Particle transport in turbulent MHD structures

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Topic

Topic: Transport of charged particles in turbulent MHD fields

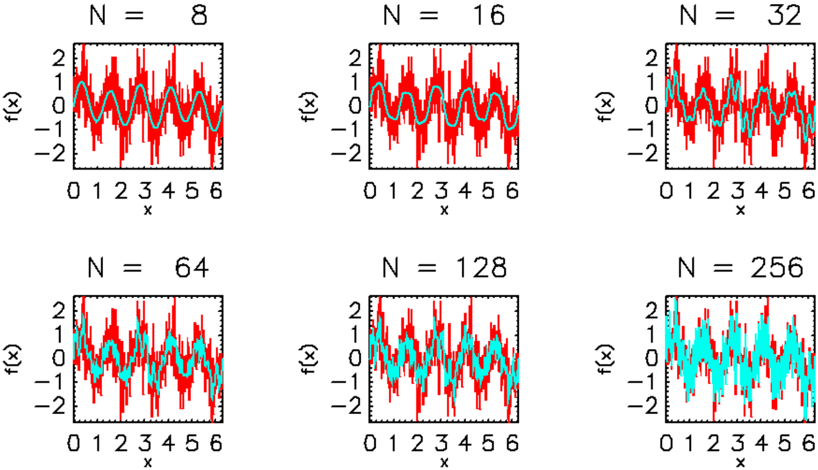
MHD: The MHD equations are solved in wavenumber-space (via Fourier transformation)

Focus: Contribution of high wavenumbers in this fields to the particle transport:

- highly resolved computations are costly regarding time, memory and disk space:
- high wave-numbers: fine structures on top of “averaged” structure
- idea: use lower resolution and replace high-wavenumber contributions by transport parameters such as an external force

Reduction of Fourier modes

Representation of a fine structure by superposition of Fourier modes:



Reduction of Fourier modes

Fourier transformation in 1D with N grid points:

$$f(x_\alpha) = \sum_{\beta=1}^{N} F(k_\beta) e^{i x_\alpha k_\beta}, \qquad 1 \leq \alpha \leq N$$

N determines:

- the number of modes to be summed up
- the grid resolution of each mode, β, in space: $x_1, \ldots, x_\alpha, \ldots, x_N$

$\rightarrow$ reducing the **number of modes** reduces also the **grid resolution**

But, there is a second way to reduce the number of modes:

reduction 1: *reduce* N to $N_0 < N$ and, thus, also the grid resolution $(\uparrow)$

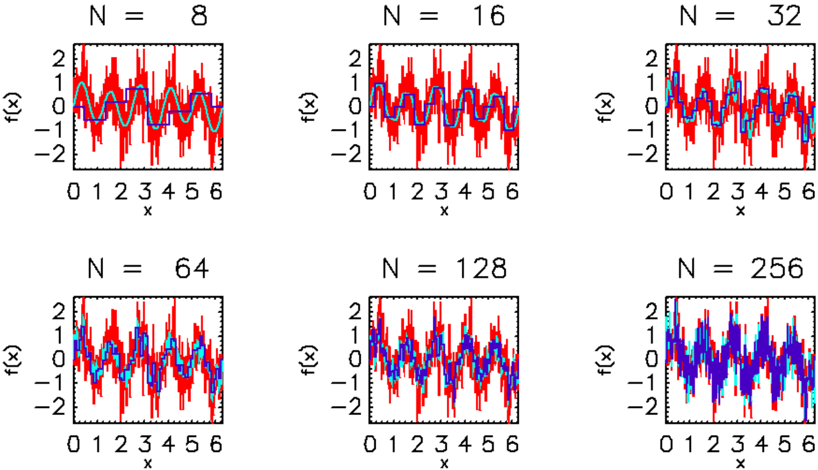
reduction 2: *keep* N, but set $F(k_\beta) = 0$ for $\beta \geq N_0$

$\rightarrow$ same high resolution* with less modes

*drawback: time, memory requirements etc. also remain the same

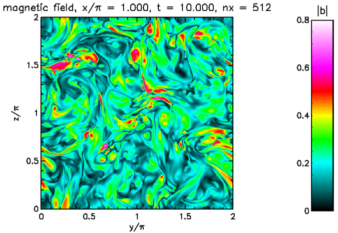
Reduction of Fourier modes

Taking the resolution into account, reduction 1 actually gives:



Application to MHD: full field ($n_x = 512$)

Magnetic field: real and wavenumber spaces: $\vec{b}(\vec{r},t) = \sum_{|\vec{k}|<256} \vec{B}(\vec{k},t)e^{i\vec{k}\cdot\vec{r}}$:



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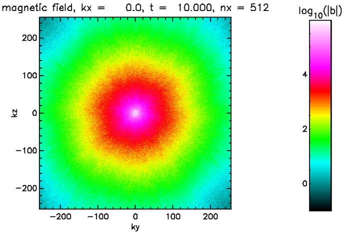

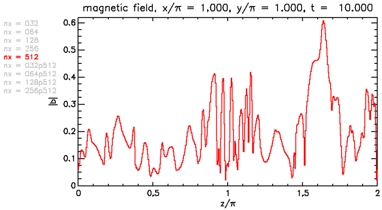

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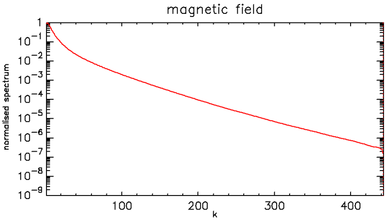

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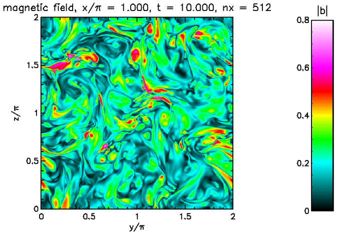

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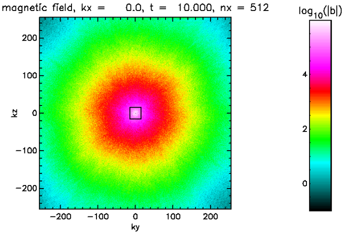

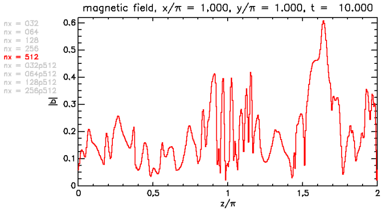

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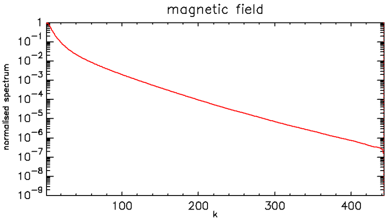
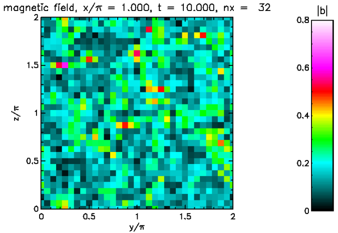


Application to MHD: reduction 1 ($n_x = 32$)

Reduce resolution, cut off all $|\vec{k}| \geq 16$: $\vec{b}(\vec{r}, t) = \sum_{|\vec{k}|<16} \vec{B}(\vec{k}, t) e^{i\vec{k}\cdot\vec{r}}$:



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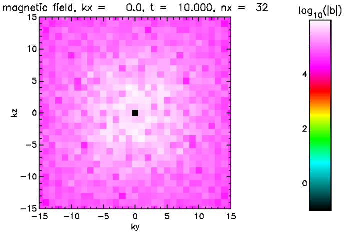

