initial control $p^{(0)}$ (e.g. $p^{(0)} \equiv 0$, or random initialization, or result from previously solved problem)

Increasing sequence $\mu^{(0)}, \ldots, \mu^{(M)}$ of penalty parameters

Decreasing sequence $\delta^{(0)}, \ldots \delta^{(M)}$ of error tolerances for each unconstrained minimization problem

**Output:**

Control $p^{(M)}$

Action $S\left[p^{(M)}\right]$

Observable value $a^{(M)}$ for $p^{(M)}$

**for** $m = 0,1,2,\ldots,M-1$ **do**

Starting from $p^{(m)}$, approximately determine a minimum $p^{(*)}$ of $R\left[p,\mu^{(m)}\right]$ with

$$\left\| \frac{\delta R}{\delta p}\left[p^{(*)},\mu^{(m)}\right] \right\|_{L^2\left(\Omega\times[-T,0],\,\mathbb{R}^d\right)} < \delta^{(m)}$$

where $R$ is the quadratic target functional

$$R[p,\mu] = S[p] + \frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'}^2$$

and possible minimization algorithms are described soon.

Set $p^{(m+1)} \leftarrow p^{(*)}$

**end for**

Evaluate $S\left[p^{(M)}\right]$ and $a^{(M)} = O\left[u\left[p^{(M)}\right](\cdot,0)\right]$

## Conversion to unconstrained problems: Augmented Lagrangian method

Combination: Lagrange multiplier $\mathscr{F} \in \mathbb{R}^{d'}$ and penalty parameter $\mu > 0$

$$L_A[p, \mathscr{F}, \mu] = S[p] + (\mathscr{F}, O[u[p](\cdot,0)] - a)_{d'} + \frac{\mu}{2} \|O[u[p](\cdot,0)] - a\|_{d'}^2$$

Again bounded from below.

Now we have a series of optimization problems for an increasing sequence of penalty parameters $\left(\mu^{(m)}\right)_{m=0,\ldots,M}$. However, it can be shown that, by updating the Lagrange multiplier $\mathscr{F}^{(m)}$ according to

$$\mathscr{F}^{(m+1)} = \mathscr{F}^{(m)} + \mu^{(m)} \left( O\left[u\left[p^{(m)}\right](\cdot,0)\right] - a \right)$$

where $p^{(m)}$ denotes the solution of the $m$-th unconstrained optimization problem, the convergence of $O\left[u\left[p^{(m)}\right](\cdot,0)\right]$ towards $a$ can be accelerated. As a result, it suffices to consider smaller values of $\mu^{(M)}$ for this method compared to the pure penalty approach. This in turn avoids potential issues with ill-conditioning caused by large penalty parameters.

**Input:**

Target observable value $a \in \mathbb{R}^{d'}$

Initial control $p^{(0)}$ (e.g. $p^{(0)} \equiv 0$, or random initialization, or result from previously solved problem)

Initial guess for the Lagrange multiplier $\mathscr{F}^{(0)} \in \mathbb{R}^{d'}$

Increasing sequence $\mu^{(0)}, \ldots, \mu^{(M)}$ of penalty parameters

Decreasing sequence $\delta^{(0)}, \ldots \delta^{(M)}$ of error tolerances for each unconstrained minimization problem

**Output:**

Control $p^{(M)}$

Action $S\left[p^{(M)}\right]$

Observable value $a^{(M)}$ for $p^{(M)}$

**for** $m = 0,1,2,\ldots,M-1$ **do**

Starting from $p^{(m)}$, approximately determine a minimum $p^{(*)}$ of $L_{\mathrm{A}}\left[p, \mathscr{F}^{(m)}, \mu^{(m)}\right]$ with

$$\left\| \frac{\delta L_{\mathrm{A}}}{\delta p}\left[p^{(*)}, \mathscr{F}^{(m)}, \mu^{(m)}\right] \right\|_{L^2\left(\Omega \times [-T,0], \mathbb{R}^d\right)} < \delta^{(m)}$$

where $L_A$ is the quadratic target functional

$$L_A[p, \mathscr{F}, \mu] = S[p] + (\mathscr{F}, O[u[p](\cdot,0)] - a)_{d'} + \frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'}^2$$

and possible minimization algorithms are described soon.

Set $p^{(m+1)} \leftarrow p^{(*)}$

Set $\mathscr{F}^{(m+1)} \leftarrow \mathscr{F}^{(m)} + \mu^{(m)}\left(O\left[u\left[p^{(m)}\right](\cdot,0)\right] - a\right)$

**end for**

Evaluate $S\left[p^{(M)}\right]$ and $a^{(M)} = O\left[u\left[p^{(M)}\right](\cdot,0)\right]$

## Gradient-based minimization: Gradient descent and L-BFGS method

Former treatment are special cases of

$$L_{\mathrm{A}}[p, \mathscr{F}, \mu] = \frac{1}{2}\int_{-T}^{0} \mathrm{d}t (p, \chi * p)_{L^2(\Omega, \mathbb{R}^d)} + (\mathscr{F}, O[u[p](\cdot,0)] - a)_{d'} + \frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'}^2$$

Introduce gradient-based algorithms to minimize this objective numerically with respect to $p$ for fixed parameters $\mu > 0$ and $\mathscr{F} \in \mathbb{R}^{d'}$.

(a): derive first order necessary conditions at minima = instanton equations
In the literature (CS), these instanton equations are often solved iteratively by repeated forward and backward integration.

(b): connect this approach to gradient-based minimization by conveniently expressing the gradient $\delta L_{\mathrm{A}} / \delta p$ using an adjoint state.

(c): standard gradient descent algorithm for minimizing the objective

(d): L-BFGS scheme, better convergence properties. Just like gradient descent, only gradient evaluations are needed and it is not necessary to compute second-order information in form of a Hessian, which is typically very expensive.

(e): implementational details concerning the memory usage

### (a) Instanton equations

Introduce another field: $z$ = adjoint variable. Focus on the case $\mu = 0$ (only Lagrange multiplier, the augmented case is similar)

$$\tilde{L}[u, p, z, \mathcal{F}] = \frac{1}{2}\int_{-T}^{0} \mathrm{d}t (p, \chi * p)_{L^2(\Omega, \mathbb{R}^d)} + \int_{-T}^{0} \mathrm{d}t \left(z, \partial_t u + N(u) - \chi * p\right)_{L^2(\Omega, \mathbb{R}^d)}$$
$$+ \left(z(\,\cdot\,, -T), u(\,\cdot\,, -T) - u_0\right)_{L^2(\Omega, \mathbb{R}^d)} + (\mathcal{F}, O[u(\cdot,0)] - a)_{d'}$$

first order necessary conditions

$$\begin{cases} \dfrac{\delta\tilde{L}}{\delta u} = -\partial_t z + \nabla N(u)^\top z = 0, \quad z(\cdot,0) = -\left[\dfrac{\delta O}{\delta u}(u(0))\right]^\top \mathcal{F} \\ \dfrac{\delta\tilde{L}}{\delta p} = \chi * [p - z] = 0 \\ \dfrac{\delta\tilde{L}}{\delta z} = \partial_t u + N(u) - \chi * p = 0, \quad u(\,\cdot\,, -T) = u_0 \\ \nabla_{\mathcal{F}}\tilde{L} = O[u(\cdot,0)] - a = 0 \end{cases}$$

stationary points $\left(u_{\mathrm{I}}, p_{\mathrm{I}}, z_{\mathrm{I}}, \mathscr{F}_{\mathrm{I}}\right)$ of the Lagrange function, the equality $p_{\mathrm{I}} = z_{\mathrm{I}}$ holds. This results in the instanton equations

$$\begin{cases} \partial_t u_{\mathrm{I}} + N\left(u_{\mathrm{I}}\right) = \chi * p_{\mathrm{I}}, & u_{\mathrm{I}}(\,\cdot\,, -T) = u_0, \\ \partial_t p_{\mathrm{I}} - \nabla N\left(u_{\mathrm{I}}\right)^{\top} p_{\mathrm{I}} = 0, & p_{\mathrm{I}}(0) = -\left[\frac{\delta O}{\delta u}\left(u_{\mathrm{I}}(0)\right)\right]^{\top} \mathscr{F}_{\mathrm{I}} \end{cases}$$

with $\mathscr{F}_{\mathrm{I}}$ being chosen such that final time constraint $O[u(\cdot,0)] - a = 0$ is satisfied.

CS solved these saddle-point equations numerically by an iterative forward and backward solution. The connection to gradient-based minimization methods will be become clear soon.

### (b) Adjoint state method

How to calculate $\delta L_{\mathrm{A}}/\delta p$ with the adjoint state method (forward-backward evaluation). valid way of expressing the gradient $\delta L_{\mathrm{A}}/\delta p$ at any $p$, and not only at critical point.

Expanding $L_{\mathrm{A}}$ to first order in $\delta p$

$$L_{\mathrm{A}}[p+\delta p,\mathcal{F},\mu] = L_{\mathrm{A}}[p,\mathcal{F},\mu] + \int_{-T}^{0} \mathrm{d}t(\delta p, \chi * p)_{L^2(\Omega,\mathbb{R}^d)}$$

$$+\int_{\Omega} \mathrm{d}^d x' \int_{-T}^{0} \mathrm{d}t \int_{\Omega} \mathrm{d}^d x \left( \mathcal{F} + \mu(O[u[p](\cdot,0)] - a), \left.\frac{\delta O}{\delta u}\right|_{u(0)} (x') \underbrace{\frac{\delta u\,(x',0)}{\delta p(x,t)}}_{=:J(x',t'=0;x,t)} \delta p(x,t) \right)_{d'}$$

Now simplify second term. Define adjoint field $z : \Omega \times [-T,0] \to \mathbb{R}^d$ as the solution of

$$\begin{cases} \partial_t z - \nabla N(u)^{\top} z = 0 \\ z(0) = -\left[\frac{\delta O}{\delta u}(u[p](\cdot,0))\right]^{\top} \{\mathcal{F} + \mu(O[u[p](\cdot,0)] - a)\} \end{cases}$$

We use $z$ to rewrite the inner integral of the second term by first computing the expression

$$\partial_{t'} \int_\Omega \mathrm{d}^d x' \left( z\left(x', t'\right), J\left(x', t'; x, t\right) \delta p(x, t) \right)_d$$

$$= \int_\Omega \mathrm{d}^d x' \left( \partial_{t'} z\left(x', t'\right), J\left(x', t'; x, t\right) \delta p(x, t) \right)_d + \left( z\left(x', t'\right), \left[ \frac{\delta}{\delta p(x, t)} \partial_{t'} u\left(x', t'\right) \right] \delta p(x, t) \right)_d$$

$$= \int_\Omega \mathrm{d}^d x' \left( \nabla N^\top \left( u\left( \,\cdot\, , t'\right) \right) \left(x'\right) z\left(x', t'\right), J\left(x', t'; x, t\right) \delta p(x, t) \right)_d$$

$$+ \left( z\left(x', t'\right), \left[ - \nabla N \left( u\left( \,\cdot\, , t'\right) \right) \left(x'\right) J\left(x', t'; x, t\right) + \chi\left(x - x'\right) \delta\left(t - t'\right) \right] \delta p(x, t) \right)_d$$

$$= \left( (\chi * z)(x, t'), \delta p(x, t) \right)_d \delta\left(t - t'\right)$$

Now, integrating this from $t' = -T$ to $t' = 0$, we get (with $J\left(x', -T; x, t\right) = 0$ )

$$\int_\Omega \mathrm{d}^d x' \left( z\left(x', 0\right), J\left(x', 0; x, t\right) \delta p(x, t) \right)_d = \left( (\chi * z)(x, t), \delta p(x, t) \right)_d$$

