Turbulence & computer simulations

Axel Brandenburg (Nordita, Stockholm)
Wolfgang Dobler (Univ. Calgary)
and now many more….

(...just google for Pencil Code)

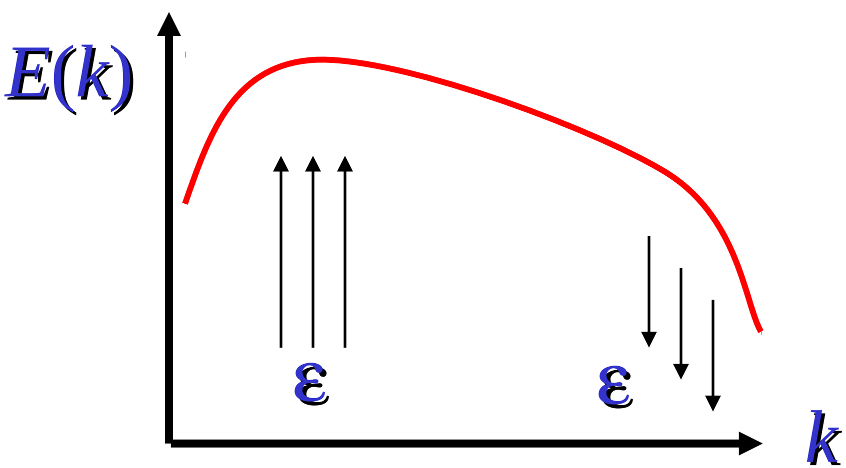
Kolmogorov spectrum

nonlinearity

$$\left(\cos kx\right)^2 = \tfrac{1}{2}\cos 2kx + \tfrac{1}{2}$$

$$k \to 2k$$

constant flux ε [cm^2/s^3]



$$\int E\left(k\right)dk = \tfrac{1}{2}\left\langle \mathbf{u}^2 \right\rangle$$ [cm^3/s^2]