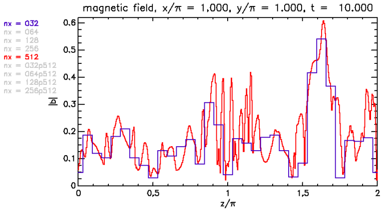

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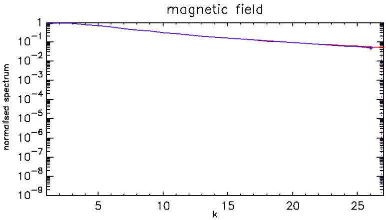
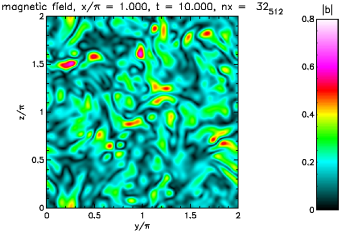


Application to MHD: reduction 2 ($n_x = 32$)

Keep resolution, but filter: $\vec{b}(\vec{r},t) = \sum_{|\vec{k}|<256} \Theta(|\vec{k}| < 16)\vec{B}(\vec{k},t)e^{i\vec{k}\cdot\vec{r}}$:



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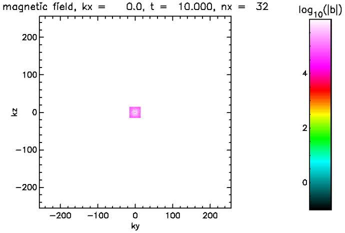

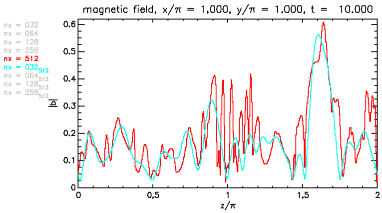

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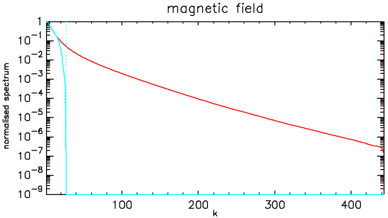
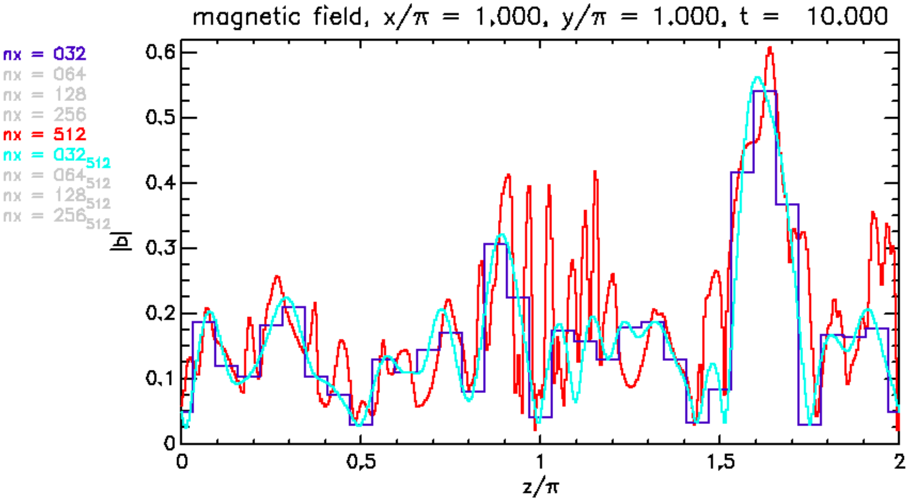


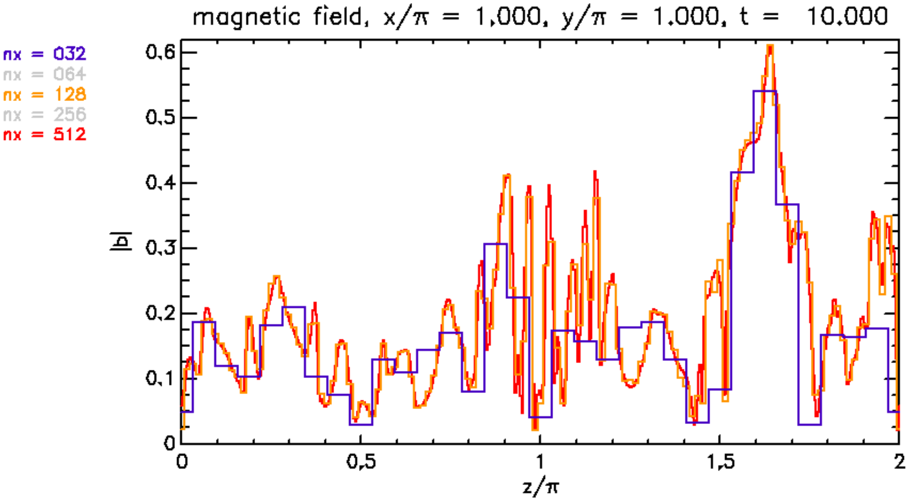
Θ: Heaviside function: $\Theta = 1$ for $|\vec{k}| < 16$, $\Theta = 0$ for $|\vec{k}| \geq 16$

Comparison of reductions 1 and 2



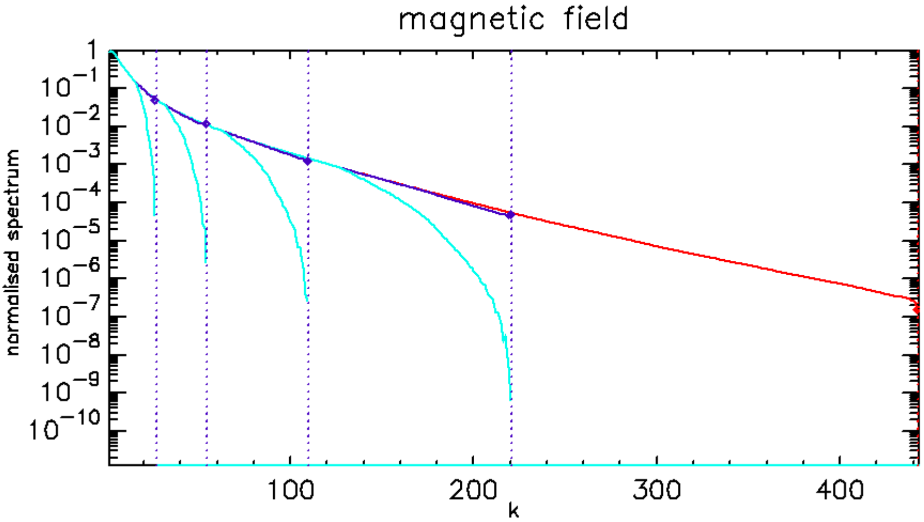
reduction 2 works as “high-order spline” interpolation of reduction 1

Comparison of $n_\mathrm{x} = 32$ and $n_\mathrm{x} = 128$ for reduction 1



$n_\mathrm{x} = 128$ catches more fine structures, rather than to interpolate $n_\mathrm{x} = 32$

Spectra of the magnetic field (normalised)



(reduced) MHD equations

Take a fluid picuture rather than a kinetic approach and assume:

- constant mass density $\rho = \rho_0$
- divergence-free plasma flow: $\vec{\nabla} \cdot \vec{u} = 0$
- periodic boundary conditions

The MHD equations read for this case:

$$\begin{aligned}
\frac{\partial \vec{u}}{\partial t} &= -\left(\vec{u} \cdot \vec{\nabla}\right)\vec{u} + \left(\vec{b} \cdot \vec{\nabla}\right)\vec{b} + \nu \Delta \vec{u} - \frac{1}{\rho}\vec{\nabla} p_{\mathrm{tot}} \\
\frac{\partial \vec{b}}{\partial t} &= -\left(\vec{u} \cdot \vec{\nabla}\right)\vec{b} + \left(\vec{b} \cdot \vec{\nabla}\right)\vec{u} + \eta \Delta \vec{b}
\end{aligned}$$