Using this

$$\int_\Omega \mathrm{d}^d x' \left( z\,(x',0), J\,(x',0;x,t)\,\delta p(x,t) \right)_d = ((\chi * z)(x,t), \delta p(x,t))_d$$

and the final condition

$$z(0) = -\left[ \frac{\delta O}{\delta u}(u[p](\cdot,0)) \right]^\top \{ \mathscr{F} + \mu(O[u[p](\cdot,0)] - a) \}$$

and combining with the first order expansion

$$L_\mathrm{A}[p+\delta p, \mathscr{F}, \mu] = L_\mathrm{A}[p, \mathscr{F}, \mu] + \int_{-T}^{0} \mathrm{d}t (\delta p, \chi * p)_{L^2(\Omega, \mathbb{R}^d)}$$

$$+ \int_\Omega \mathrm{d}^d x' \int_{-T}^{0} \mathrm{d}t \int_\Omega \mathrm{d}^d x \left( \mathscr{F} + \mu(O[u[p](\cdot,0)] - a), \left.\frac{\delta O}{\delta u}\right|_{u(0)} (x') \underbrace{\frac{\delta u\,(x',0)}{\delta p(x,t)}}_{=:J(x',t'=0;x,t)} \delta p(x,t) \right)_{d'}$$

We arrive at $\boxed{\dfrac{\delta L_\mathrm{A}}{\delta p} = \chi * (p - z)}$ ✓

For a single evaluation of the gradient of $L_{\mathrm{A}}$ with respect to $p$, we need to solve two PDEs: First, given the current control $p$, we need to integrate the nonlinear equations

$$\begin{cases} \partial_t u + N(u) = \chi * p \\ u(\,\cdot\,, -T) = u_0 \end{cases}$$

forward in time in order to determine $u[p]$. Afterwards, we need to integrate the linearized equations

$$\begin{cases} \partial_t z - \nabla N(u)^\top z = 0 \\ z(0) = -\left[\frac{\delta O}{\delta u}(u[p](\cdot,0))\right]^\top \{\mathscr{F} + \mu(O[u[p](\cdot,0)] - a)\} \end{cases}$$

backwards in time from $t = 0$ to $t = -T$. Here, both the starting condition for $z$ at $t = 0$ and the term $\nabla N(u)^\top$ will in general depend on $u$. We note that due to the negative sign in front of the term $\nabla N(u)^\top z$ in the adjoint equations, integrating these equations backwards in time is actually the natural and numerically stable choice.

### (c) Minimisation algorithms - Gradient descent

Now gradient based *iterative* minimization: update of the optimal control $p$

$$p^{(k+1)} = p^{(k)} + \sigma^{(k)} s^{(k)}$$

with $s^{(k)}$ being the search direction and $\sigma^{(k)} \in \mathbb{R}_+ \backslash \{0\}$ being the step length.

First simplest approach: steepest descent in direction $-\delta L_\mathrm{A} / \delta p$

$$s = -\chi^{-1} * \frac{\delta L_\mathrm{A}}{\delta p} = -(p - z)$$ search direction

preconditioner

Step length $\sigma$: Armijo line search with backtracking. More details soon.

Why this preconditioner ? In the case of linear $N$ and $O$ and $\mu = 0$ this would be the exact Hessian (second order variation) of $L_\mathrm{A}$ !!! With this the update looks like

$$p^{(k+1)} = p^{(k)} + \sigma^{(k)} s^{(k)} = \left(1 - \sigma^{(k)}\right) p^{(k)} + \sigma^{(k)} z^{(k)}$$

This corresponds to the CS iteration !!!

But the CS iteration use a *different strategy* for determining the step length.

Here Armijo or (sufficient decrease) condition

$$L_{\mathrm{A}}\left[p^{(k+1)}, \mathscr{F}, \mu\right] \leq L_{\mathrm{A}}\left[p^{(k)}, \mathscr{F}, \mu\right] + c\sigma^{(k)}\left(g^{(k)}, s^{(k)}\right)_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$$

where $g^{(k)}$ is the gradient at $p^{(k)}$ and $c > 0$ is the sufficient decrease constant

For our problem this reads:

$$\sigma^{(k)}\left(p^{(k)}, \chi * s^{(k)}\right)_{L^2(\Omega\times[-T,0],\mathbb{R}^d)} + \frac{\left(\sigma^{(k)}\right)^2}{2}\left(s^{(k)}, \chi * s^{(k)}\right)_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$$

$$\leq \left(\mathscr{F}, O\left[u\left[p^{(k)}\right](\cdot,0)\right] - O\left[u\left[p^{(k+1)}\right](\cdot,0)\right]\right)_{d'} + \frac{\mu}{2}\left\{\left\| O\left[u\left[p^{(k)}\right](\cdot,0)\right] - a\right\|_{d'}^2\right.$$

$$\left. - \left\| O\left[u\left[p^{(k+1)}\right](\cdot,0)\right] - a\right\|_{d'}^2\right\} + c\sigma^{(k)}\left(g^{(k)}, s^{(k)}\right)_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$$

Looks ugly, is ugly, BUT: scalar products do not depend on step length $\sigma$

$\Longrightarrow$ need to be evaluated only once for each complete line search

Gradient descent for the minimization of

$$L_\mathrm{A}[p,\mathscr{F},\mu] = \frac{1}{2}\int_{-T}^{0} \mathrm{d}t (p, \chi * p)_{L^2(\Omega,\mathbb{R}^d)} + (\mathscr{F}, O[u[p](\cdot,0)] - a)_{d'} + \frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'}^2$$

**Input:**

Target observable value $a \in \mathbb{R}^{d'}$
Penalty parameter $\mu > 0$
Lagrange multiplier $\mathscr{F} \in \mathbb{R}^{d'}$
Initial control $p^{(0)}$ (e.g. $p^{(0)} \equiv 0$, or random initialization, or result from previously solved problem)
Error tolerance $\delta$
Maximum step number $K$
Initial step size $\sigma_\mathrm{init} > 0$ (typically $\sigma_\mathrm{init} = 1$)
Minimum step size $\sigma_\mathrm{min} \ll \sigma_\mathrm{init}$
Backtracking fraction $\beta \in (0,1)$ (e.g. $\beta = 1/2$)
Sufficient decrease constant $c > 0$ (typically $c \approx 10^{-2}$ )

**Output:**

Control $p^{(*)}$ (approximate minimum of $L_\mathrm{A}$ )
Gradient norm $\left\| \delta L_\mathrm{A}/\delta p \left(p^{(*)}\right) \right\|_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$ at the approximate minimum;

Augmented Lagrangian $L_\mathrm{A}\left[p^{(*)},\mathscr{F},\mu\right]$
Observable value $a^{(*)}$ for $p^{(*)}$

**for** $k = 0,1,2,\ldots,K-1$ **do**

Compute the gradient at $p^{(k)}$:

Starting from $u_0$, integrate the forward equation

$$\partial_t u + N(u) = \chi * p\,,\ \ u(\,\cdot\,,-T) = u_0$$

with $p^{(k)}$ on the RHS and store the the solution $u^{(k)}$.

Store the current observable value $a^{(k)} = O\left[u\left[p^{(k)}\right](\cdot,0)\right]$.

Integrate the backward equation

$$\partial_t z - \nabla N(u)^\top z = 0\,,\ \ z(0) = -\left[\frac{\delta O}{\delta u}(u[p](\cdot,0))\right]' \{\mathcal{F} + \mu(O[u[p](\cdot,0)] - a)\}$$

to get $z^{(k)}$, and compute the gradient

$$g^{(k)} \leftarrow \chi * \left(p^{(k)} - z^{(k)}\right)\,.$$

Compute and store $\left\| g^{(k)} \right\|_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$.

**if** $\left\| g^{(k)} \right\|_{L^2(\Omega\times[-T,0],\mathbb{R}^d)} < \delta$ **then**

**break**

**end if**

Fix the search direction: $s^{(k)} \leftarrow -\chi^{-1} * g^{(k)}$

and perform an Armijo line search to determine the step length $\sigma^{(k)}$ :

⋮

$\vdots$

Armijo line search:

**for** $\sigma^{(k)} = \sigma_{\text{init}}, \beta\sigma_{\text{init}}, \beta^2\sigma_{\text{init}}, \ldots$ **do**

Set $p^{(k+1)} \leftarrow p^{(k)} + \sigma^{(k)} s^{(k)}$

Evaluate $L_A\left[p^{(k+1)}, \mathscr{F}, \mu\right]$ (needs another forward integration)

**if** $L_A\left[p^{(k+1)}, \mathscr{F}, \mu\right] \leq L_A\left[p^{(k)}, \mathscr{F}, \mu\right] + c\sigma^{(k)}\left(g^{(k)}, s^{(k)}\right)_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$ **then**

break current loop

**end if**

**if** $\sigma^{(k)} < \sigma_{\min}$ **then**

break current and outer loop; report.

**end if**

**end for**

**end for**

## Remark

approach here: optimize then discretize

may not converge: choose discretization very carefully

alternative approach: discretize then optimize

Stopping criteria: $\left\| g^{(k)} \right\|_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$ is smaller than given threshold

## (d) Minimisation algorithms - L-BFGS method

gradient descent: robust but slow

true Hessian of $L_\mathrm{A}$ would improve convergence, but infeasible: memory and time issues

need solvers with require only matrix-vector products: future work

here: *Quasi Newton schemes*, that take *curvature* info from past steps

well know: BFGS scheme (Broyden-Fletcher-Goldfarb-Shanno)
1970 1970 1970 1970 4 separate publications

limited memory: L-BFGS (Liu, Nocedal 1989)

store last $m$ updates (typically $3 \leq m \leq 30$)

$$\Delta p^{(k-1)} := p^{(k)} - p^{(k-1)}, \ldots, \Delta p^{(k-m)} := p^{(k-m+1)} - p^{(k-m)} \qquad \text{control}$$

$$\Delta g^{(k-1)} := g^{(k)} - g^{(k-1)}, \ldots, \Delta g^{(k-m)} := g^{(k-m+1)} - g^{(k-m)} \qquad \text{gradient}$$

$\Longrightarrow$ construct low-rank approximation of the inverse of Hessian $H^{(k)} = \delta^2 L_\mathrm{A}\left[p^{(k)}, \mathscr{F}, \mu\right]$

apply as preconditioner to gradient descent direction $-g^{(k)}$ without storing it.

more details on standard BFGS

computation of the approximate inverse Hessian, start with an initial symmetric and positive definite estimate $B^{(0)}$ for the inverse Hessian $H^{(0)}$.

Good choices: $B^{(0)} = \mathrm{Id}$ or here $B^{(0)} = \chi^{-1}$

standard BFGS: update of search direction $s^{(k+1)} = -B^{(k+1)} g^{(k+1)}$ and

$$B^{(k+1)} = B^{(k)} + \rho^{(k)} \left[ w^{(k)} \otimes \Delta p^{(k)} + \Delta p^{(k)} \otimes w^{(k)} \right]$$
$$- \left[\rho^{(k)}\right]^2 \left( w^{(k)}, \Delta g^{(k)} \right)_{L^2(\Omega \times [-T,0], \mathbb{R}^d)} \Delta p^{(k)} \otimes \Delta p^{(k)}$$
$$= \left[ V^{(k)} \right]^\top B^{(k)} V^{(k)} + \rho^{(k)} \Delta p^{(k)} \otimes \Delta p^{(k)}$$

with $w^{(k)} = \Delta p^{(k)} - B^{(k)} \Delta g^{(k)}$ and

$$\rho^{(k)} = \left[ \left( \Delta g^{(k)}, \Delta p^{(k)} \right)_{L^2(\Omega \times [-T,0], \mathbb{R}^d)} \right]^{-1} \text{ and } V^{(k)} = \mathrm{Id} - \rho^{(k)} \Delta g^{(k)} \otimes \Delta p^{(k)}$$

Line search: Armijo (and not Powell-Wolf, too expensive) no guarantee about positive definiteness of $B^{(\bar{k})}$ $\Longrightarrow$ safety checks like angle condition

$$\left(-g^{(k)}, s^{(k)}\right)_{L^2\left(\Omega\times[-T,0],\mathbb{R}^d\right)} \geq \tilde{c}\ \| g^{(k)} \|_{L^2\left(\Omega\times[-T,0],\mathbb{R}^d\right)} \| s^{(k)} \|_{L^2\left(\Omega\times[-T,0],\mathbb{R}^d\right)}$$

with a small constant $\tilde{c}$.

condition guarantees that angle between

search direction $s^{(k)}$ and negative gradient $-g^{(k)}$

is smaller than 90 degrees

If violated, reset BFGS memory.