$$E\left(k\right) = C_K \varepsilon^a k^b$$

$$\text{cm}: \quad 3 = 2a - 1$$

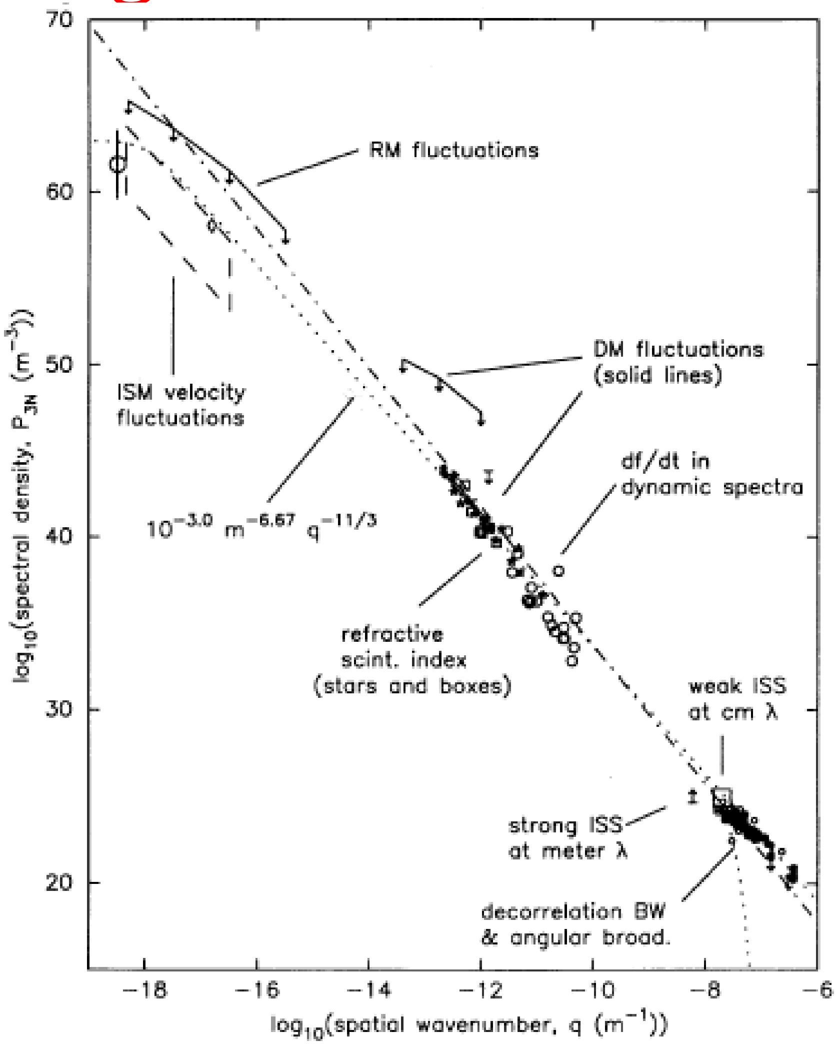
$$\text{s}: \quad 2 = 3a$$

a=2/3, b= –5/3

Scintillations

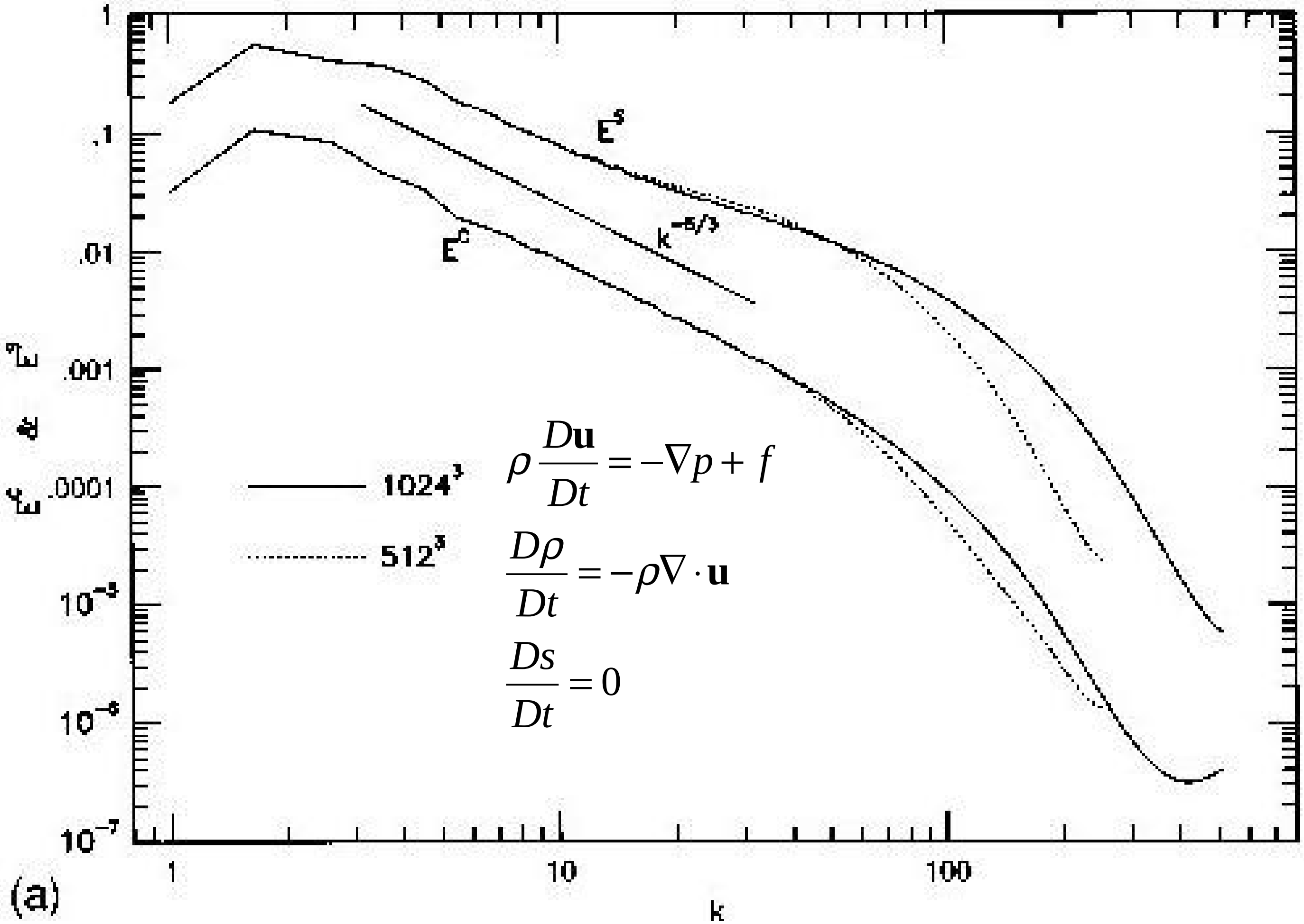
- Armstrong, Cordes, Rickett 1981, Nature
- Armstrong, Rickett, Spangler 1995, ApJ

Big Power Law in Sky



Simulation of turbulence at 1024^3

(Porter, Pouquet,& Woodward 1998)



$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + f$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{u}$$

$$\frac{Ds}{Dt} = 0$$

Direct vs hyper at 512^3

Biskamp & Müller (2000, Phys Fluids 7, 4889)

D. Biskamp and W.-C. Müller

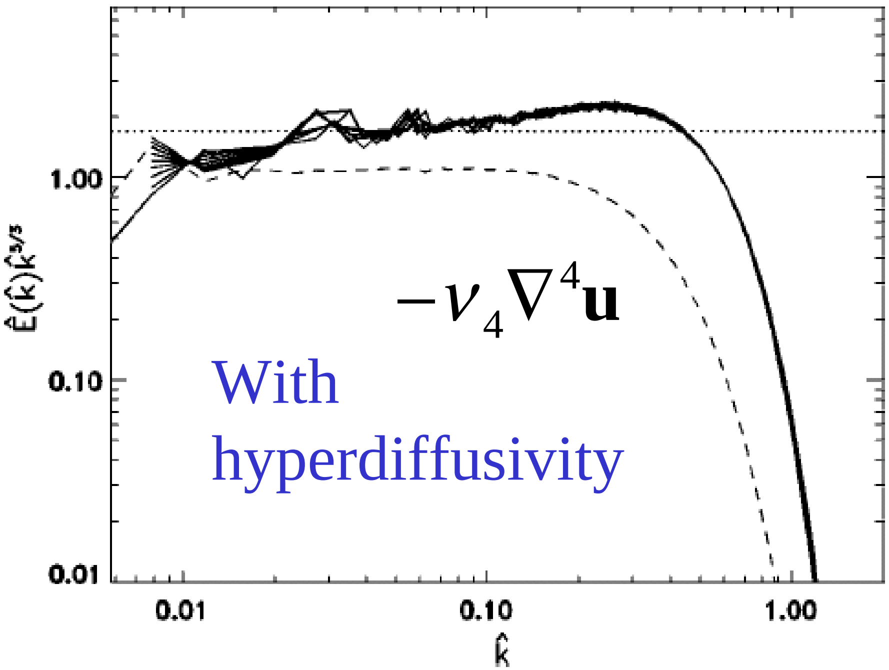


FIG. 11. Scatter plot of the normalized energy spectrum compensated by $k^{5/3}$ from the hyperdiffusive run 10. The dotted line is identical to the one in Fig. 8 for normal diffusion, indicating the same inertial range spectrum outside the bottleneck hump. The dashed line gives the one-dimensional spectrum $E(|k_z|)=E(k_z)+E(-k_z)$.

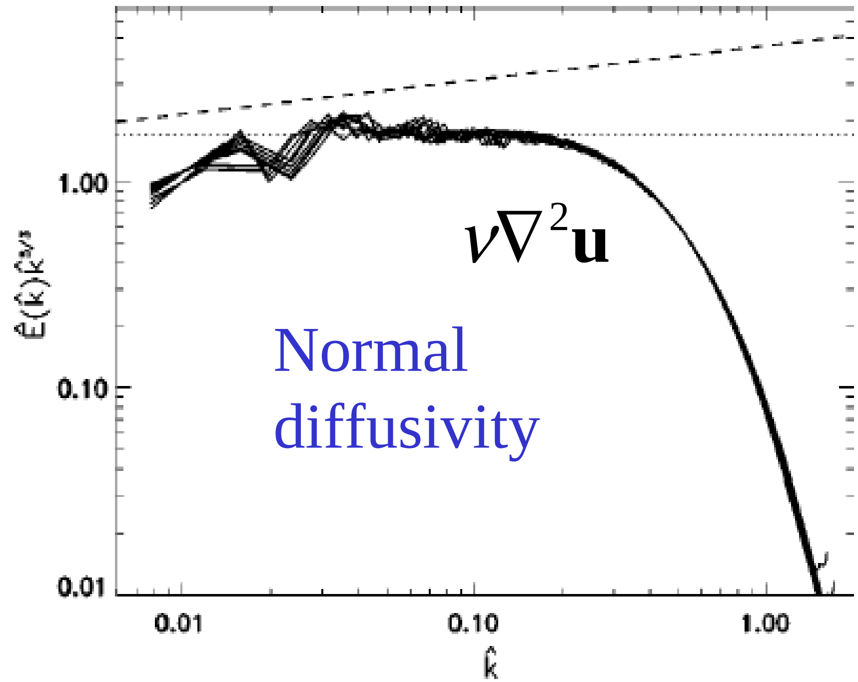


FIG. 8. Scatter plot of the normalized angle-integrated energy spectrum compensated by $k^{5/3}$ from run 6 taken during the period $t=4.5-10$. The dashed line indicates the IK-spectrum $k^{3/2}$, the dotted line the Kolmogorov spectrum with $C'=1.7$.