- fluid velocity $\vec{u}$
- magnetic field $\vec{B}$ $\rightarrow$ Alfvén velocity $\vec{b} = \frac{1}{\sqrt{\mu_0 \rho}}\vec{B}$
- viscosity ν and resistivity η
- total (gas plus magnetic) pressure p_{tot}

Fourier transformation

The MHD equations are solved in Fourier space (sum over grid indices):

$$\vec{U}(\vec{k},t) = \sum_{\vec{r}} \vec{u}(\vec{r},t)e^{-i\vec{k}\cdot\vec{r}}$$

$$\vec{B}(\vec{k},t) = \sum_{\vec{r}} \vec{b}(\vec{r},t)e^{-i\vec{k}\cdot\vec{r}}$$

(operators reduce: $\vec{\nabla}\cdot\vec{u} \to i\vec{k}\cdot\vec{U}$ or $\vec{\nabla}\times\vec{b} \to i\vec{k}\times\vec{B}$)

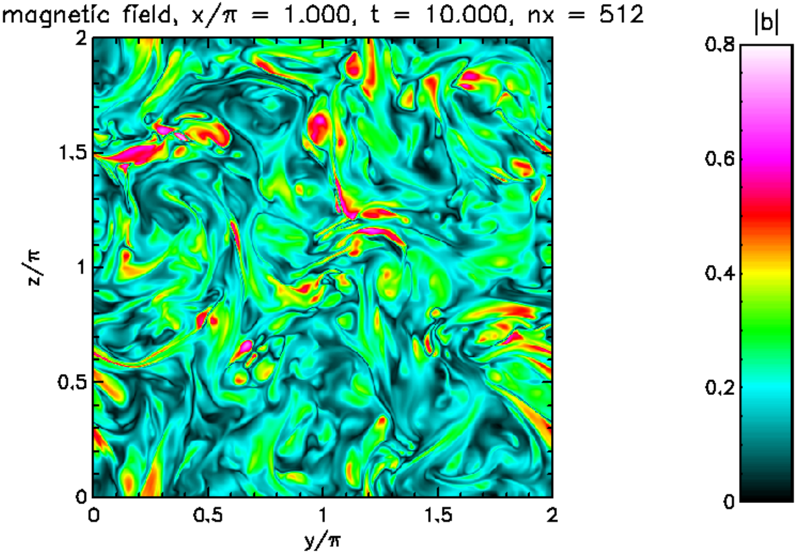
$\to$ Solve (with p_{tot} being set into the first equation)

$$\frac{\partial U_\alpha(\vec{k},t)}{\partial t} = \ldots$$

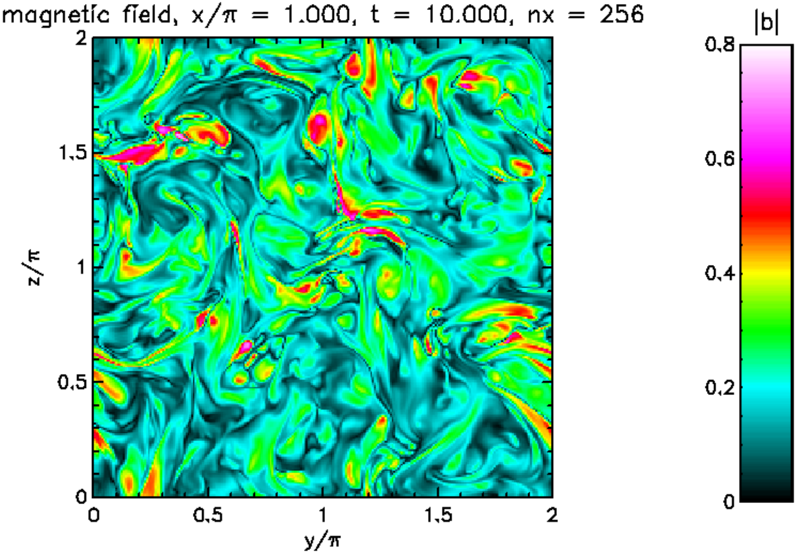
$$\frac{\partial B_\alpha(\vec{k},t)}{\partial t} = \ldots$$

with `TURBO`. The time integration is performed with a modified Williamson/Runge-Kutta scheme

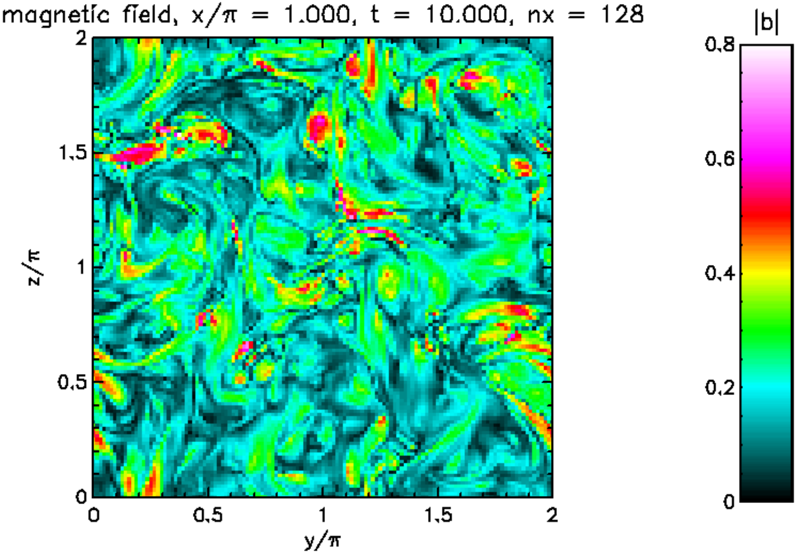
$\vec{B}(\vec{r})$ ($n_x = 512$)



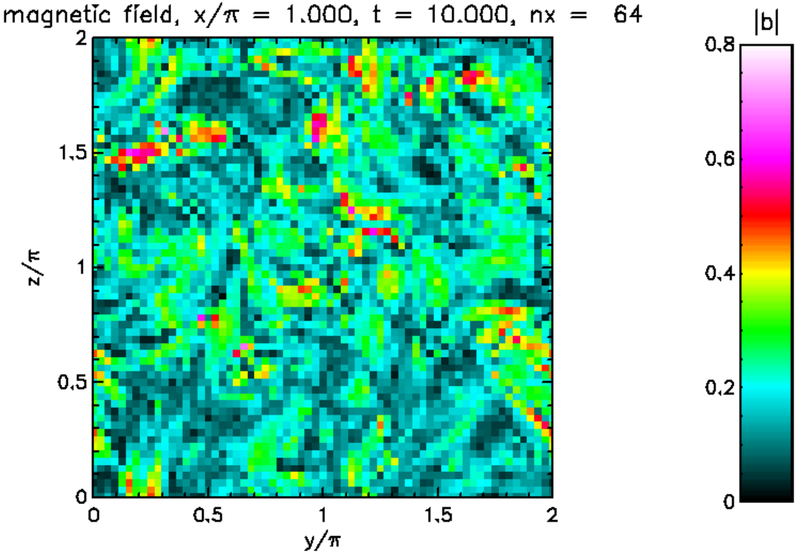
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (1) to $n_x = 256$)