above formula for $B^{(k+1)}$ not recommended for large-scale problems since approximation matrix is dense

rewrite the algorithm to deduce a limited memory version

BFGS preconditioner can be written recursively as

$$
\begin{aligned}
B^{(k+1)} &= \left[V^{(k)}\right]^{\top} B^{(k)} V^{(k)} + \rho^{(k)} \Delta p^{(k)} \otimes \Delta p^{(k)} \\
&= \left[V^{(k-1)} V^{(k)}\right]^{\top} B^{(k-1)} \left[V^{(k-1)} V^{(k)}\right] \\
&\quad + \rho^{(k-1)} \left[V^{(k)}\right]^{\top} \Delta p^{(k-1)} \otimes \Delta p^{(k-1)} V^{(k)} + \rho^{(k)} \Delta p^{(k)} \otimes \Delta p^{(k)} \\
&= \cdots = \\
&= \left[V^{(k-m+1)} \ldots V^{(k)}\right]^{\top} B^{(k-m+1)} \left[V^{(k-m+1)} \ldots V^{(k)}\right] \\
&\quad + \rho^{(k-m+1)} \left[V^{(k-m+2)} \ldots V^{(k)}\right]^{\top} \Delta p^{(k-m+1)} \otimes \Delta p^{(k-m+1)} \left[V^{(k-m+2)} \ldots V^{(k)}\right] \\
&\quad + \rho^{(k-m+2)} \left[V^{(k-m+3)} \ldots V^{(k)}\right]^{\top} \Delta p^{(k-m+2)} \otimes \Delta p^{(k-m+2)} \left[V^{(k-m+3)} \ldots V^{(k)}\right] \\
&\quad + \cdots + \rho^{(k)} \Delta p^{(k)} \otimes \Delta p^{(k)}
\end{aligned}
\qquad (*)
$$

Thus can write $B^{(k+1)}$ using the matrix $B^{(k-m+1)}$ and vector products that involve $\Delta p^{(k)}, \ldots, \Delta p^{(k-m+1)}$ as well as $\Delta g^{(k)}, \ldots, \Delta g^{(k-m+1)}$.

now L-BFGS: replace potentially dense matrix $B^{(k-m+1)}$ by initial sparse guess $B_0^{(k+1)}$

Important: not necessary to store full matrices. Only the last $m$ entries for $\Delta p$ and $\Delta g$ need to be stored in order to construct the preconditioner.

popular choice for initial guess: $B_0^{(k+1)} = \gamma^{(k)}\,\mathrm{Id} = \dfrac{\left(\Delta p^{(k)}, \Delta g^{(k)}\right)_{L^2\left(\Omega\times[-T,0],\,\mathbb{R}^d\right)}}{\left(\Delta g^{(k)}, \Delta g^{(k)}\right)_{L^2\left(\Omega\times[-T,0],\,\mathbb{R}^d\right)}}\,\mathrm{Id}$

Here: $B_0^{(k+1)} = \gamma^{(k)}\chi^{-1}$. $B^{(k+1)}$ can be applied to $-g^{(k+1)}$ to compute the search direction $s^{(k+1)}$ without explicitly storing it via the two-loop recursion that is summarised in next algorithm. The algorithm for the full L-BFGS method follows thereafter.

## Two-loop recursion for the evaluation of $s^{(k)} = -B^{(k)} g^{(k)}$

**Input:**

Current gradient $g^{(k)}$

$m$ previous gradient updates $\Delta g^{(k-1)}, \ldots, \Delta g^{(k-m)}$

$m$ previous control updates $\Delta p^{(k-1)}, \ldots, \Delta p^{(k-m)}$

$m$ previous weights $\rho^{(k-1)}, \ldots, \rho^{(k-m)}$

**Output:**

$s^{(k)} = -B^{(k)} g^{(k)}$ given by (*)

$r \leftarrow -s^{(k)}$

**for** $i = k-1, \ldots, k-m$ **do**

$\alpha^{(i)} \leftarrow \rho^{(i)} \left(\Delta p^{(i)}, r\right)_{L^2\left(\Omega \times [-T,0], \mathbb{R}^d\right)}$

$r \leftarrow r - \alpha^{(i)} \Delta g^{(i)}$

**end for**

$r \leftarrow B_0^{(k)} r$

**for** $i = k-m, \ldots, k-1$ **do**

$h \leftarrow \rho^{(i)} \left(\Delta g^{(i)}, r\right)_{L^2\left(\Omega \times [-T,0], \mathbb{R}^d\right)}$

$r \leftarrow r + \left[\alpha^{(i)} - h\right] \Delta p^{(i)}$

**end for**

**return** $r$

## L-BFGS minimization

**Input:**

Target observable value $a \in \mathbb{R}^{d'}$

Penalty parameter $\mu > 0$

Lagrange multiplier $\mathscr{F} \in \mathbb{R}^{d'}$

Initial control $p^{(0)}$ (e.g. $p^{(0)} \equiv 0$, or random initialisation, or result from previously solved problem)

Error tolerance $\delta$

Maximum step number $K$

Initial step size $\sigma_{\text{init}} > 0$ (typically $\sigma_{\text{init}} = 1$)

Minimum step size $\sigma_{\min} \ll \sigma_{\text{init}}$

Backtracking fraction $\beta \in (0,1)$ (e.g. $\beta = 1/2$)

Sufficient decrease constant $c > 0$ (typically $c \approx 10^{-2}$ )

Number of stored previous updates $m$ (typically $3$ to $20$)

Angle condition constant $\tilde{c}$ (typically $\tilde{c} \approx 10^{-4}$ )

**Output:**

Control $p^{(*)}$ (approximate minimum of $L_{\mathrm{A}}$)

Gradient norm $\left\| \delta L_{\mathrm{A}} / \delta p \left(p^{(*)}\right) \right\|_{L^2\left(\Omega \times [-T,0], \mathbb{R}^d\right)}$ at the approximate minimum

Augmented Lagrangian $L_{\mathrm{A}}\left[p^{(*)}, \mathscr{F}, \mu\right]$

Observable value $a^{(*)}$ for $p^{(*)}$

**for** $k = 0,1,2,\ldots,K-1$ **do**

Compute the gradient $g^{(k)}$ at $p^{(k)}$ as before:

**if** $k \geq m+1$ **then**

Delete $\Delta g^{(k-m-1)}$, $\Delta p^{(k-m-1)}$ and $\rho^{(k-m-1)}$

**end if**

**if** $k \geq 1$ **then**

Store $\Delta p^{(k-1)}$, $\Delta g^{(k-1)}$ and $\rho^{(k-1)} \leftarrow 1/\left(\Delta g^{(k-1)}, \Delta p^{(k-1)}\right)_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$

**end if**

Compute and store $\left\| g^{(k)} \right\|_{L^2(\Omega\times[-T,0],\mathbb{R}^d)}$

**if** $\left\| g^{(k)} \right\|_{L^2(\Omega\times[-T,0],\mathbb{R}^d)} < \delta$ **then**

**break**

**end if**

Fix the search direction: $s^{(k)} \leftarrow$ Two-loop $\left(-g^{(k)}, \Delta g, \Delta p, \rho\right)$

and $B_0^{(k+1)} = \gamma^{(k)}\chi^{-1}$ as initial guess for $B_0^{(k)}$ (use $s^{(k)} \leftarrow -\chi^{-1} * g^{(k)}$ for $k = 0$ )

**if** angle condition is violated **then**

Reset to $s^{(k)} \leftarrow -\chi^{-1} * g^{(k)}$ and delete all $\Delta g, \Delta p, \rho$

**end if**

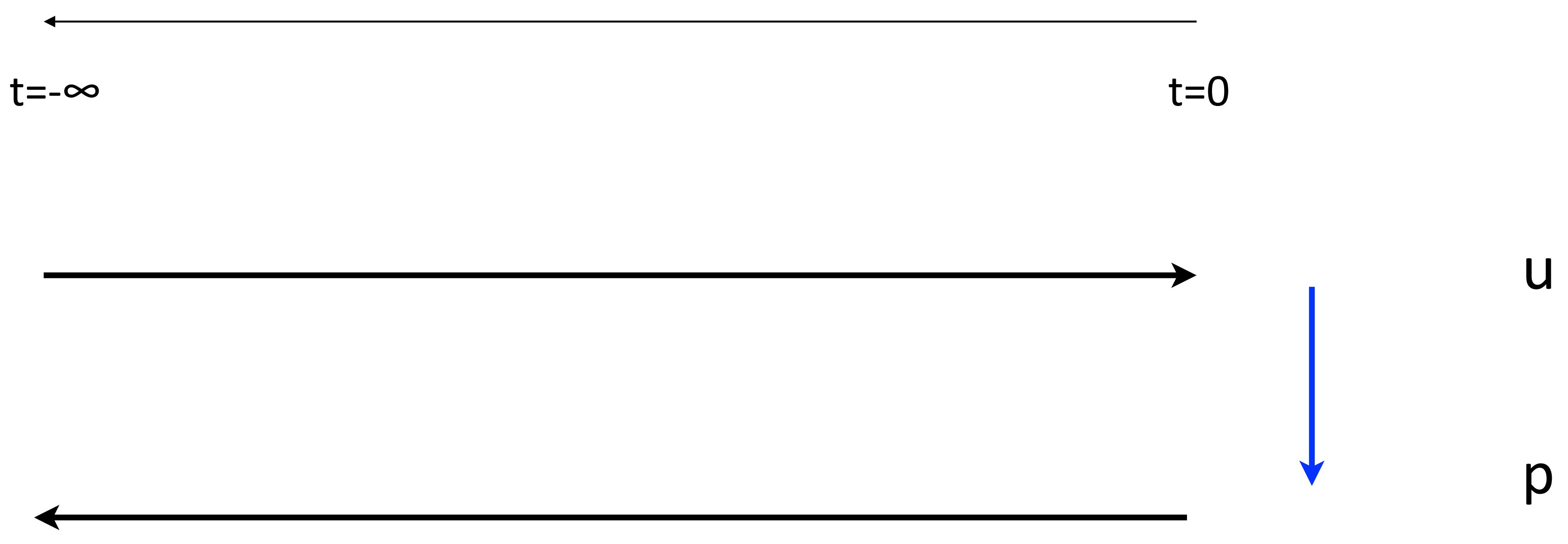
Perform an Armijo line search for $s^{(k)}$ to determine the step length $\sigma^{(k)}$

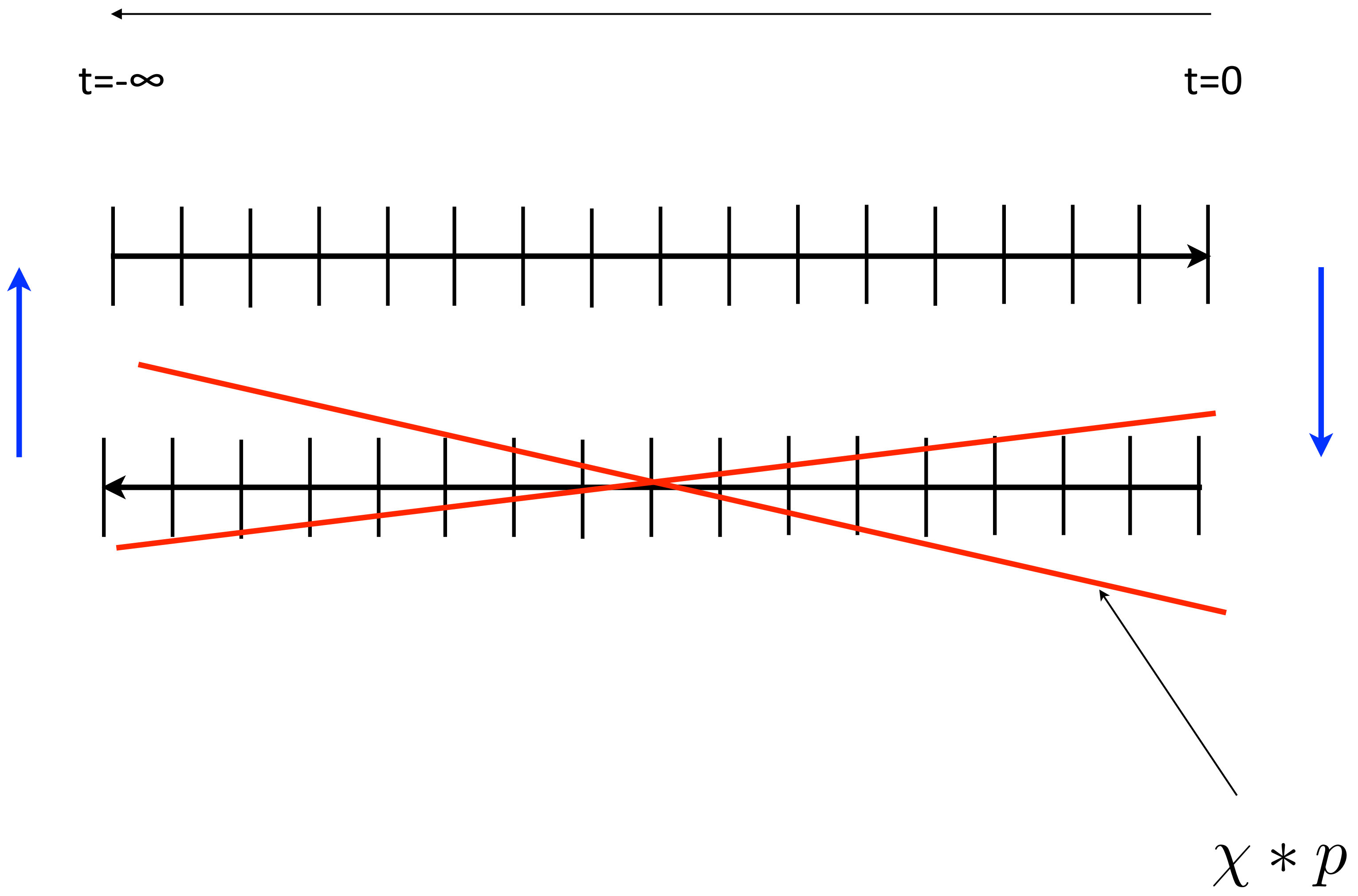
update $p^{(k+1)} \leftarrow p^{(k)} + \sigma^{(k)}s^{(k)}$