Ideal hydro: should we be worried?

- Why this k^{-1} tail in the power spectrum?
  - Compressibility?
  - PPM method
  - Or is real??
- Hyperviscosity destroys entire inertial range?
  - Can we trust any ideal method?
- Needed to wait for 4096^3 *direct* simulations

Non-ideal equations

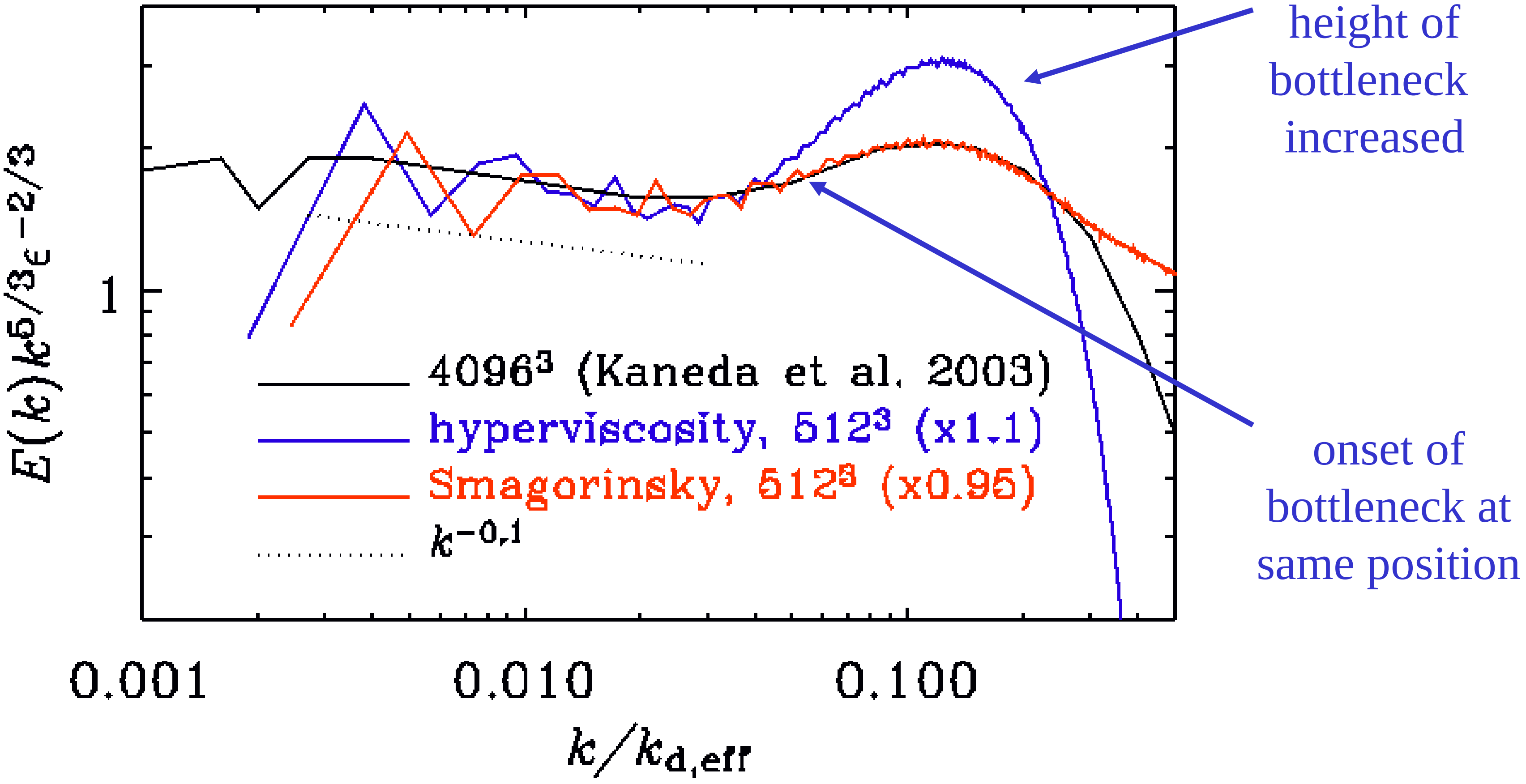
$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + f + \nu\left(\nabla^2\mathbf{u} + \tfrac{1}{3}\nabla\nabla\cdot\mathbf{u} + 2\mathrm{S}\nabla \ln\rho\right)$$

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\mathbf{u}$$

$$T\frac{Ds}{Dt} = 2\nu\,\mathrm{S}^2$$

$$\mathrm{S}_{\mathrm{ij}} = \tfrac{1}{2}\left(u_{i,j} + u_{j,i}\right) - \tfrac{1}{3}\delta_{\mathrm{ij}}u_{k,k}$$