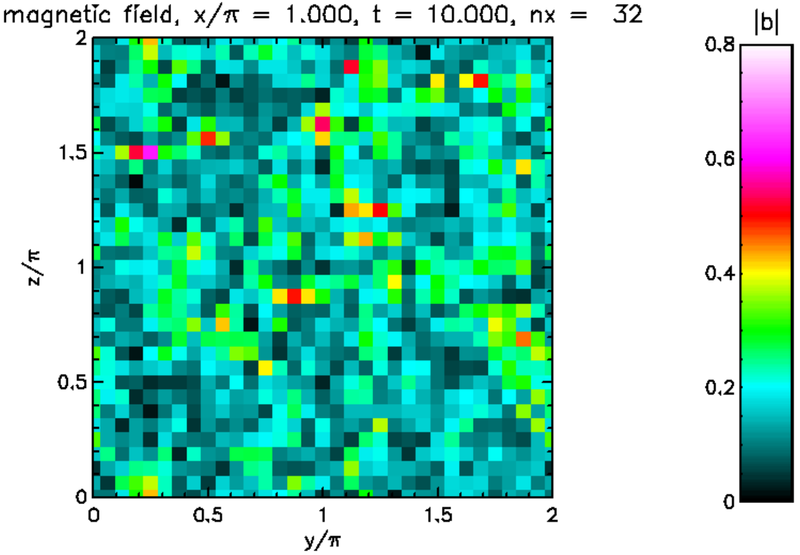
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (1) to $n_x = 128$)



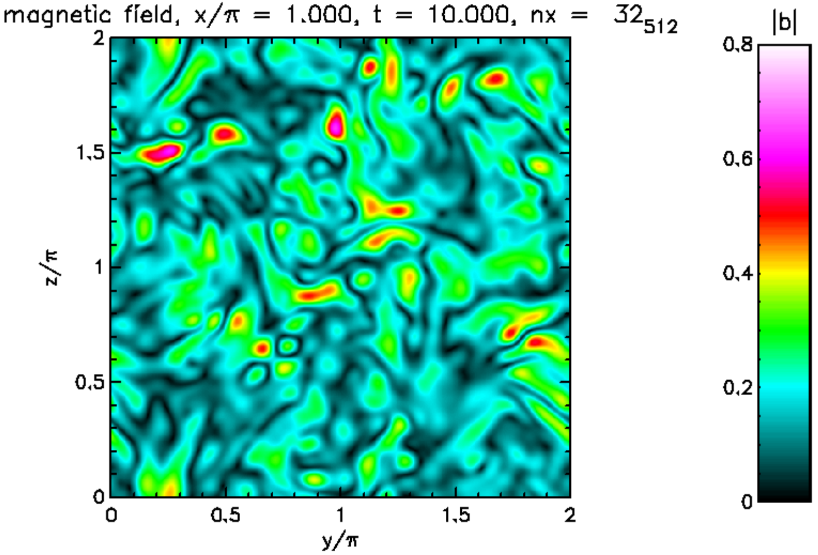
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (1) to $n_x = 64$)



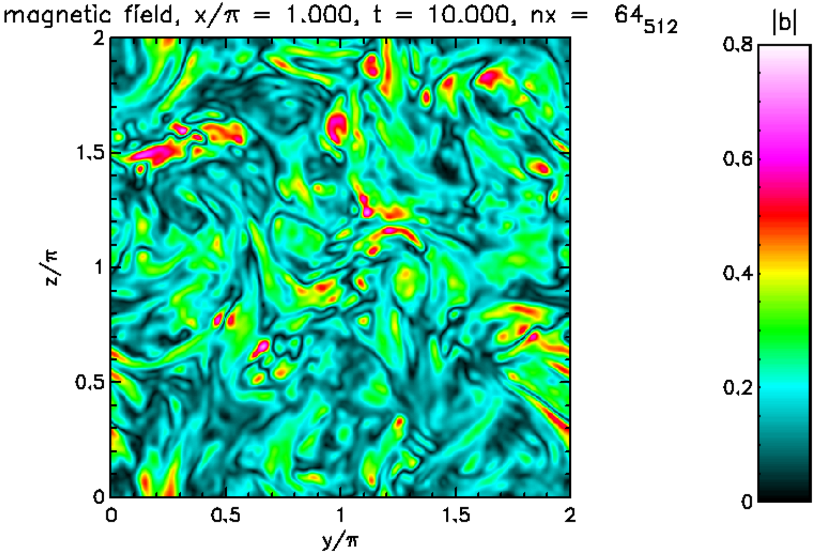
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (1) to $n_x = 32$)



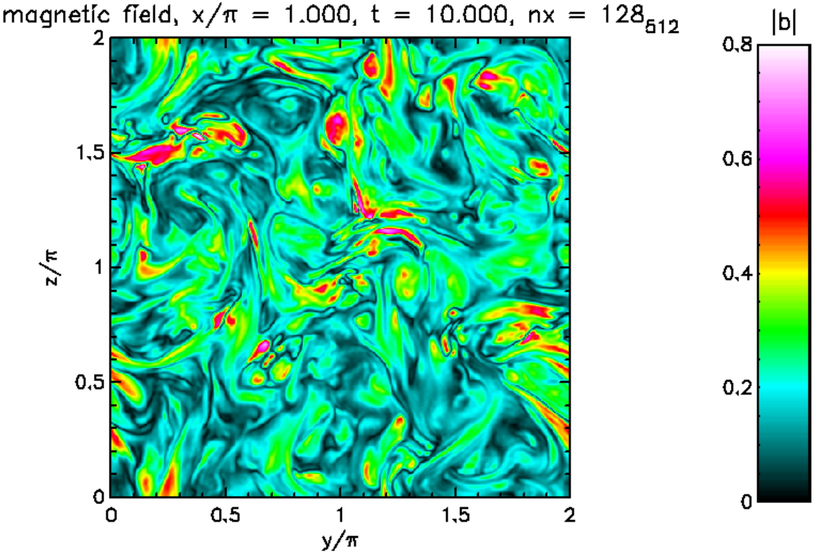
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (2) to $n_x = 32$)



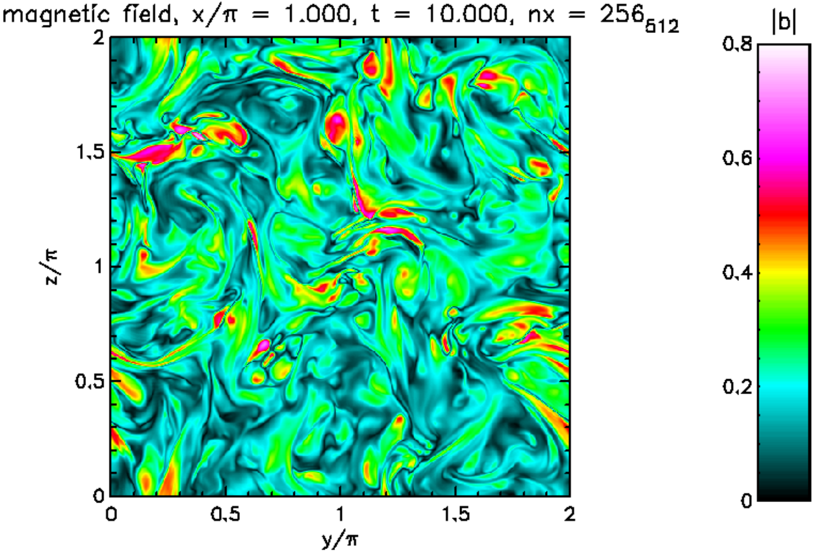
$\vec{B}(\vec{r})$ ($n_{\rm x} = 512$, reduced (2) to $n_{\rm x} = 64$)