**end for**

(e) Memory reduction techniques

- store only $\widehat{\chi * p}(k) = \hat{\chi}(k)\hat{p}(k)$ and reduced modes for the gradient $g^{(k)}$ and the previous updates $\Delta p^{(k)}$ and $\Delta g^{(k)}$
- Checkpointing on a logarithmically spaced subgrid in time

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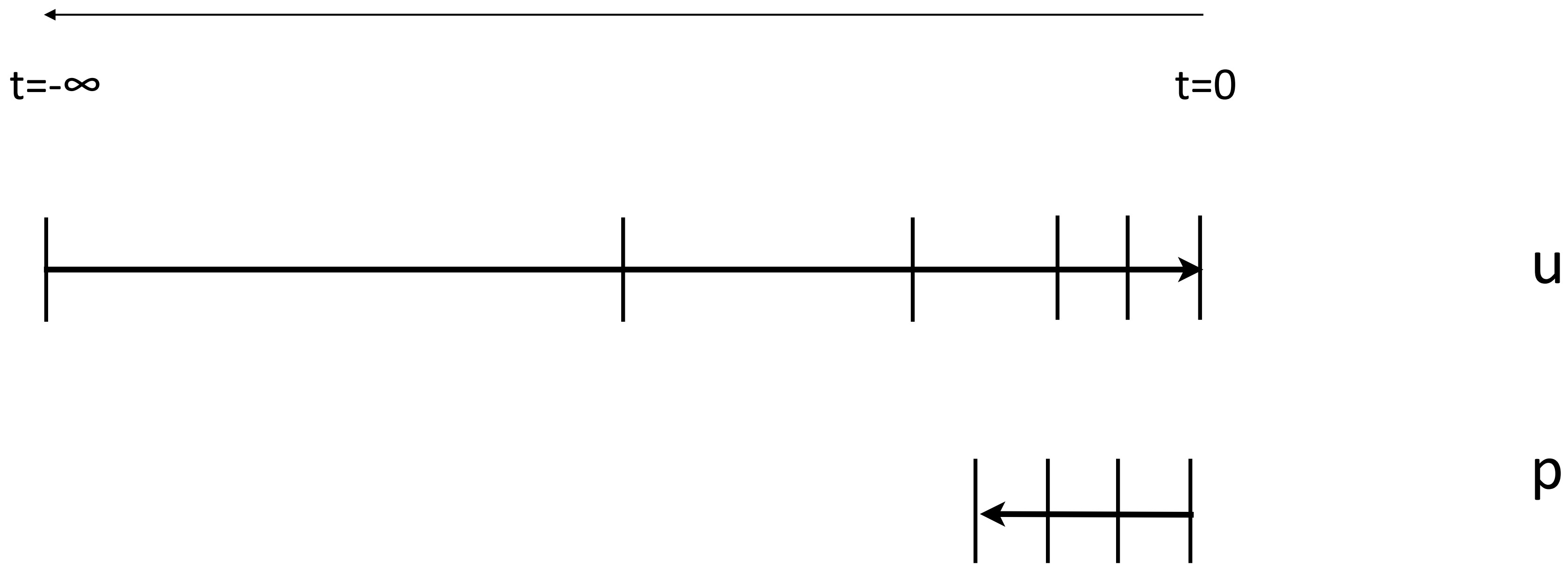
t=0
u
p
$\chi * p$



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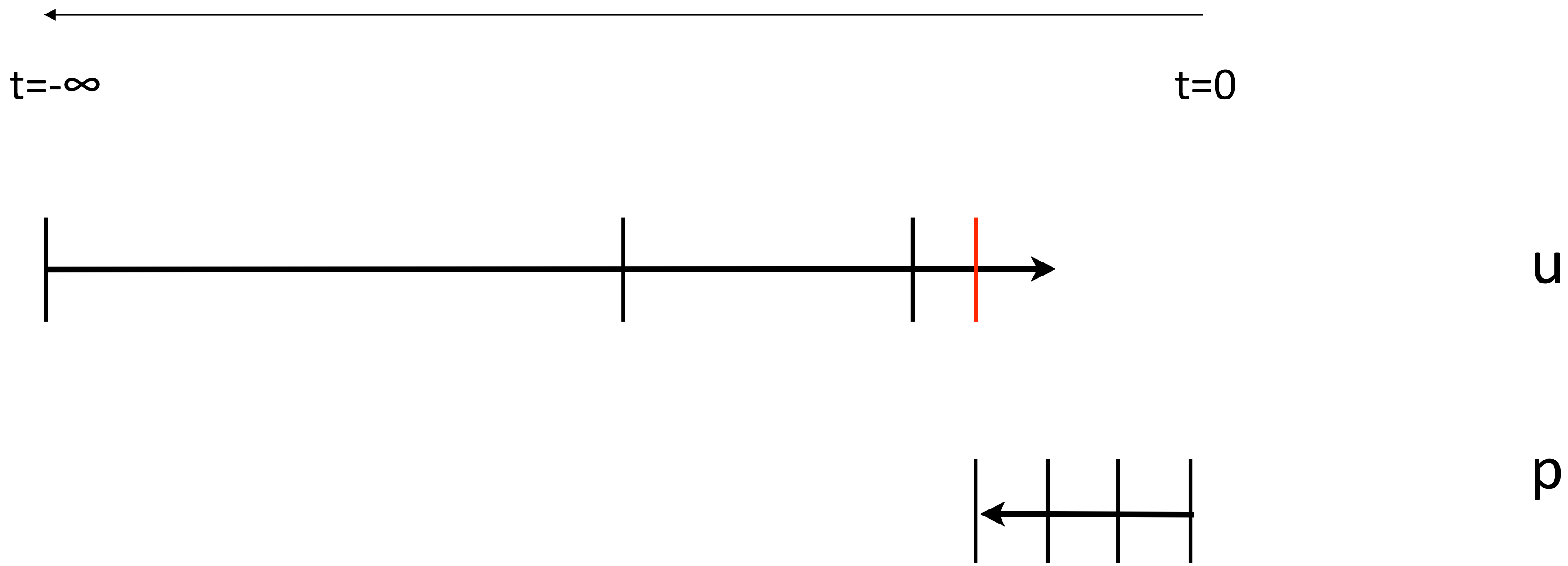

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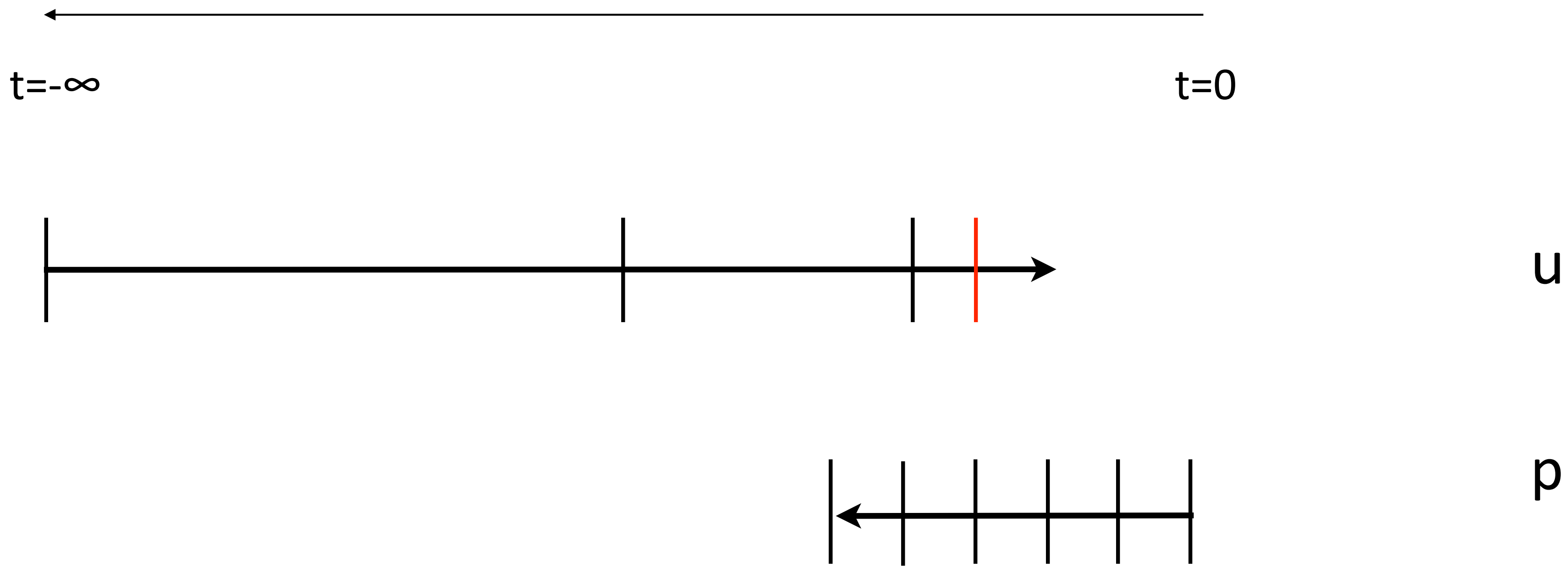
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t=0
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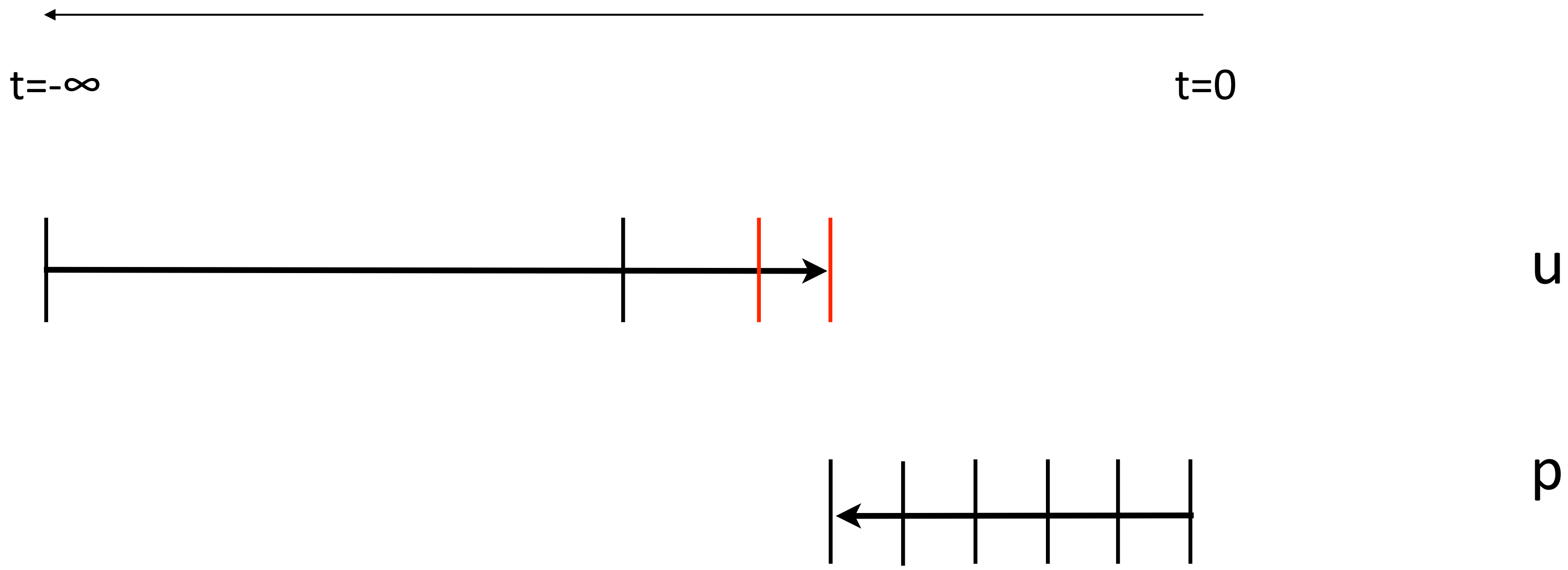