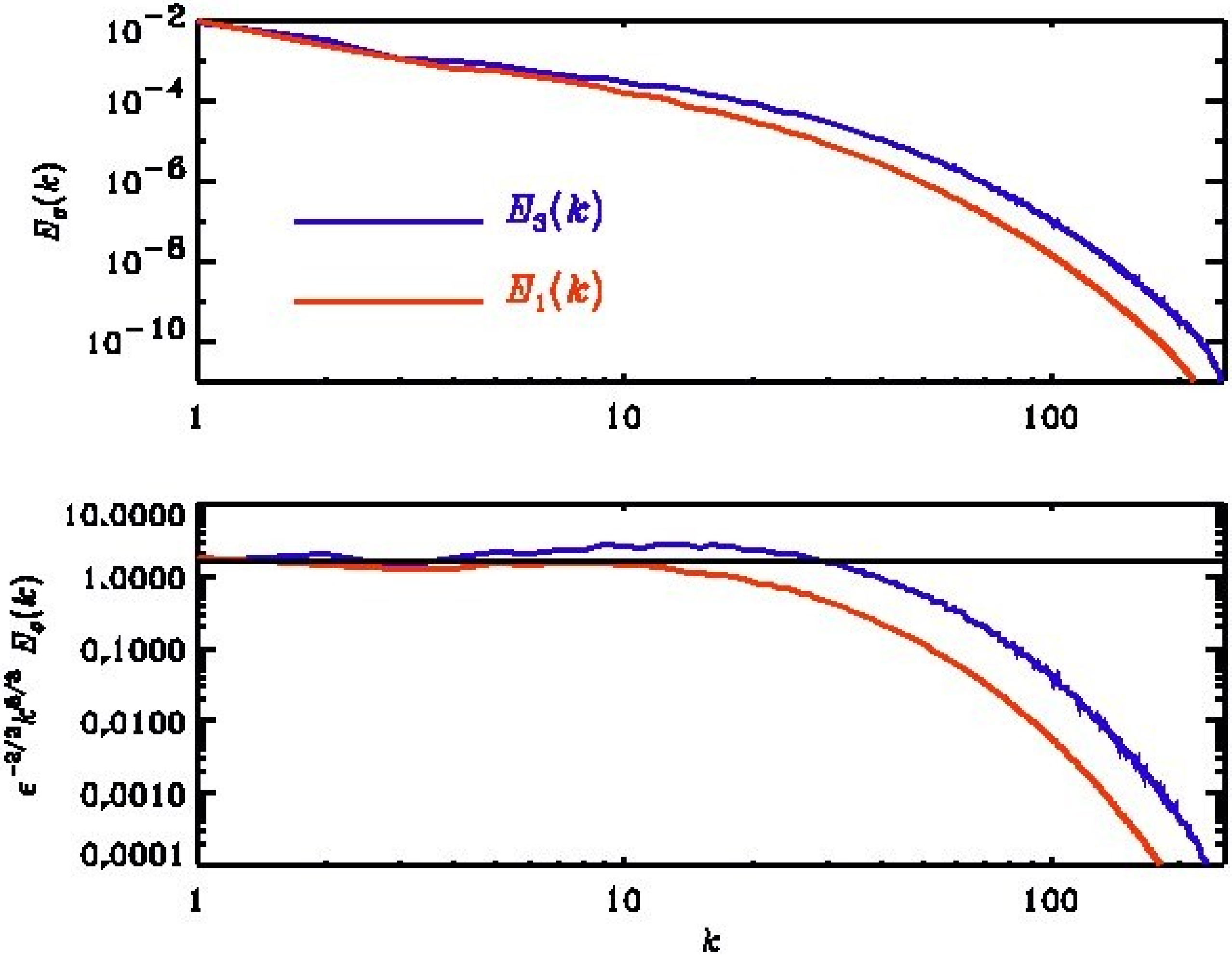
Hyperviscous, Smagorinsky, normal



Inertial range unaffected by artificial diffusion

Bottleneck effect: 1D vs 3D spectra

Why did wind tunnels not show this?



Compensated spectra (1D vs 3D)

Relation to 'laboratory' 1D spectra

$$E_{3D} = \int \left|\mathbf{u}(\mathbf{k})\right|^2 k^2 d\Omega_k = 4\pi k^2 \left\langle \left|\mathbf{u}(\mathbf{k})\right|^2 \right\rangle$$

$$E_{1D}(k_z) = 2\int \left\langle \left|\mathbf{u}(x,y,k_z)\right|^2 \right\rangle \mathrm{d}x\,\mathrm{d}y$$

$k_z > 0$

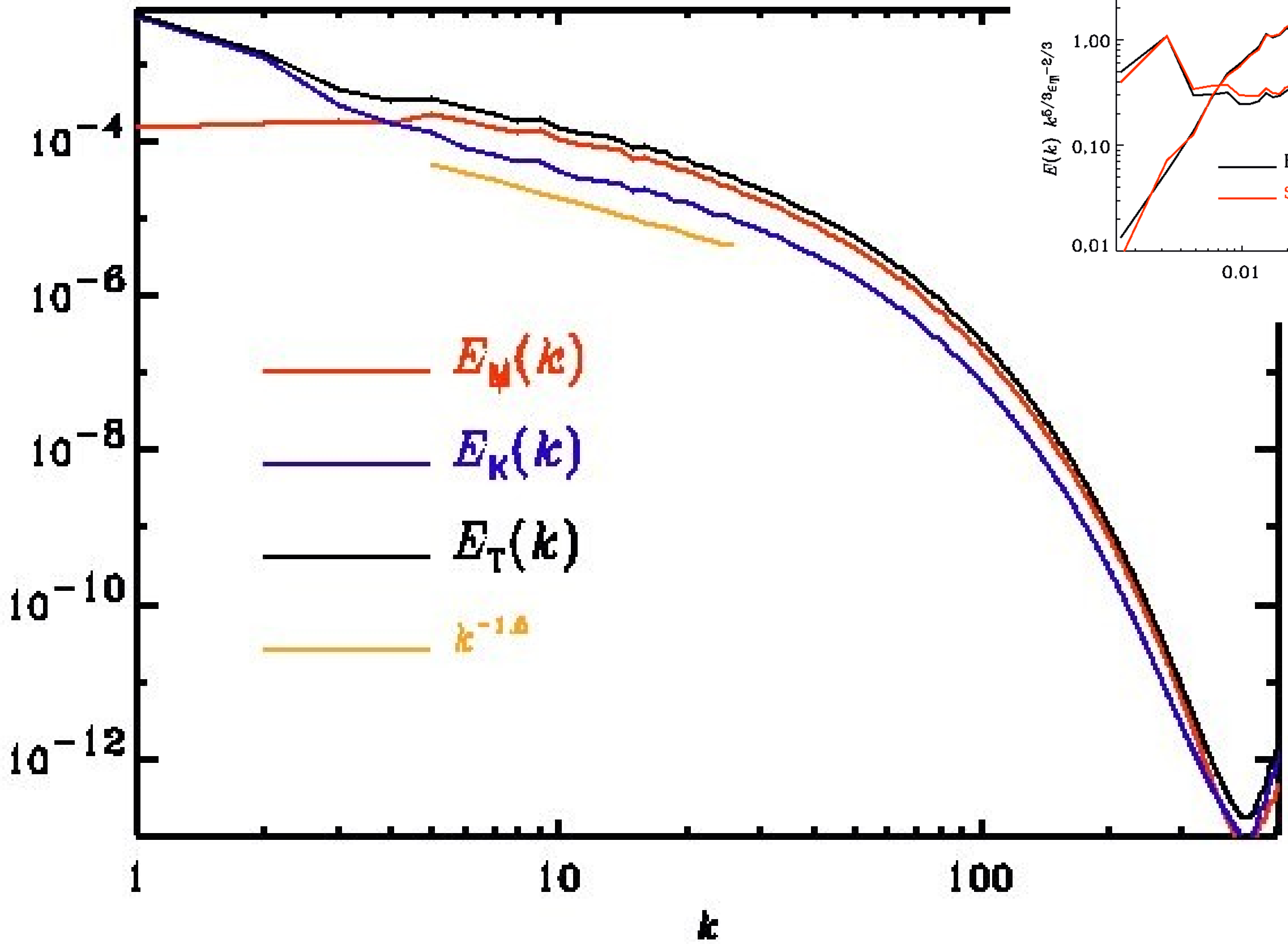
$$= 4\pi \int_0^\infty \left\langle \left|\mathbf{u}(k_\varpi, k_z)\right|^2 \right\rangle k_\varpi \,\mathrm{d}k_\varpi = 4\pi \int_{k_z}^\infty \left\langle \left|\mathbf{u}(k)\right|^2 \right\rangle k\,\mathrm{d}k$$