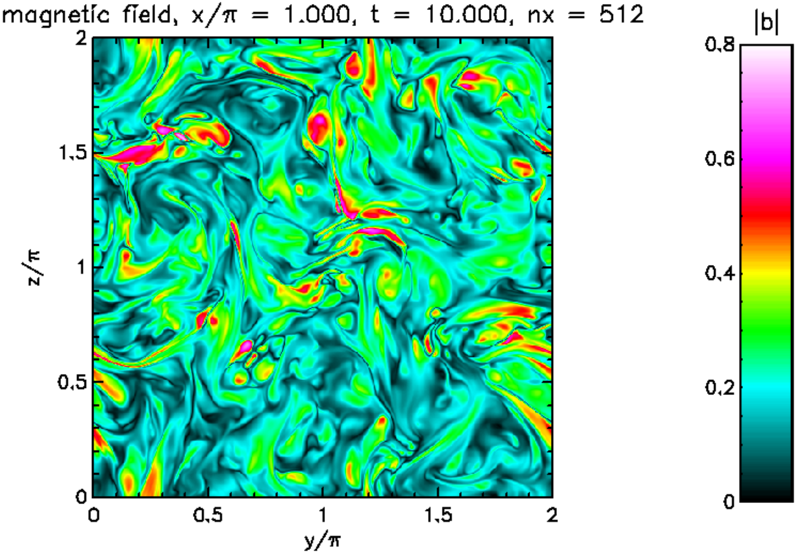
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (2) to $n_x = 128$)



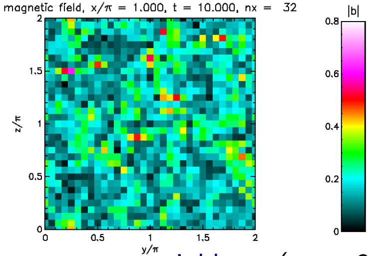
$\vec{B}(\vec{r})$ ($n_x = 512$, reduced (2) to $n_x = 256$)



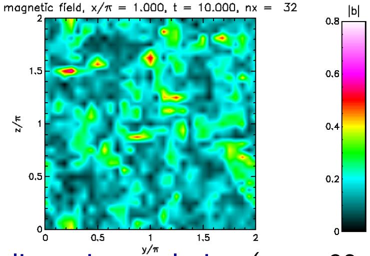
$\vec{B}(\vec{r})$ ($n_x = 512$)



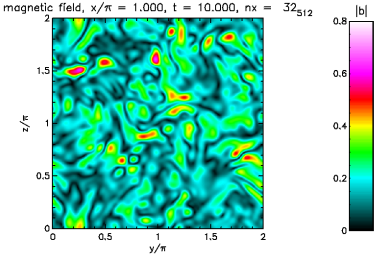
$\vec{B}(\vec{r})$: comparisons for $n_{\mathrm{x}} = 32$



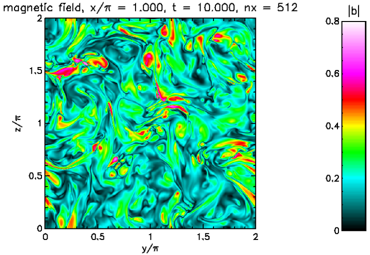
nearest neighbour ($n_{\mathrm{x}} = 32$)



linear interpolation ($n_{\mathrm{x}} = 32 \to 512$)



"Fourier interpolation" ($n_{\mathrm{x}} = 32_{512}$)



full field ($n_{\mathrm{x}} = 512$)

Particle transport in MHD fields

The TURBO particle code:

- propagates a set of charged particles with mass m_{p} and velocity $\vec{v}_{\mathrm{p}}(t)$, resulting in trajectories $\vec{r}_{\mathrm{p}}(t)$
- the initial values are $\vec{r}_{\mathrm{p},0}$ and $\vec{v}_{\mathrm{p},0}$ at time $t = 0$:

  $\vec{r}_{\mathrm{p},0}$: two cases:

  all particles at the same place or randomly distributed

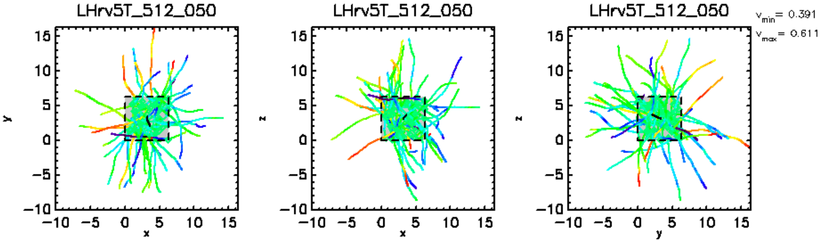
  $\vec{v}_{\mathrm{p},0}$: random direction with same speed v_0

  $p \in \{1, \ldots, N_p\}$
- the MHD fields are frozen in time, but TURBO also allows to simulate the evolutions of both fields and particles
- Runge-Kutta scheme with spline-interpolation of the MHD fields and control of the time-step

Code validation: energy conservation

Particle trajectories

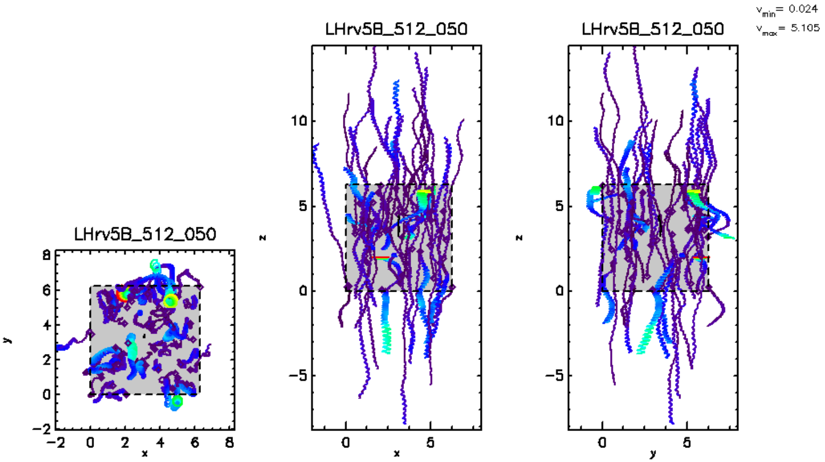
Sample trajectories with no background magnetic field:



(colour = speed, random starting points with $v_0 = 0.5$)

Particle trajectories

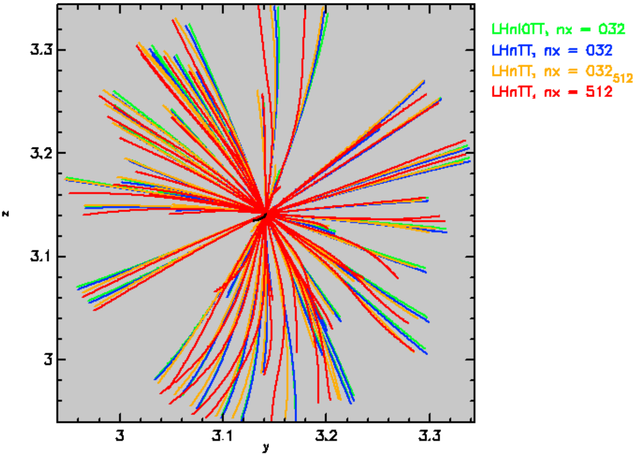
Sample trajectories with a background magnetic field, $b_{0,z}$:



(colour = speed, random starting points with $v_0 = 0.5$)

Particle trajectories

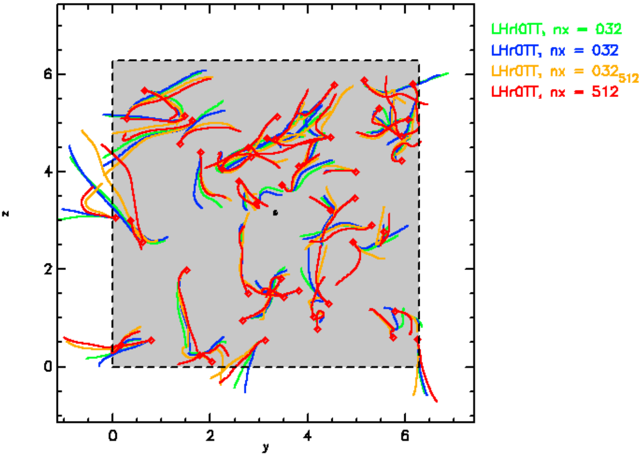
Early time, trajectories for different resolutions, same starting point:



(green: linear interpolation, else: 6-point splines)

Particle trajectories

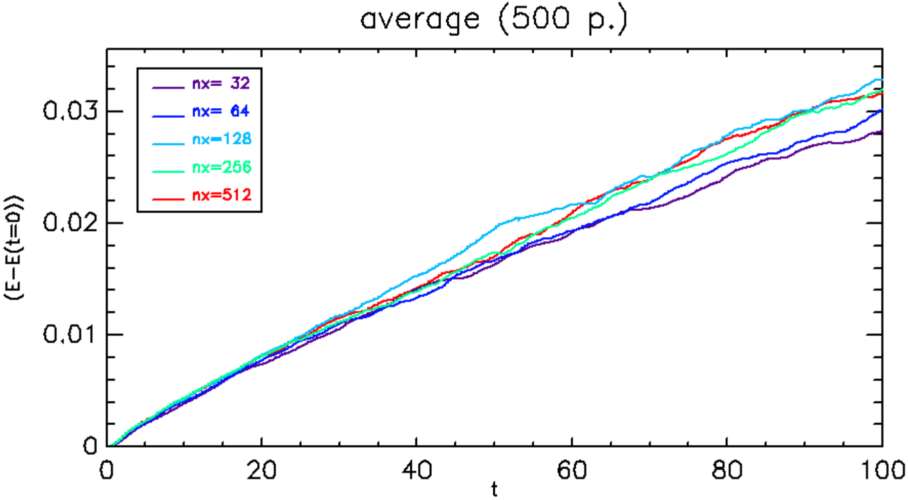
Early time, trajectories for different resolutions, random starting points:



(green: linear interpolation, else: 6-point splines)

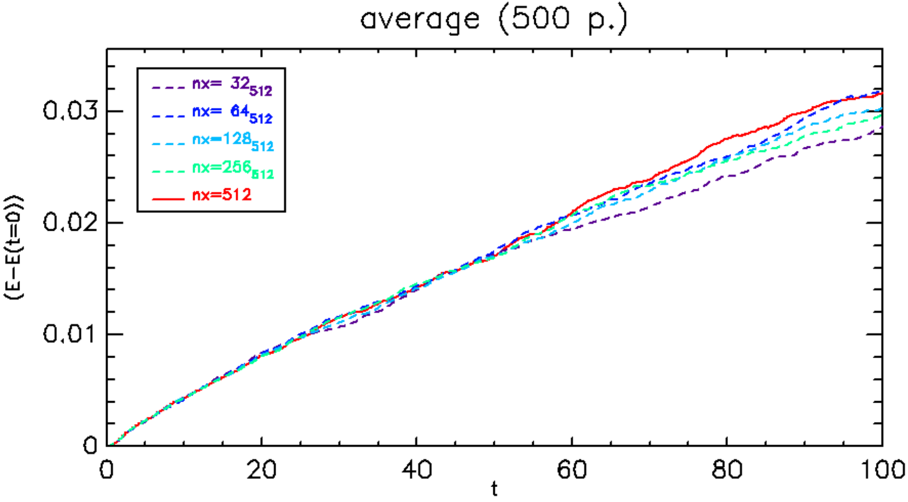
Kinetic energy

Averaged kinetic energy for different resolutions and reduction 1:



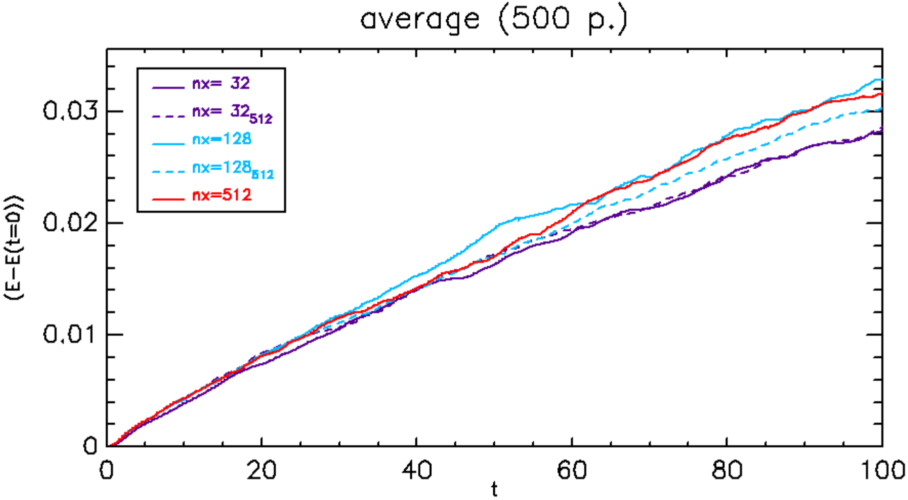
Kinetic energy

Averaged kinetic energy for different resolutions and reduction 2:



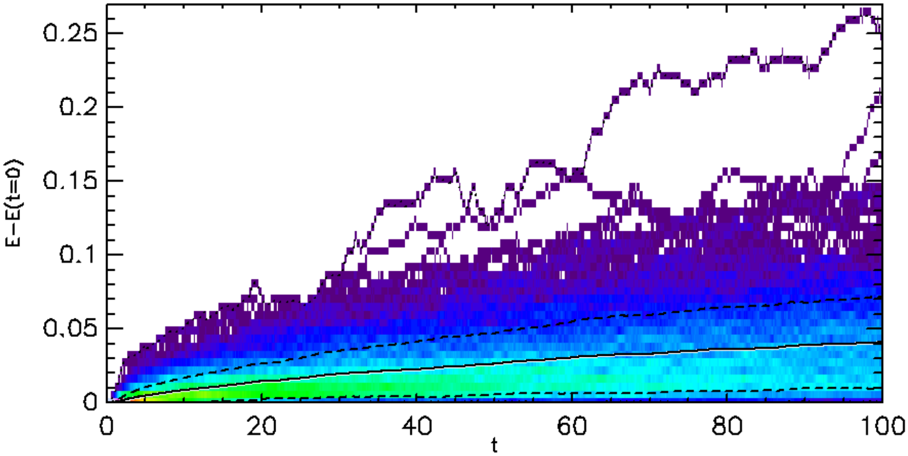
Kinetic energy

Averaged kinetic energy for different resolutions and both reductions:



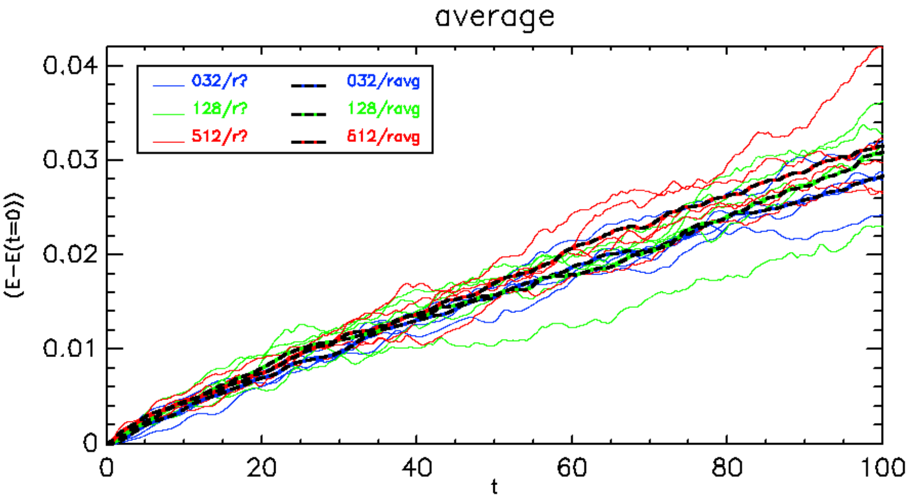
Kinetic energy

Binning of E_{kin} for $n_{\mathrm{x}} = 512$:



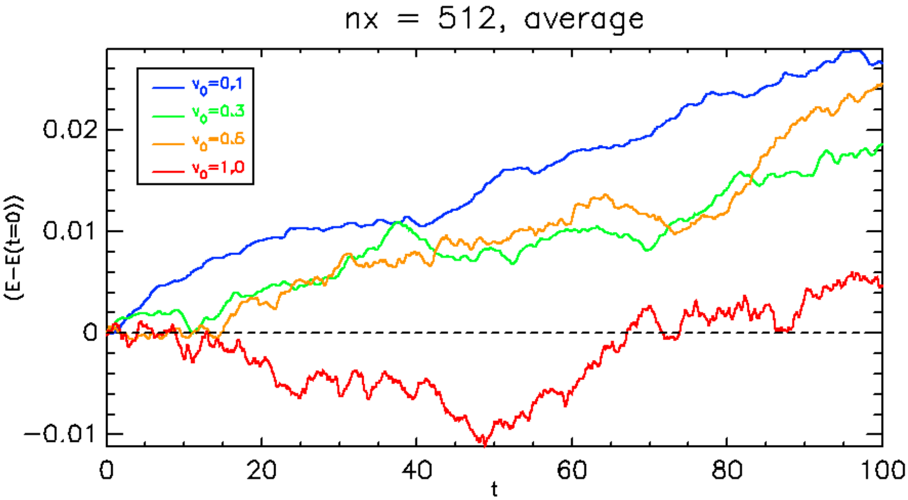
Kinetic energy

Sets of 5×50 particles and **average** for different n_x:



Kinetic energy

Runs with $b_{0,z}$: averages for different initial speeds:



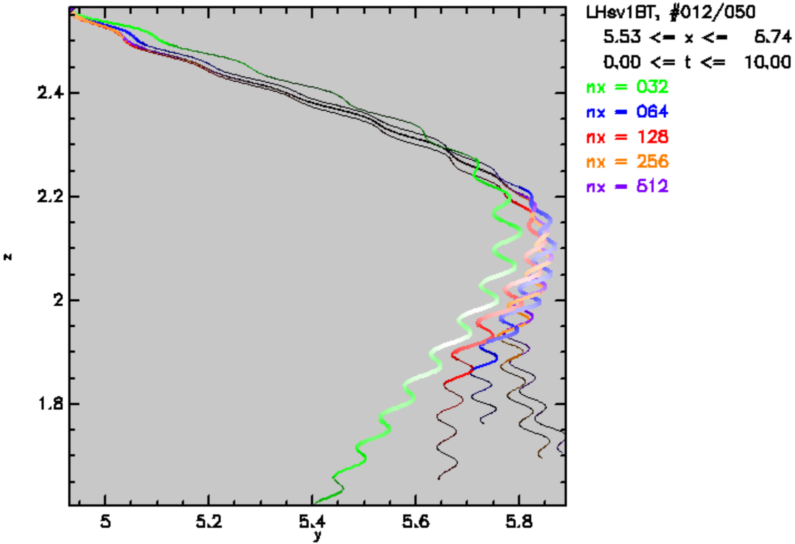
Expectation and findings

- The expectation for E_{kin} could have been:
  - the averages show at least some trend regarding the grid resolution

  → formulation of transport parameters (e.g. a diffusion coefficient) or even of an external force
- But:
  - spread around each average is large compared to the differences between the averages for different cases
  - no trend or systematics visible so far
  - reason could be some kind of "chaotic behaviour" of the particles:

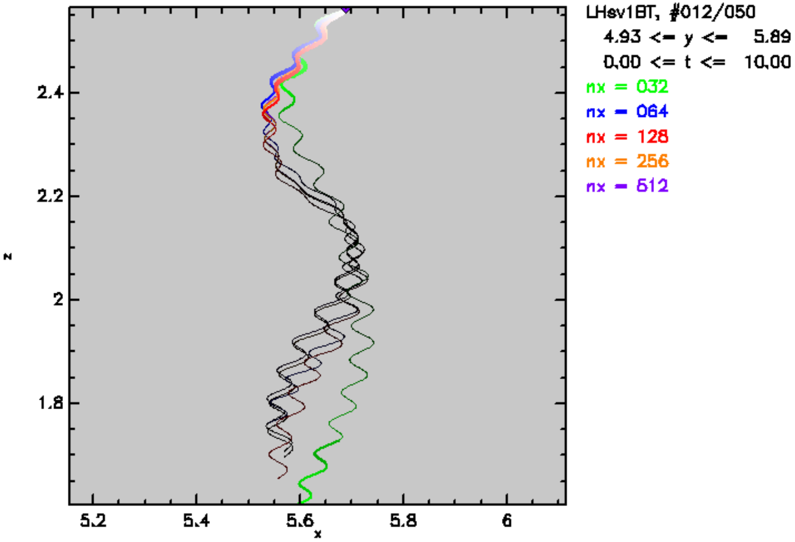
Particle trajectories

One particle (x=const.) for different resolutions, reduction 1:



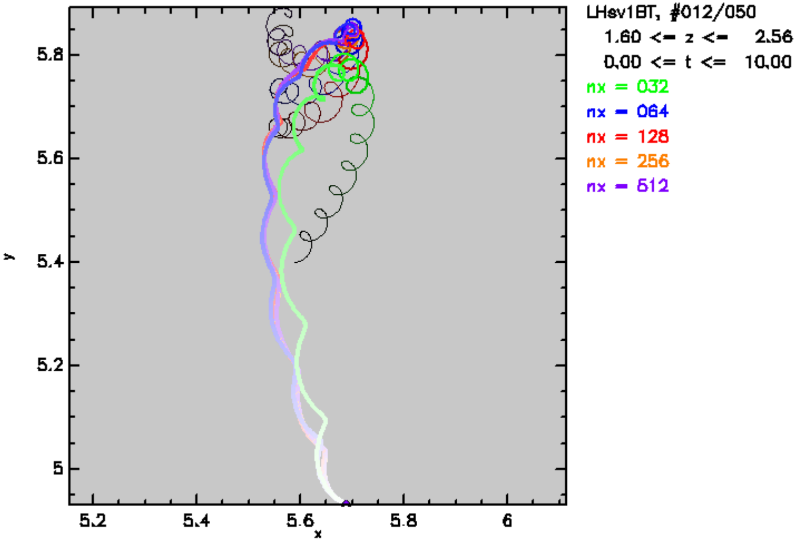
Particle trajectories

One particle (y=const.) for different resolutions, reduction 1:



Particle trajectories

One particle (z=const.) for different resolutions, reduction 1:



Conclusions and outlook

- small differences in the background field may lead to large deviations in the *individual* trajectories during the time-evolution
- these, however, are *not systematic*, but rather randomly in nature
- these, however, compensate essentially in the *average*

- do even higher grid resolutions help...?
- do even more particles help...?