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t=0
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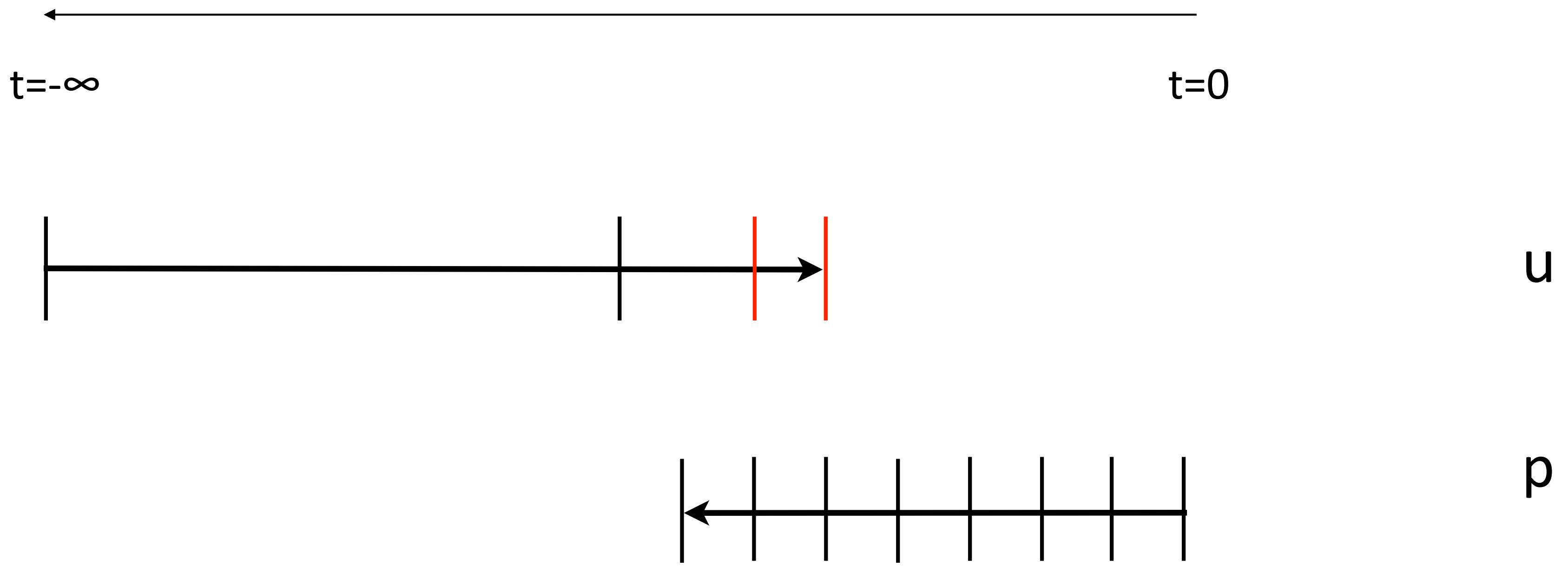
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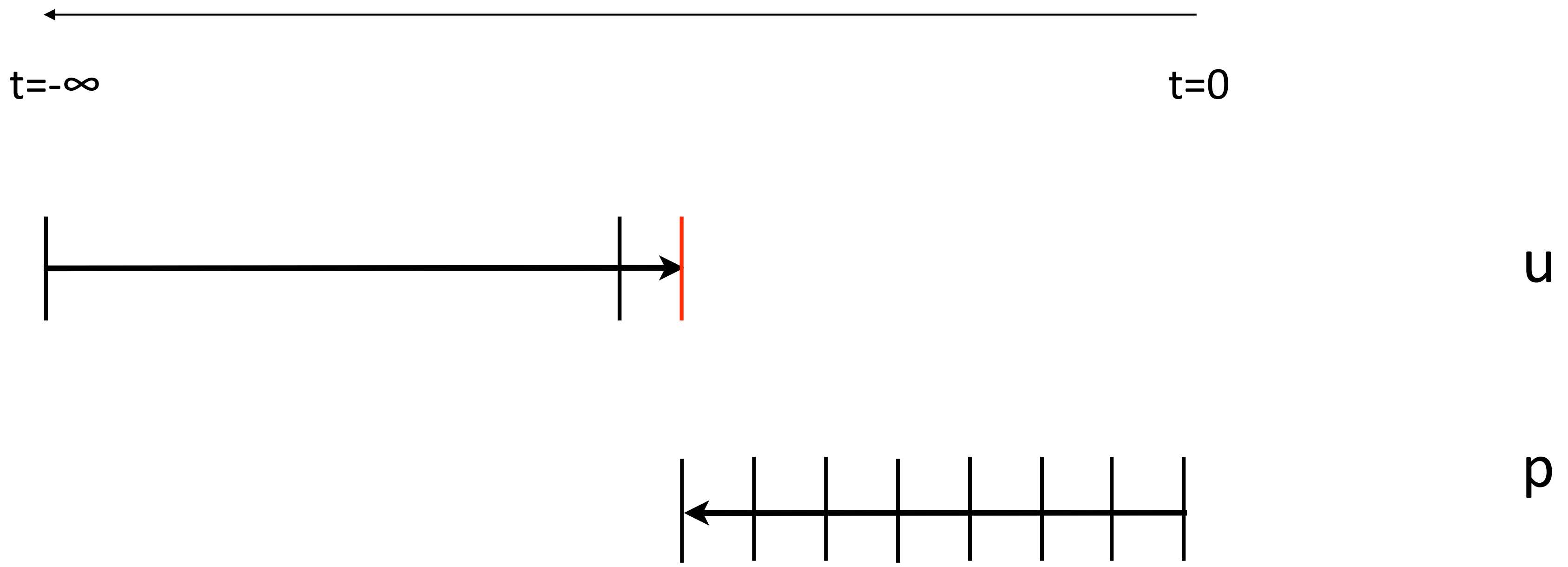
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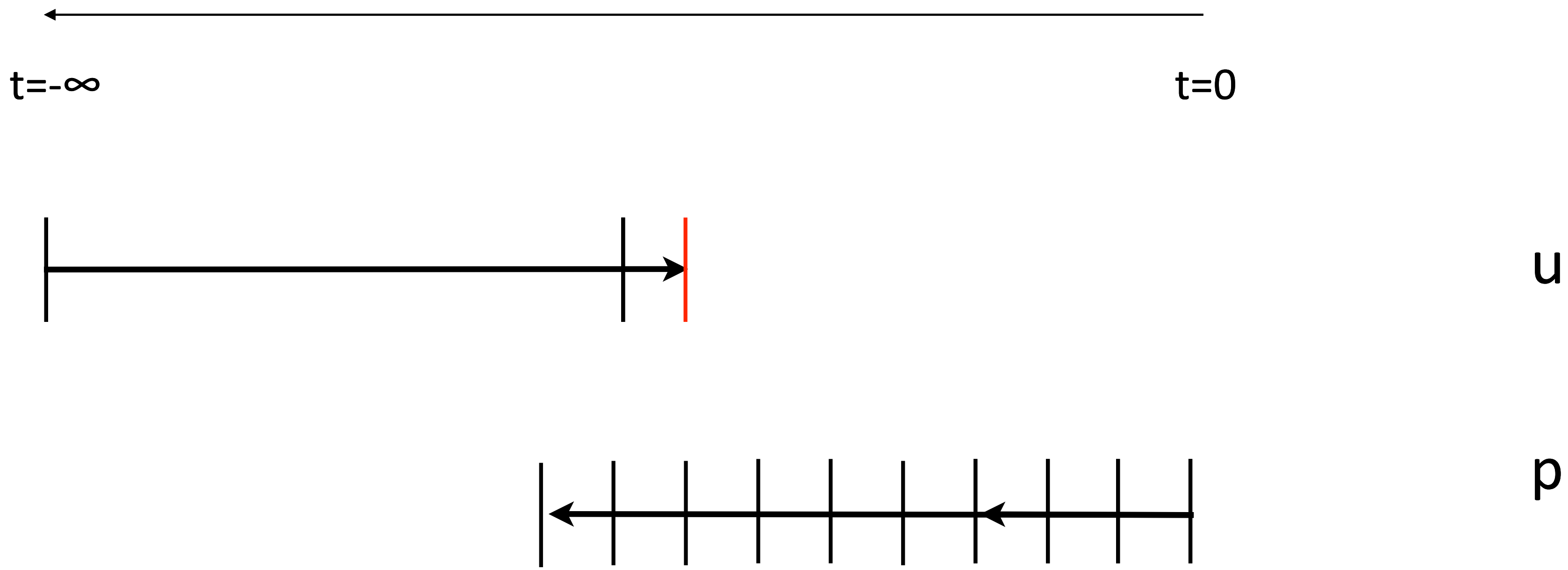

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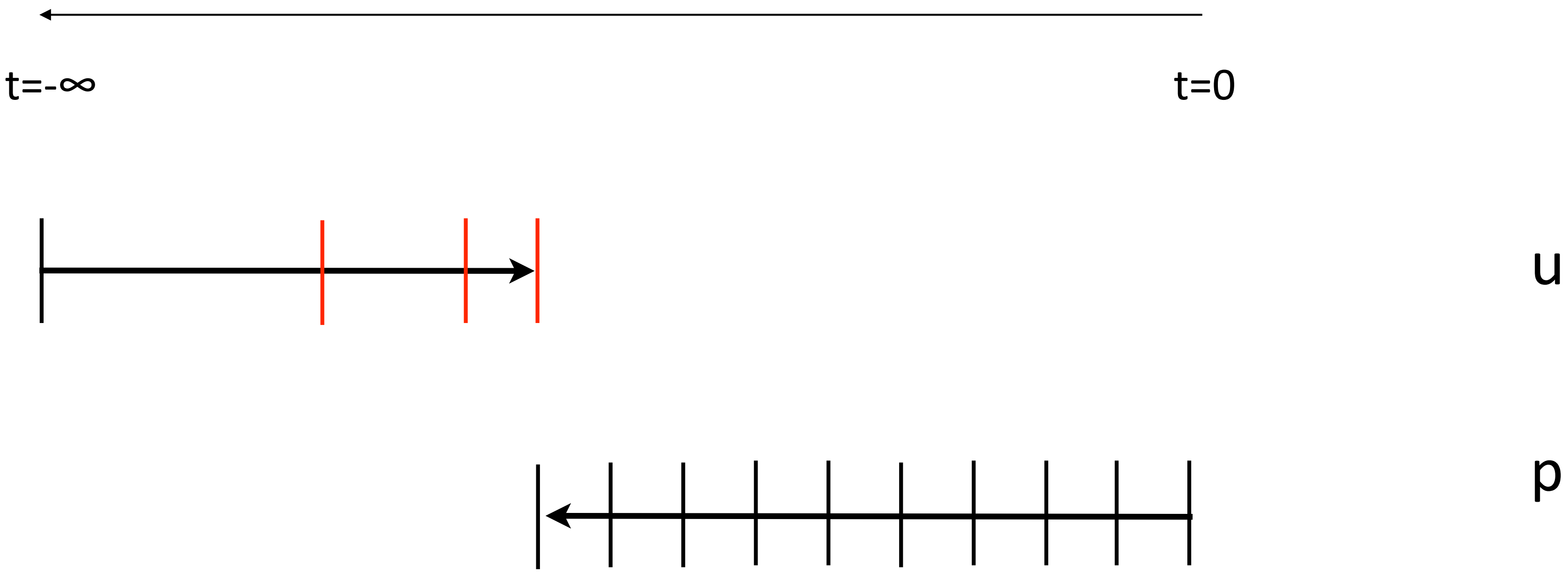
t=0
u
p