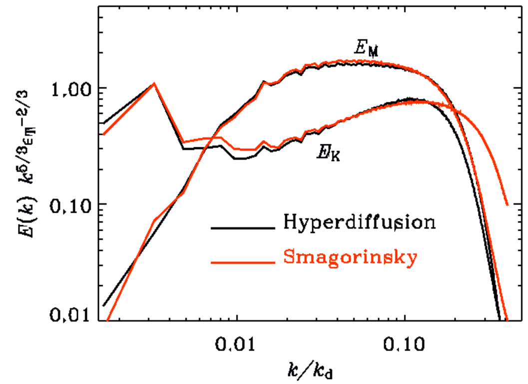
$$= \int_{k_z}^\infty \frac{E_{3D}}{k}\,\mathrm{d}k$$

$k^2 = k_\varpi^2 + k_z^2$

Dobler, et al
(2003, PRE 68, 026304)

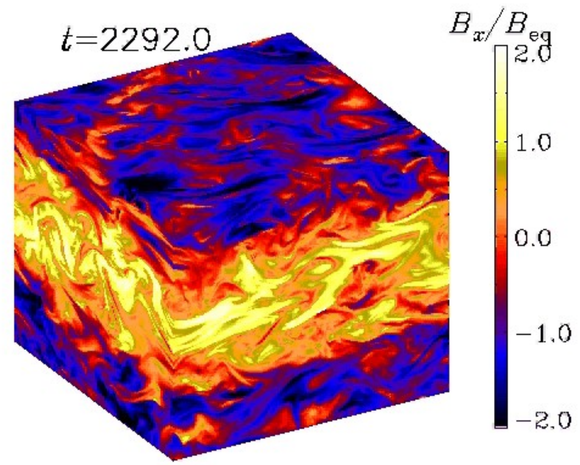
Nonhelical MHD turbulent spectrum

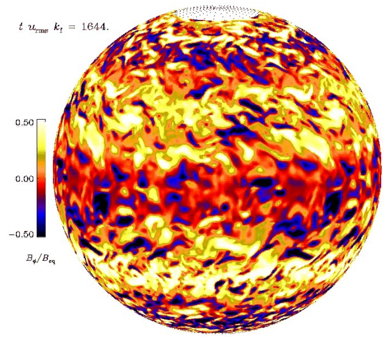




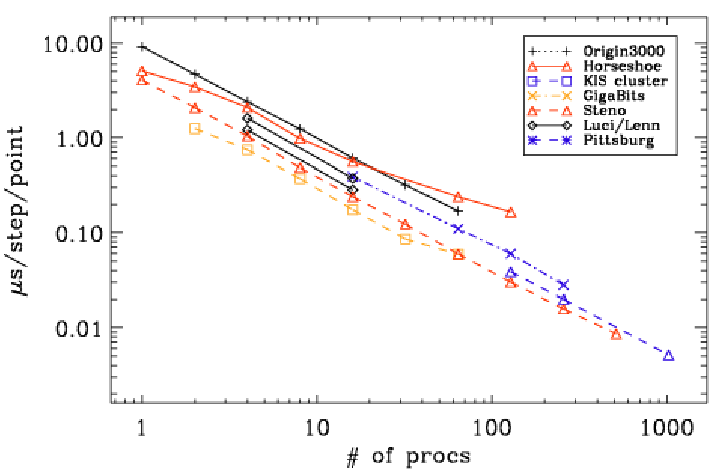
Pencil code

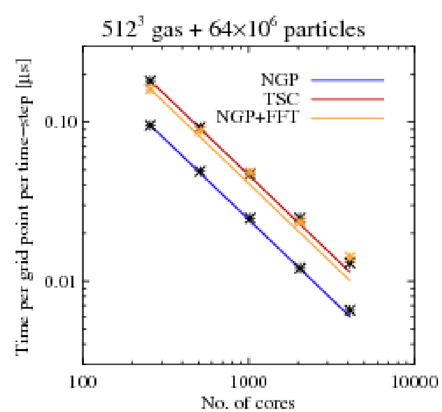
- Started in Sept. 2001 with Wolfgang Dobler
- High order (6th order in space, 3rd order in time)
- Cache & memory efficient
- MPI, can run PacxMPI (across countries!)
- Maintained/developed by ~80 people (SVN)
- Automatic validation (over night or any time)
- 0.0013 μs/pt/step at 1024^3, 2048 procs
- http://pencil-code.googlecode.com





- Isotropic turbulence
  - MHD, passive scl, CR
- Stratified layers
  - Convection, radiation
- Shearing box
  - MRI, dust, interstellar
  - Self-gravity
- Sphere embedded in box
  - Fully convective stars
  - geodynamo
- Other applications
  - Chemistry, combustion
  - Spherical coordinates





Pencil formulation

- In CRAY days: worked with full chunks *f(nx,ny,nz,nvar)*
  - Now, on SGI, nearly 100% cache misses
- Instead work with *f(nx,nvar)*, i.e. one *nx*-pencil
- No cache misses, negligible work space, just *2N*
  - Can keep all components of derivative tensors
- Communication before sub-timestep
- Then evaluate all derivatives, e.g. *call curl(f,iA,B)*
  - Vector potential *A=f(:,:,:,iAx:iAz)*, *B=B(nx,3)*