Backup slides

MHD equations

Set of resistive MHD equations:

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\vec{\nabla} \cdot (\rho \vec{u}) \\
\frac{\partial (\rho \vec{u})}{\partial t} &= -\vec{\nabla} \cdot (\rho \vec{u} \otimes \vec{u}) + \nu \rho \Delta \vec{u} - \vec{\nabla} p + \frac{1}{\mu_0} \left(\vec{\nabla} \times \vec{B} \right) \times \vec{B} \\
\frac{\partial \vec{B}}{\partial t} &= \vec{\nabla} \times \left(\vec{u} \times \vec{B} \right) + \eta \Delta \vec{B} \\
\frac{\partial p}{\partial t} &= -\vec{\nabla} \cdot (p \vec{u}) + (\gamma - 1) \left(-p \vec{\nabla} \cdot \vec{u} + \eta \vec{\jmath}^{\,2} \right)
\end{aligned}
$$

- ρ plasma mass density
- $\vec{u}$ plasma flow velocity (with viscosity ν)
- $\vec{B}$ magnetic field (with resistivity η)
- p plasma gas pressure (with adiabatic index γ)

MHD equations

Assume:

- constant mass density $\rho = \rho_0$
- divergence-free plasma flow: $\vec{\nabla} \cdot \vec{u} = 0$
- periodic boundary conditions

$$
\begin{aligned}
0 &= 0 \\
\frac{\partial \vec{u}}{\partial t} &= -\left(\vec{u} \cdot \vec{\nabla}\right) \vec{u} + \frac{1}{\mu_0 \rho} \left(\vec{B} \cdot \vec{\nabla}\right) \vec{B} + \nu \Delta \vec{u} - \frac{1}{\rho} \vec{\nabla} \underbrace{\left(p + \frac{\vec{B}^2}{2\mu_0}\right)}_{p_{\mathrm{tot}}} \\
\frac{\partial \vec{B}}{\partial t} &= -\left(\vec{u} \cdot \vec{\nabla}\right) \vec{B} + \left(\vec{B} \cdot \vec{\nabla}\right) \vec{u} + \eta \Delta \vec{B} \\
\Delta p_{\mathrm{tot}} &= -\left(\vec{\nabla} \otimes \vec{u}\right) : \left(\vec{\nabla} \otimes \vec{u}\right)
\end{aligned}
$$

(last equation: $\vec{\nabla} \cdot (\partial \vec{u} / \partial t) = 0$)

MHD equations

Define the Alfvén velocity

$$\vec{b} = \frac{1}{\sqrt{\mu_0 \rho}} \vec{B}.$$

The MHD equations reduce to:

$$\begin{aligned}
\frac{\partial \vec{u}}{\partial t} &= -\left(\vec{u} \cdot \vec{\nabla}\right) \vec{u} + \left(\vec{b} \cdot \vec{\nabla}\right) \vec{b} + \nu \Delta \vec{u} - \frac{1}{\rho} \vec{\nabla} p_{\mathrm{tot}} \\
\frac{\partial \vec{b}}{\partial t} &= -\left(\vec{u} \cdot \vec{\nabla}\right) \vec{b} + \left(\vec{b} \cdot \vec{\nabla}\right) \vec{u} + \eta \Delta \vec{b}
\end{aligned}$$

(with p_{tot} still to be inserted)

Fourier transformation

The MHD equations are solved in Fourier space with TURBO

$$\mathcal{F}[\vec{u}(\vec{r},t)] = \vec{U}(\vec{k},t) = \int \vec{u}(\vec{r},t)e^{-i\vec{k}\cdot\vec{r}}d^3\vec{r}$$

$$\mathcal{F}[\vec{b}(\vec{r},t)] = \vec{B}(\vec{k},t) = \int \vec{b}(\vec{r},t)e^{-i\vec{k}\cdot\vec{r}}d^3\vec{r}$$

- $\vec{\nabla}\cdot\vec{u} \to i\vec{k}\cdot\vec{U}$, $\vec{\nabla}\times\vec{b} \to i\vec{k}\times\vec{B}$
- but products such as $\mathcal{F}[\vec{u}\cdot\vec{b}]$ result in terms like (dealiasing!)

$$ik_\beta N^{u,b}_{\alpha\beta}(\vec{k}) = \sum_\beta \int ik_\beta u_\beta(\vec{q}) b_\alpha(\vec{k}-\vec{q})d^3\vec{q}$$

- the pressure can now easily computed as

$$P(\vec{k},t) = -\sum_{\beta,\gamma} \frac{k_\gamma k_\beta}{k^2}\left(N^{u,u}_{\gamma\beta}(\vec{k},t) - N^{b,b}_{\gamma\beta}(\vec{k},t)\right)$$

MHD equations in Fourier space

$$
\begin{aligned}
\frac{\partial U_\alpha(\vec{k},t)}{\partial t} &= \sum_{\beta,\gamma} M_{\alpha\beta\gamma}\left(N^{u,u}_{\gamma\beta}(\vec{k},t) - N^{b,b}_{\gamma\beta}(\vec{k},t)\right) - \nu k^2 U_\alpha(\vec{k},t) \\
\frac{\partial B_\alpha(\vec{k},t)}{\partial t} &= \sum_{\beta,\gamma} M_{\alpha\beta\gamma}\left(N^{u,b}_{\gamma\beta}(\vec{k},t) - N^{b,u}_{\gamma\beta}(\vec{k},t)\right) - \eta k^2 B_\alpha(\vec{k},t)
\end{aligned}
$$

with the projection operators:

$$
\begin{aligned}
M_{\alpha\beta\gamma} &= -\frac{i}{2}\left(k_\beta P_{\alpha\gamma} + k_\gamma P_{\alpha\beta}\right) \\
P_{\alpha\zeta} &= \delta_{\alpha\zeta} - \frac{k_\alpha k_\zeta}{k^2}
\end{aligned}
$$

The time integration in `TURBO` is performed with a modified Williamson/Runge-Kutta scheme

Particle transport in MHD fields

The TURBO particle code:

- propagates a set of charged particles with mass m_p and velocity $\vec{v}_\mathrm{p}(t)$, resulting in trajectories $\vec{r}_\mathrm{p}(t)$
- the initial values are $\vec{r}_{\mathrm{p},0}$ and $\vec{v}_{\mathrm{p},0}$ at time $t = 0$:

  $\vec{r}_{\mathrm{p},0}$: two cases:

  all particles at the same place or randomly distributed

  $\vec{v}_{\mathrm{p},0}$: random direction with same speed v_0

  $p \in \{1, \dots, N_p\}$
- the MHD fields are frozen in time, but TURBO also allows to simulate the evolutions of both fields and particles
- Runge-Kutta scheme with spline-interpolation of the MHD fields and control of the time-step

Postprocessing with binning or averaging over the set of particles

Code validation: energy conservation

Equation of motion (with: $\alpha = \Omega t_{\mathrm{A}} = \frac{q}{m_{\mathrm{p}}} b \frac{L}{v_{\mathrm{A}}}$):

$$\frac{d\vec{v}_{\mathrm{p}}}{dt} = \alpha \left(\vec{e} + \vec{v}_{\mathrm{p}} \times \vec{b} \right), \qquad \vec{e} = \underbrace{-\vec{\nabla}\varphi}_{\vec{e}_{\mathrm{nsl}}} \underbrace{-\frac{\partial \vec{a}}{\partial t}}_{\vec{e}_{\mathrm{sol}}}$$

Kinetic energy:

$$\int \vec{v}_{\mathrm{p}} \cdot \frac{d\vec{v}_{\mathrm{p}}}{dt} dt = \alpha \int \left(\vec{e} \cdot \vec{v}_{\mathrm{p}} \right) dt = \alpha \int \left(\left(-\vec{\nabla}\varphi - \frac{\partial \vec{a}}{\partial t} \right) \cdot \vec{v}_{\mathrm{p}} \right) dt,$$

so that

$$\frac{1}{2} \vec{v}_{\mathrm{p}}(t_2)^2 - \frac{1}{2} \vec{v}_{\mathrm{p}}(t_1)^2 = -\alpha \Big(\varphi(r_{\mathrm{p}}(t_2)) - \varphi(r_{\mathrm{p}}(t_1)) \Big) \underbrace{-\alpha \left(\int_{t_1}^{t_2} \left(\vec{e}_{\mathrm{sol}} \cdot \vec{v}_{\mathrm{p}} \right) dt \right)}_{M(t_1, t_2)}$$

Code validation: energy conservation

Comparison of different contributions ($\alpha = 1,\ t_2 = t,\ t_1 = 0$):