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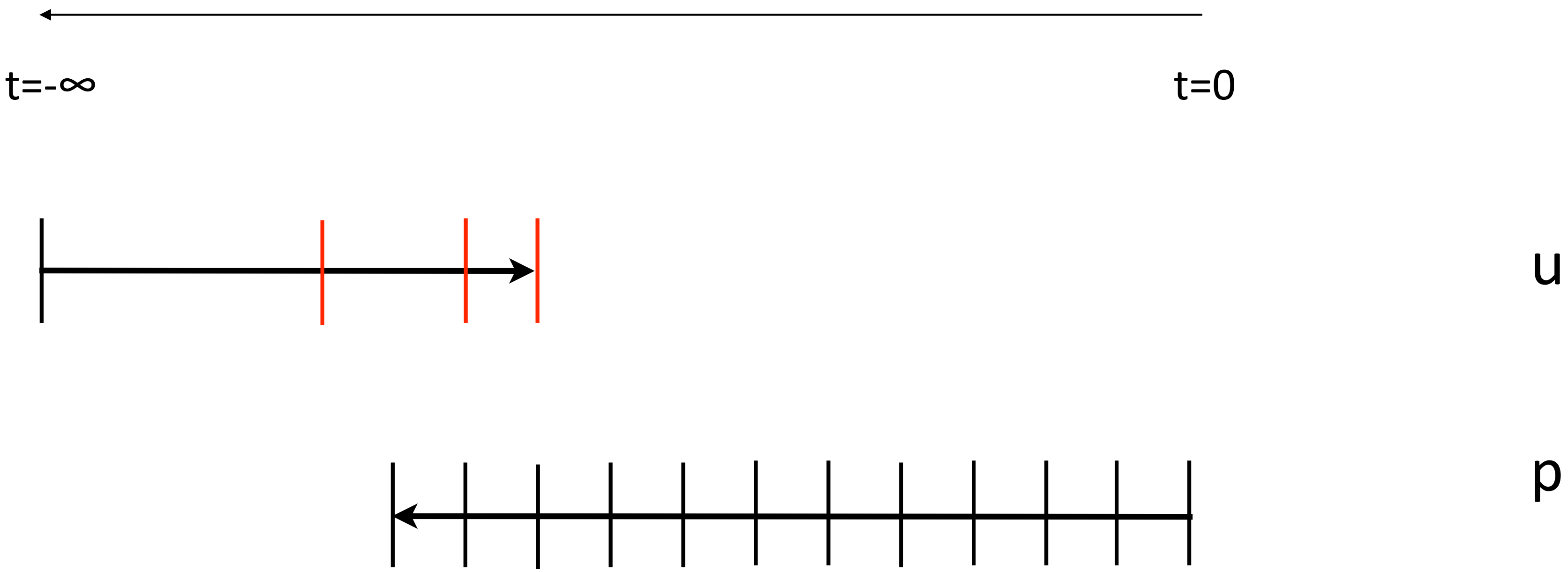
t=0
u
p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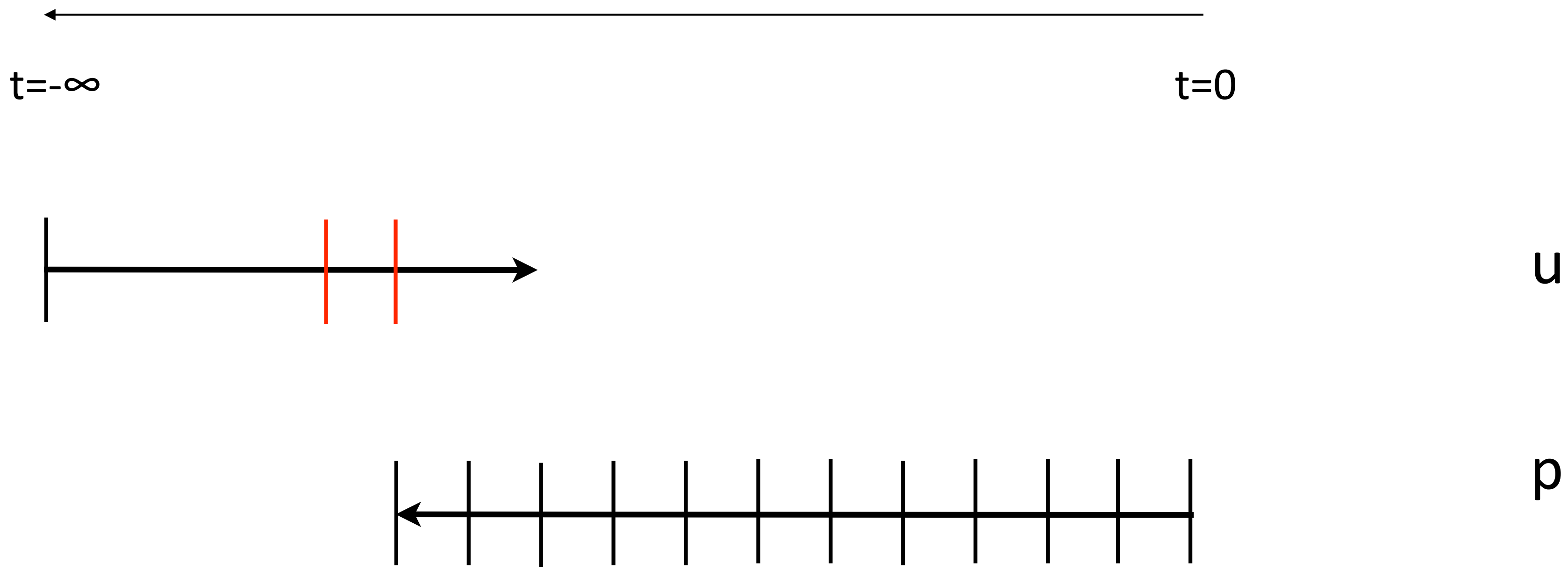
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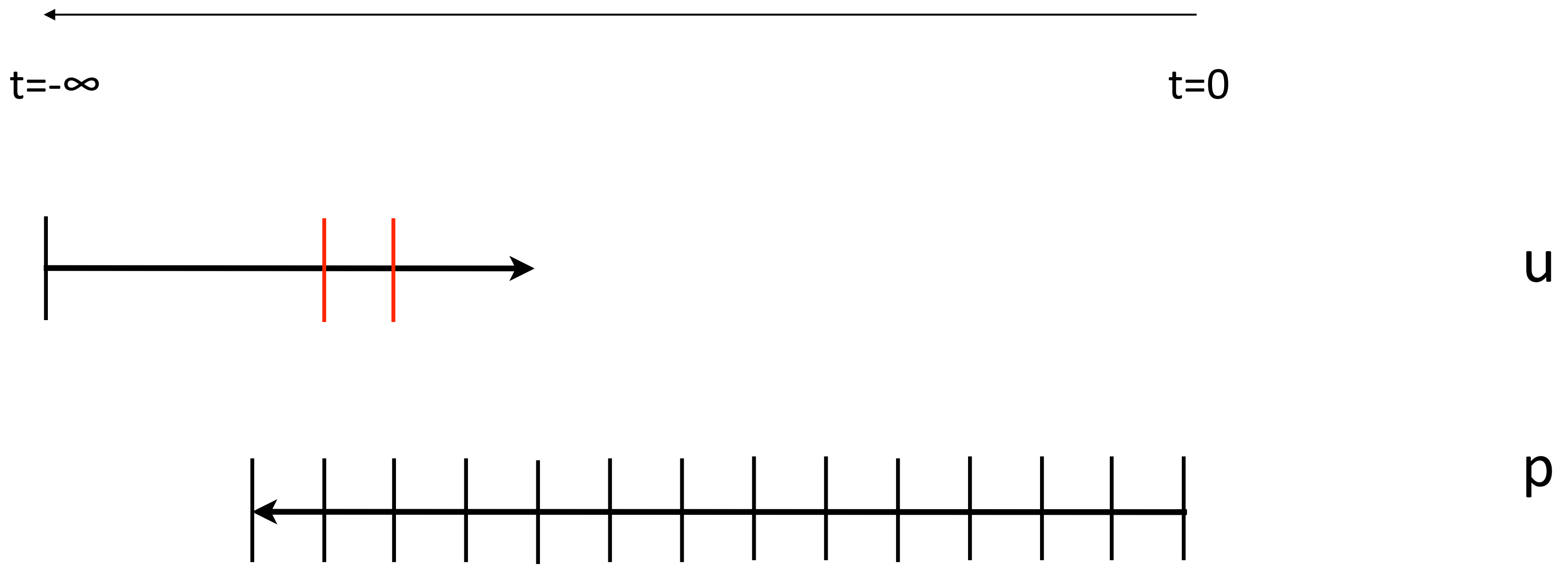
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t=0