Switch modules

- magnetic or nomagnetic (e.g. just hydro)
- hydro or nohydro (e.g. kinematic dynamo)
- density or nodensity (burgulence)
- entropy or noentropy (e.g. isothermal)
- radiation or noradiation (solar convection, discs)
- dustvelocity or nodustvelocity (planetesimals)
- Coagulation, reaction equations
- Chemistry (reaction-diffusion-advection equations)

Other physics modules: MHD, radiation, partial ionization, chemical reactions, selfgravity

High-order schemes

- Alternative to spectral or compact schemes
  - Efficiently parallelized, no transpose necessary
  - No restriction on boundary conditions
  - Curvilinear coordinates possible (except for singularities)
- 6th (or other) order central differences in space
- Non-conservative scheme
  - Allows use of logarithmic density and entropy
  - Copes well with strong stratification and temperature contrasts

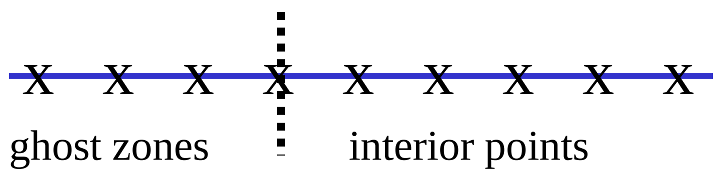
(i) High-order spatial schemes

Main advantage: low *phase* errors

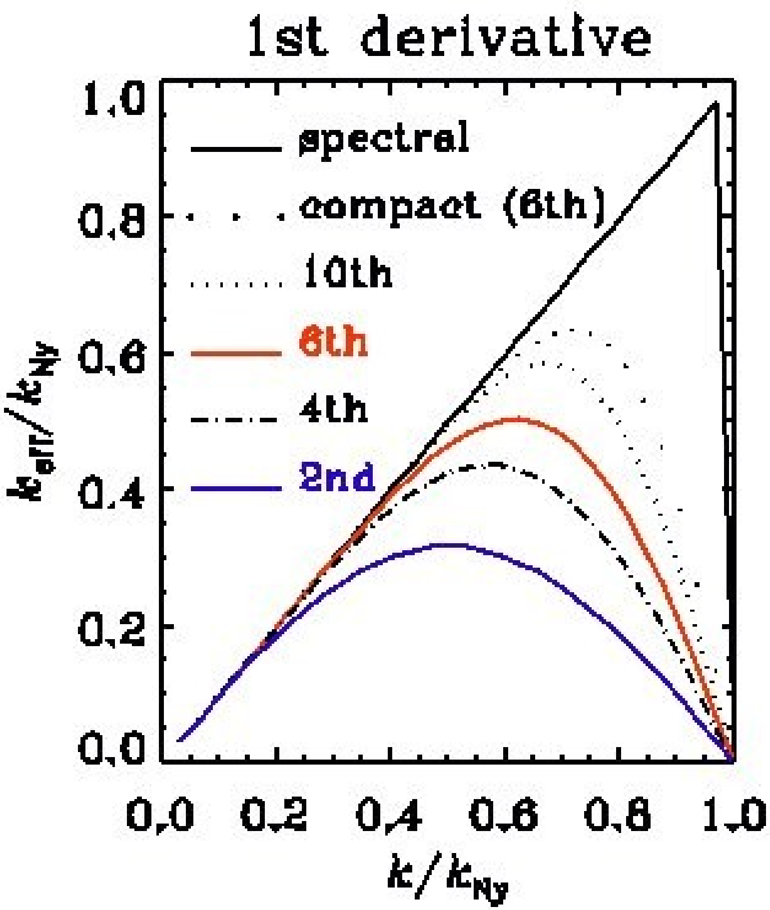
$$f_i' = \frac{-f_{i-3} + 9f_{i-2} - 45f_{i-1} + 45f_{i+1} - 9f_{i+2} + f_{i+3}}{60\delta x}$$

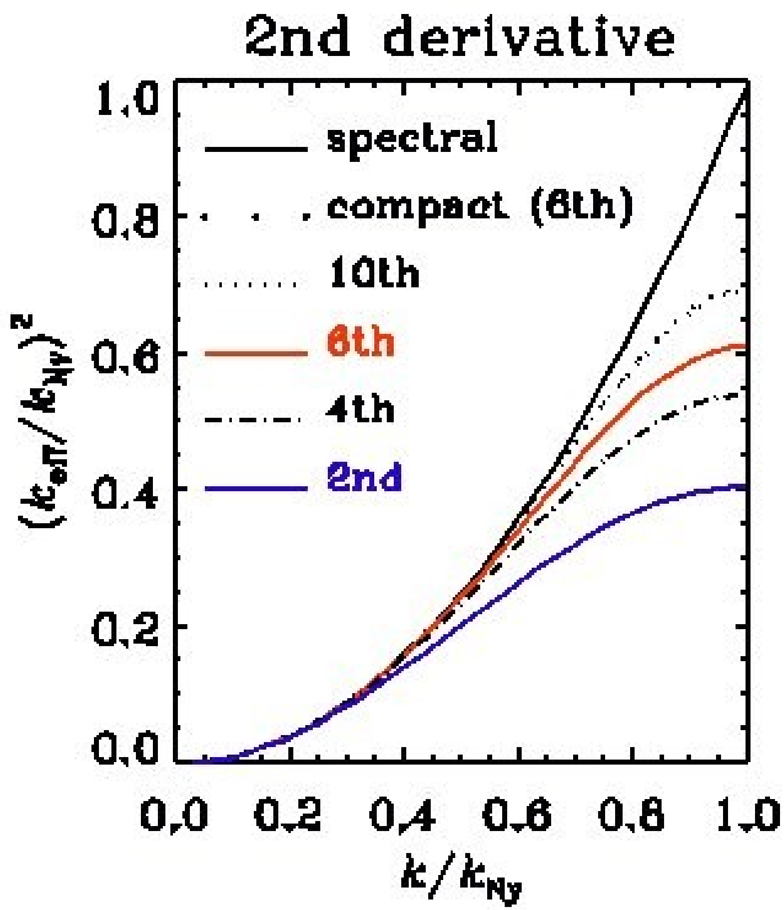
$$f_i'' = \frac{2f_{i-3} - 27f_{i-2} + 270f_{i-1} - 490f_i + 270f_{i+1} - 27f_{i+2} + 2f_{i+3}}{180\delta x^2}$$