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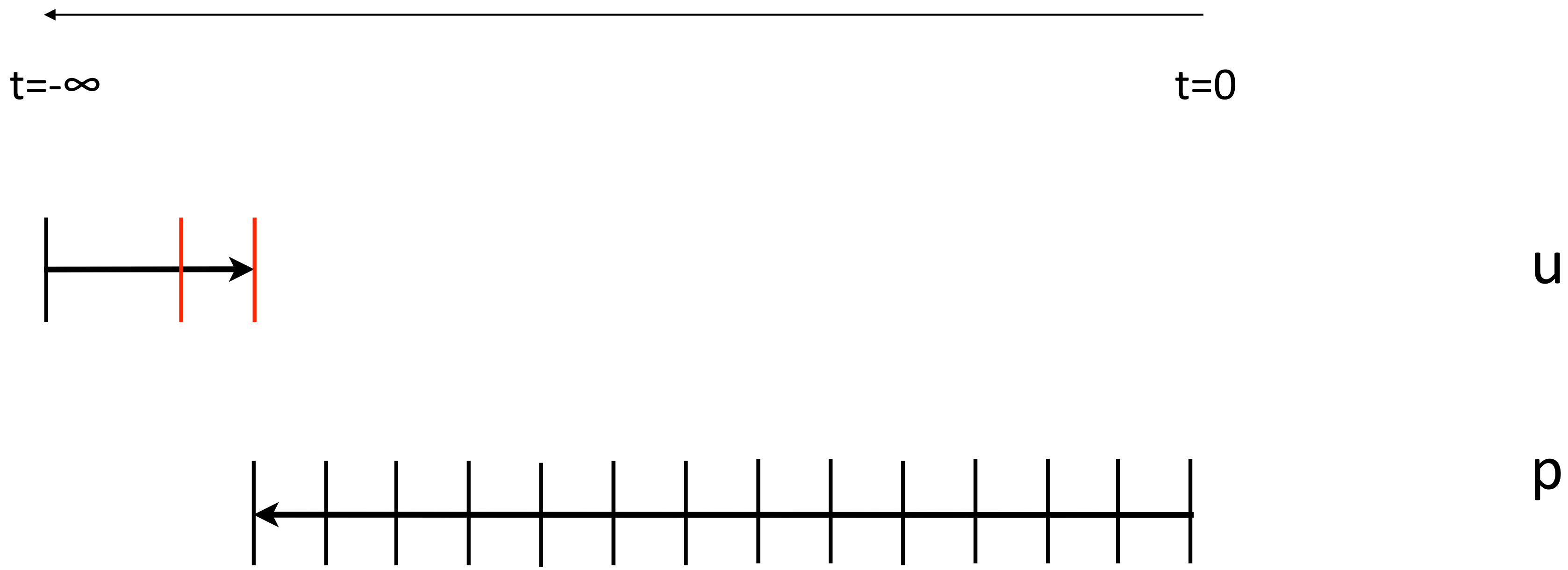
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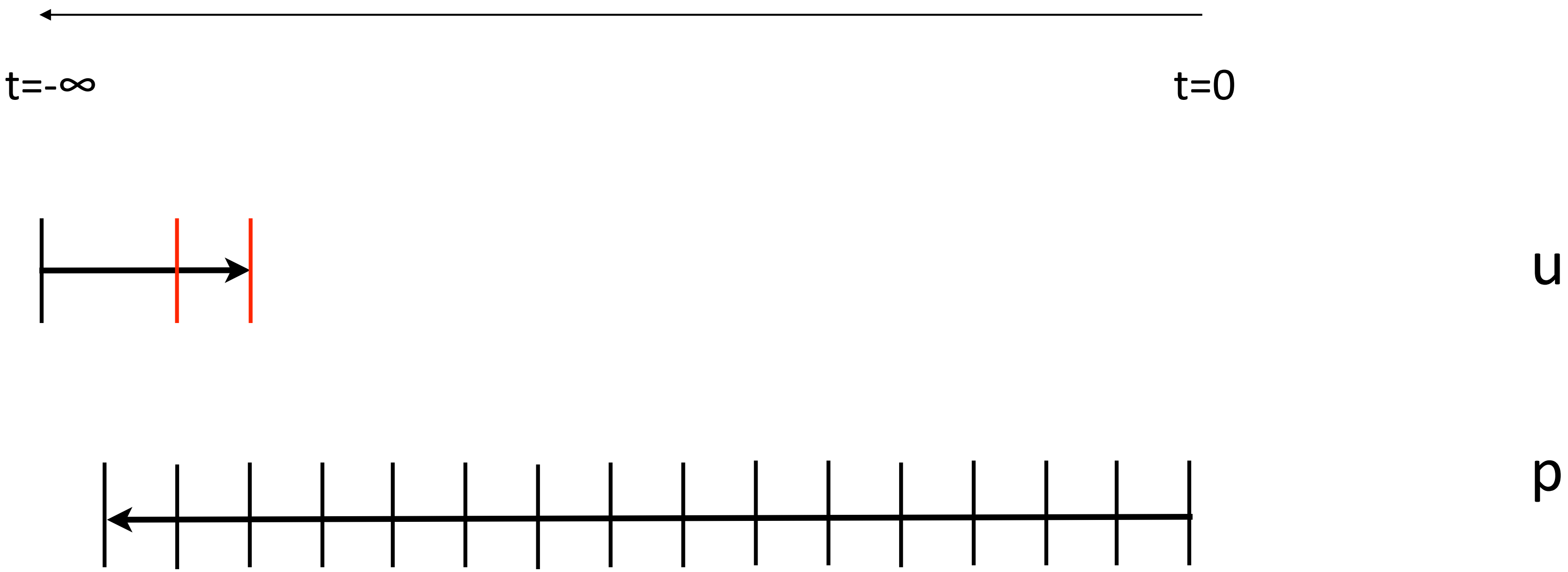
t=0
u
p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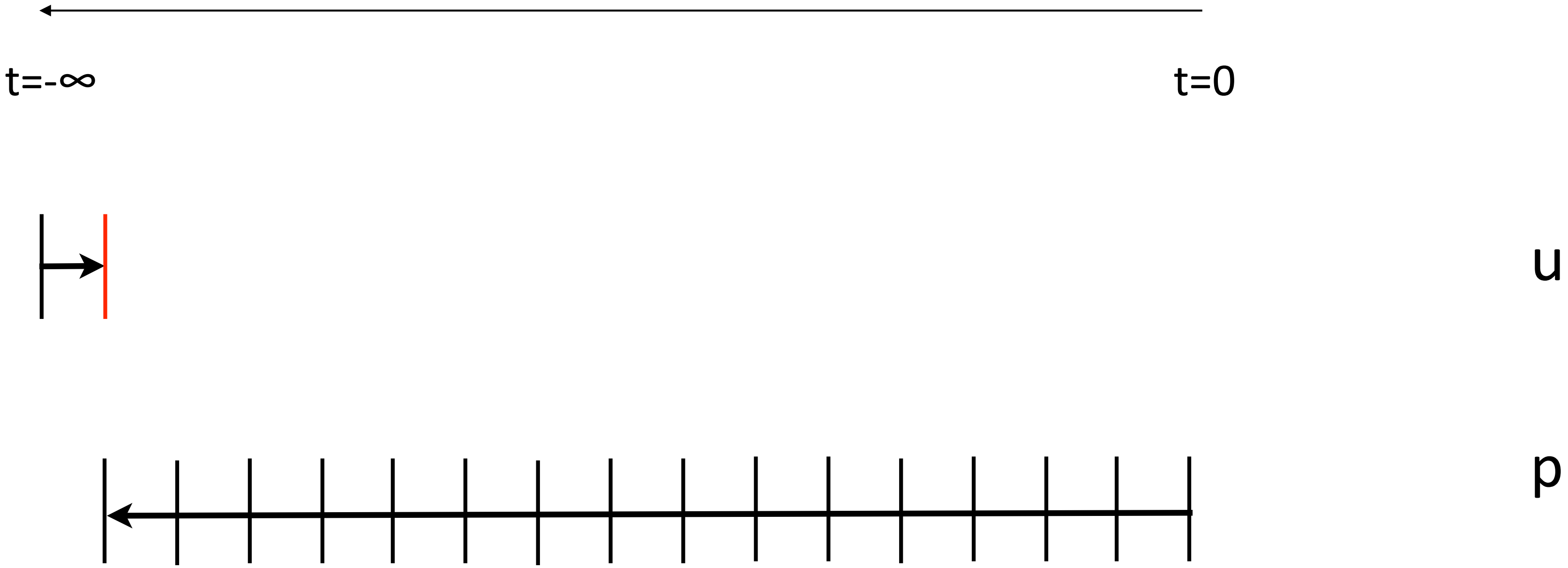
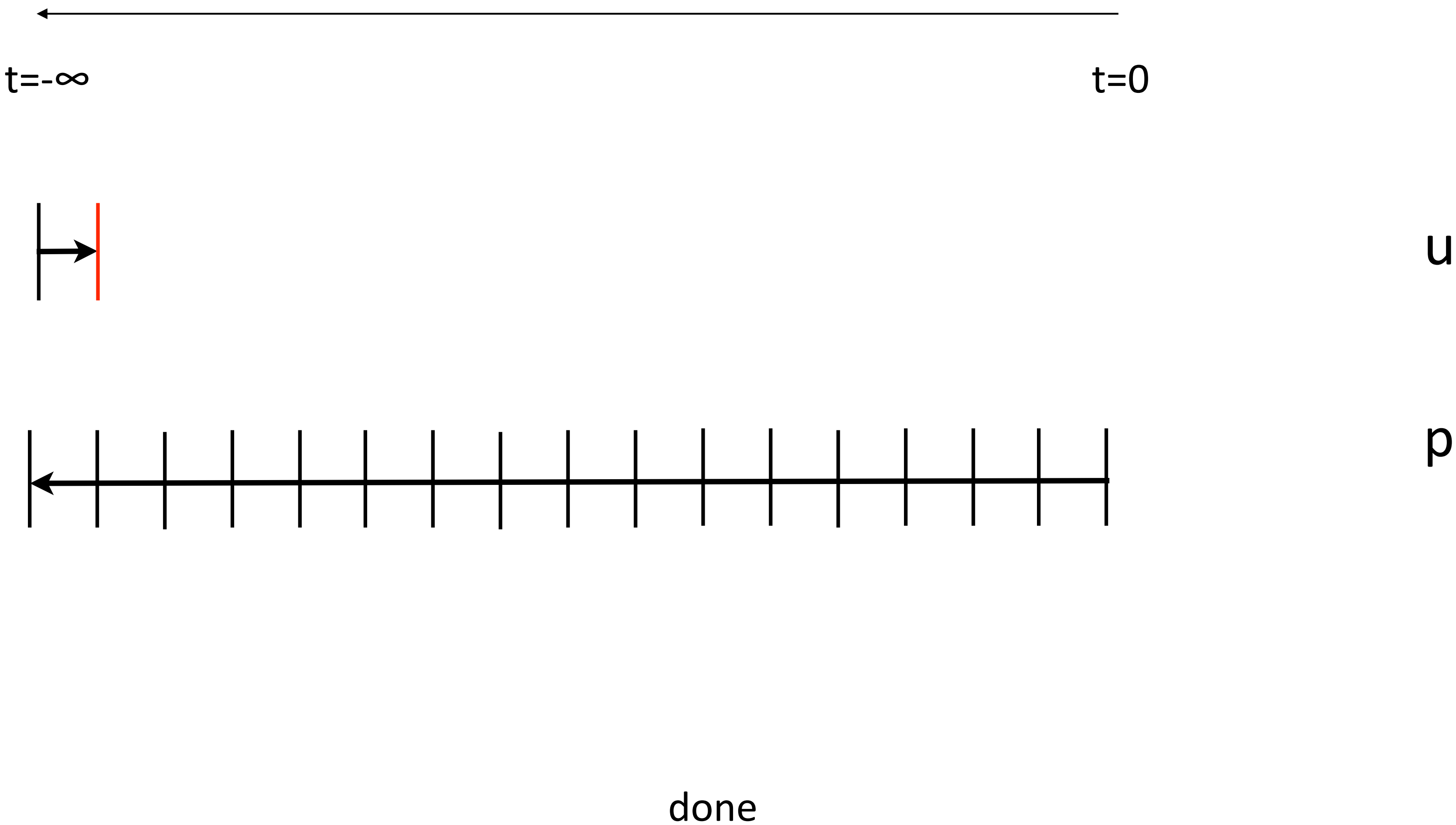
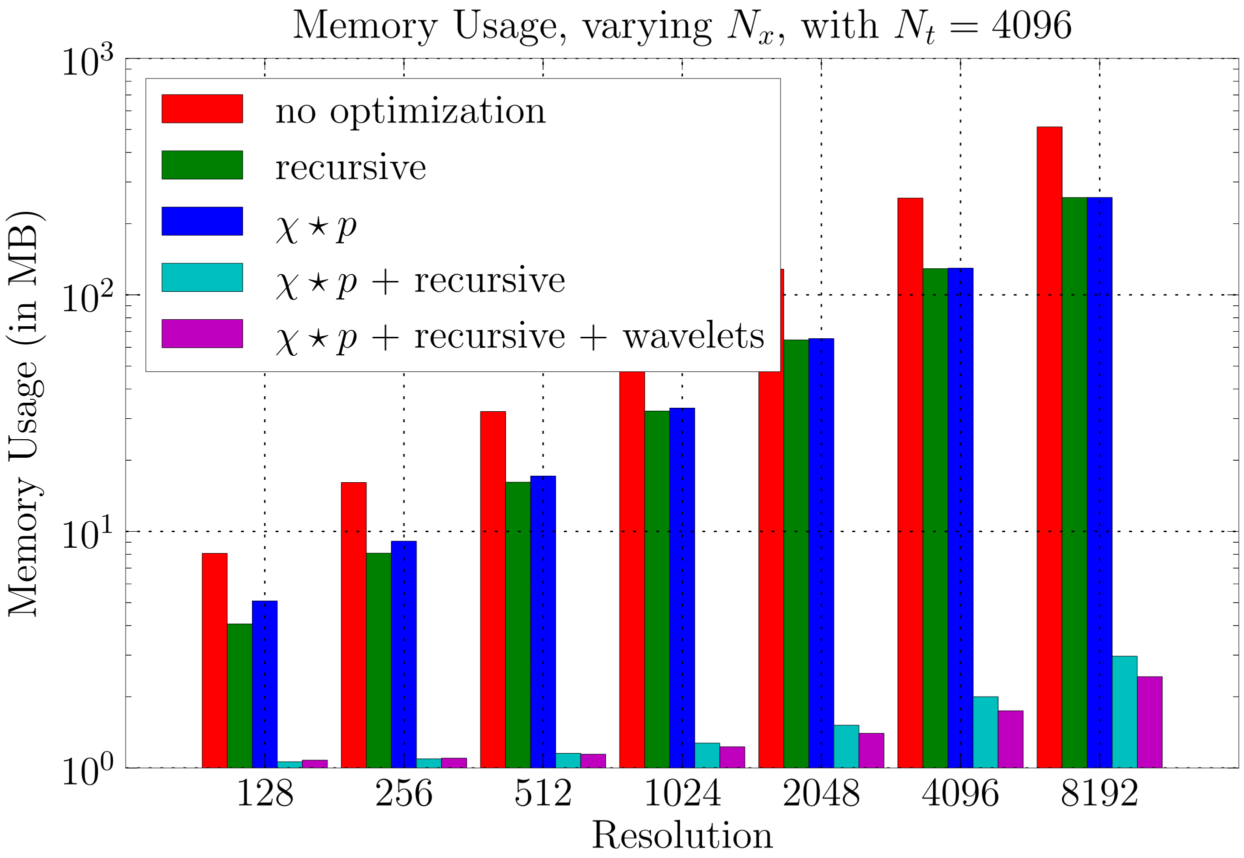
t=0
u
p