Near boundaries:



Wavenumber characteristics

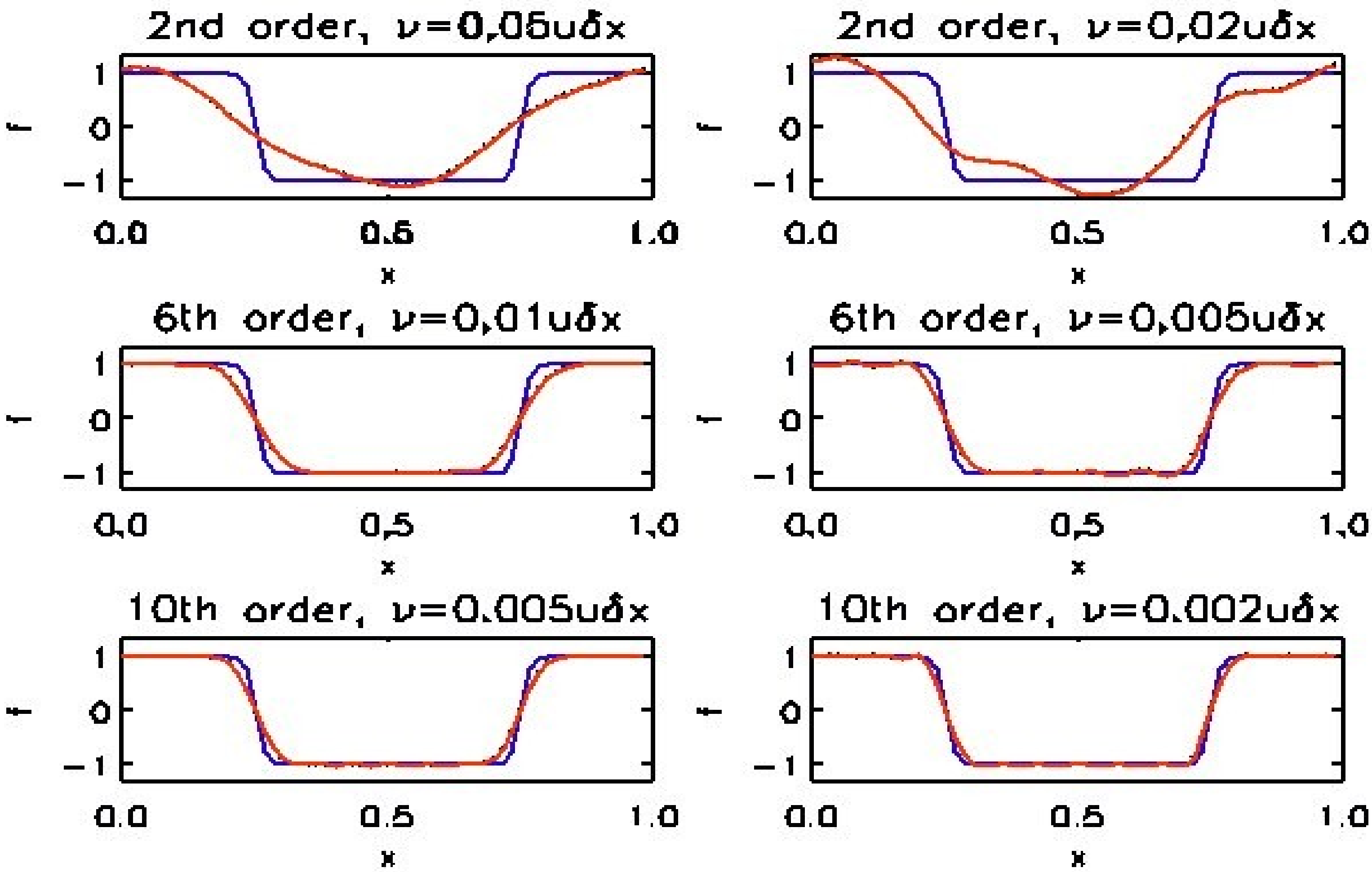




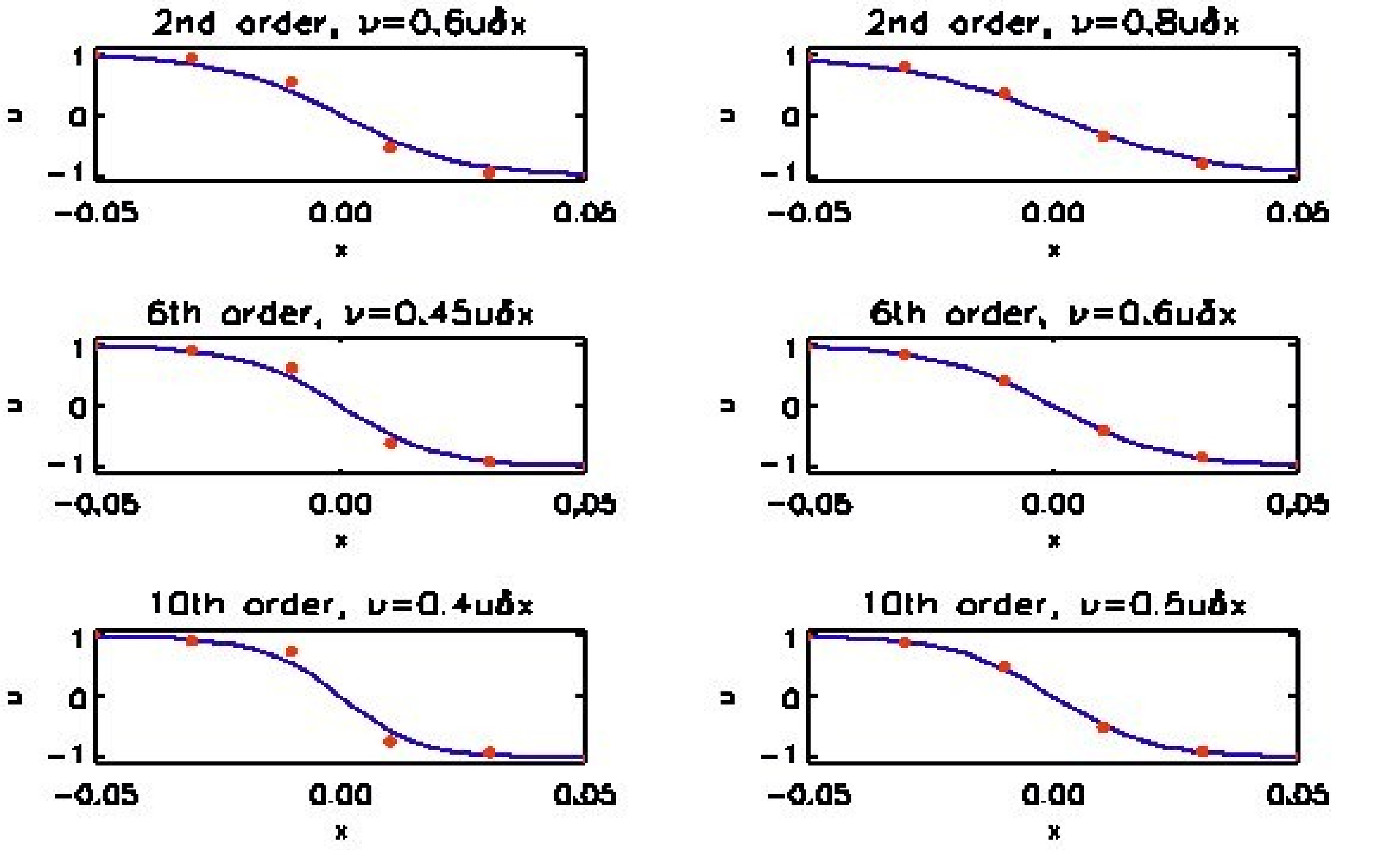
$$k_{eff} = \frac{d(\cos kx)/dx}{-\sin kx}$$