t=-∞
t=0
u
p

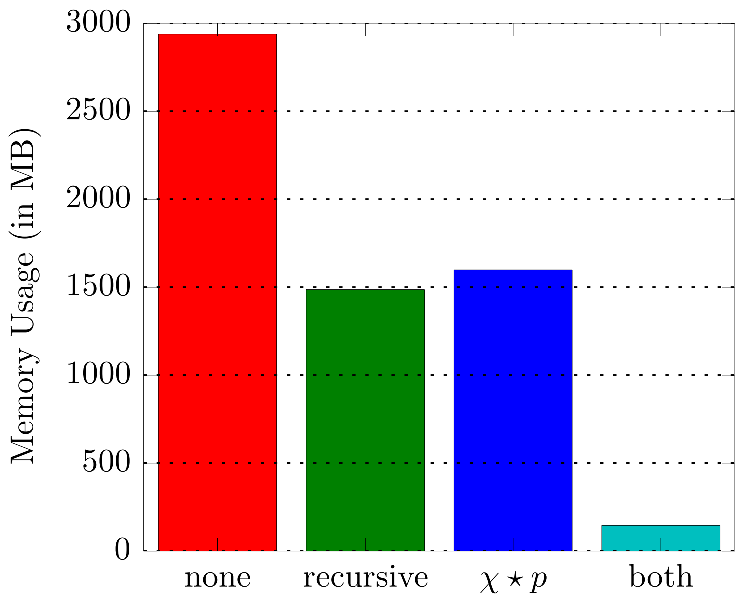

t=-∞
t=0
u
p
done

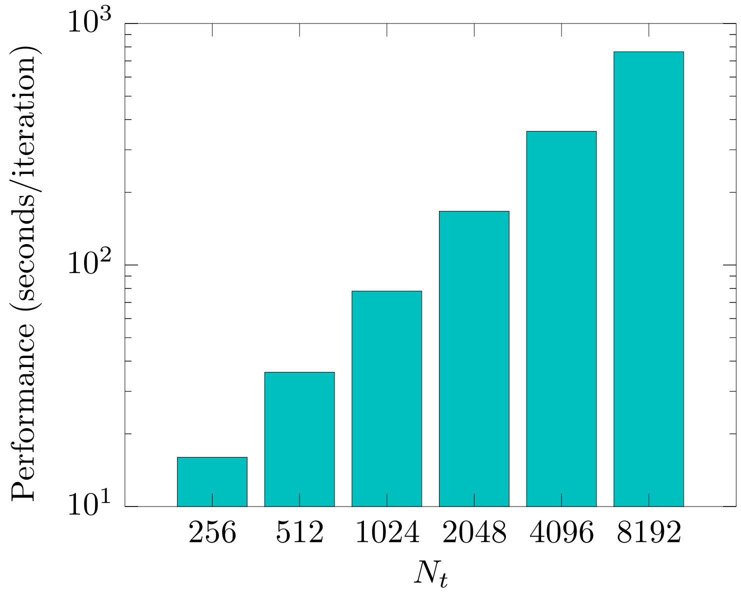
# 1D Burgers




257MB naive vs. 2MB optimized

# 2D Burgers

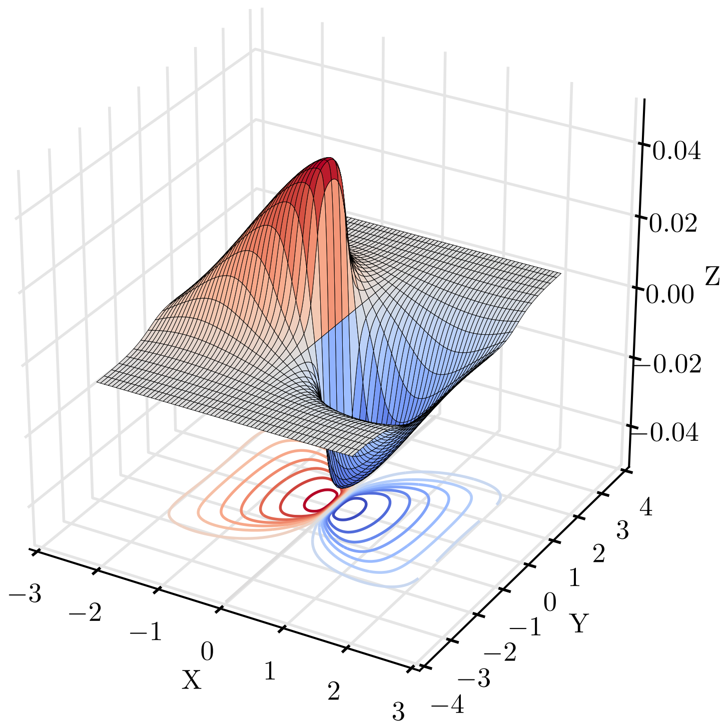


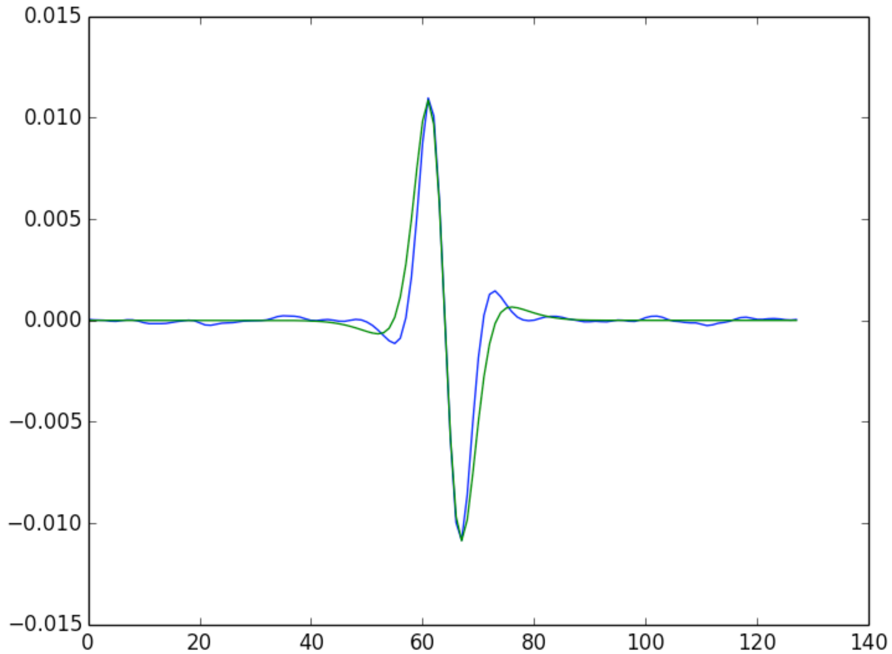

Left: The total memory saving of the combined algorithm exceeds a factor of 200.

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

Example: crude approximation of Burgers equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_1 \\ 4u_2 \end{pmatrix} + \begin{pmatrix} u_1 u_2 \\ -u_1^2 \end{pmatrix} = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}, \quad \left\langle \eta(t)\eta^\top(t') \right\rangle = \varepsilon \,\mathrm{diag}\left(\chi_1, \chi_2\right) \delta\left(t - t'\right)$$

Observable: $O(u) = -\left(u_1 + 2u_2\right)$ (mimics the gradient)

Augmented Lagrangian:

$$L_A[p, \mathcal{F}, \mu] = S[p] + (\mathcal{F}, O[u[p](\cdot,0)] - a)_{d'} + \frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'}^2$$

Action:

$$S[p] = \frac{\varepsilon}{2}\int_{-T}^{0} \mathrm{d}t\,(p, \chi * p)_{L^2(\Omega, \mathbb{R}^d)} = \frac{\varepsilon}{2}\int_{-T}^{0} \mathrm{d}t\,\left(p_1\chi_1 p_1 + p_2\chi_2 p_2\right)$$

Linear constraint:

$$(\mathcal{F}, O[u[p](\cdot,0)] - a)_{d'} = \mathcal{F}\left( -(u_1(0) + 2u_2(0)) - a\right)$$

Quadratic constraint:

$$\frac{\mu}{2}\|O[u[p](\cdot,0)] - a\|_{d'}^2 = \frac{\mu}{2}\left( -(u_1(0) + 2u_2(0)) - a\right)^2$$

Forward equation: $\partial_t u + N(u) = \chi * p^{(k)}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_1 \\ 4u_2 \end{pmatrix} + \begin{pmatrix} u_1 u_2 \\ -u_1^2 \end{pmatrix} = \varepsilon \begin{pmatrix} \chi_1 p_1^{(k)} \\ \chi_2 p_2^{(k)} \end{pmatrix}, \quad \begin{pmatrix} u_1(-T) \\ u_2(-T) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Backward equation:

$$\partial_t z - \nabla N(u)^\top z = 0\,,\ \ z(0) = -\left[\frac{\delta O}{\delta u}(u[p](\cdot,0))\right]'\{\mathscr{F} + \mu(O[u[p](\cdot,0)] - a)\}$$

$$\begin{aligned} &-\partial_t z_1 + z_1 + z_1 u_2 - 2z_2 u_1 = 0 \qquad && z_1(0) = \mathscr{F} + \mu(\,-(u_1(0) + 2u_2(0)) - a) \\ &-\partial_t z_2 + 4z_2 + z_1 u_1 = 0 && z_2(0) = 2\big(\mathscr{F} + \mu(\,-(u_1(0) + 2u_2(0)) - a)\big) \end{aligned}$$

Compute gradient: $g^{(k)} \leftarrow \chi * \left(p^{(k)} - z^{(k)}\right)$

## What do we need?

put most functions in a problem specific class

```
def compute_grad(self, p, z):
    ⋮
    return gradient

def compute_L_A(self, z, u, dt)
    ⋮
    return action, loss

def solve_forward(self, p, u, dt):
    ⋮
    return u for all times

def step_forward(self, p, u, dt):
    ⋮
    return u at next tilmestep

def solve_adjoint(self, z, u, dt):
    ⋮
    return z_next

def step_adjoint(self, z, u, dt):
    ⋮
    return z for all times

def gradObsT(self):
    ⋮
    return gradient of observable transposed

def delta(self)
def chi_F(self)
def actionDensity(self, p)
def delta_x(self)
def observable(self, u)
def integrate(self, f)
```

**Wishlist instantons** (= possible projects)

i) store $p$ on a reduced grid fitting to $\chi * p$ — easy
   for large scale forcing we need only a few Fourier modes

ii) Implement CS using grad and cost for 2D MHD — easy

iii) implement LBFGS using grad and cost for 2D MHD — medium

iv) implement checkpointing using pyRevolve — medium++

v) Implement mai parallel MHD + MPI revolve — hard

**Wishlist tensor network + wavelets** (= possible projects)

i) model 3D instantons — easy

ii) 3D instant gas — easy

iii) compression of 3D field with Tucker — medium

iv) compression of 3D field with Tucker + wavelets — medium++