$$k_{eff}^2 = \frac{d^2(\cos kx)/dx^2}{-\cos kx}, \qquad k_{Ny} = \pi/\delta x$$

Higher order – less viscosity



Less viscosity – also in shocks



(ii) High-order temporal schemes

Main advantage: low *amplitude* errors

2N-RK3 scheme (Williamson 1980)

$$w_i = \alpha_i w_{i-1} + \delta t\, F(t_{i-1}, u_{i-1})$$

$$u_i = u_{i-1} + \beta_i w_i$$

$$u_0 = u^{(n)}, \quad u^{(n+1)} = u_3$$

2nd order

$$\alpha_1 = 0, \quad \alpha_2 = -1/2$$

$$\beta_1 = 1/2, \quad \beta_2 = 1$$

3rd order

$$\alpha_1 = 0, \quad \alpha_2 = -2/3, \quad \alpha_3 = -1$$

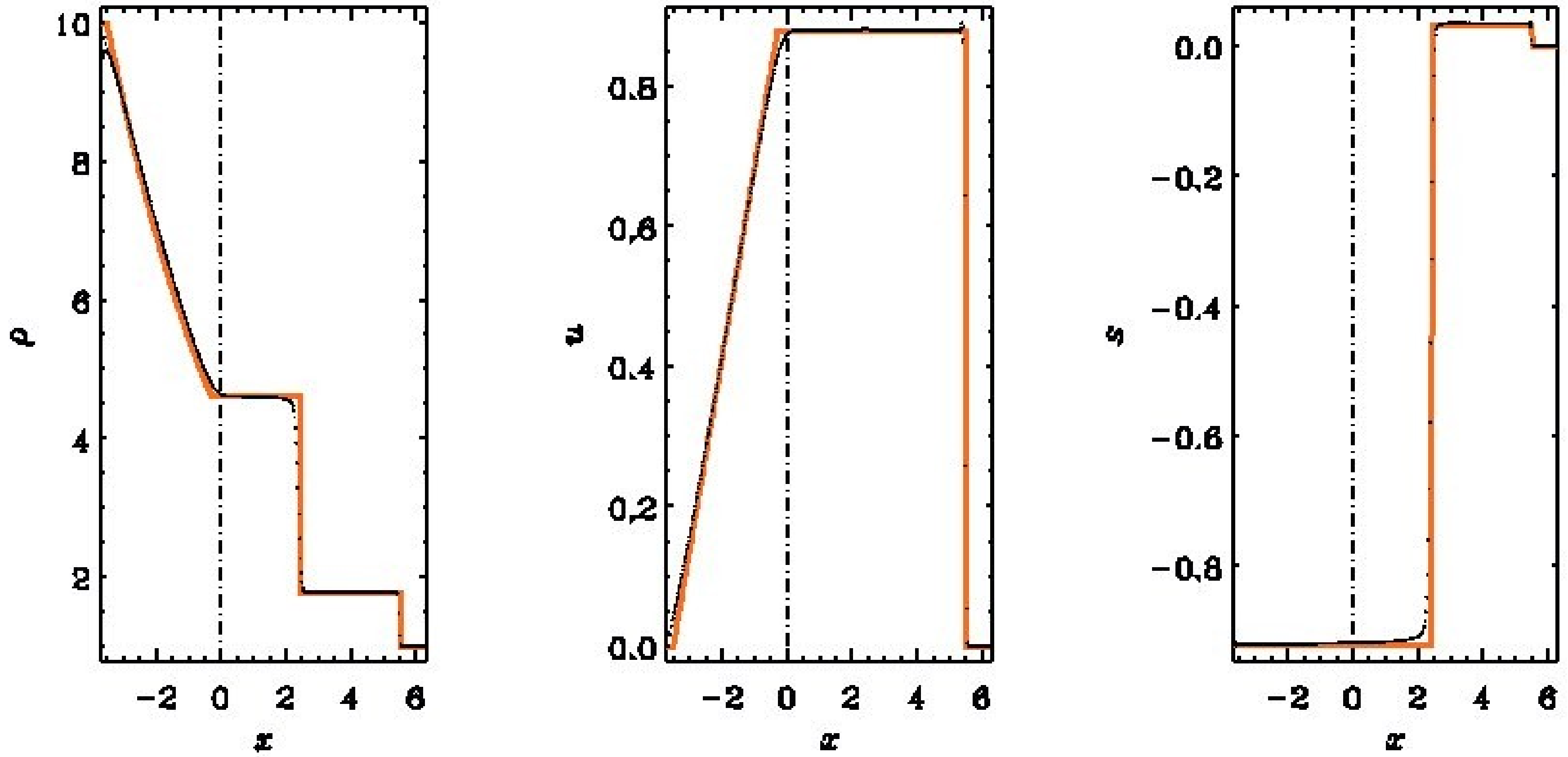
$$\beta_1 = 1/3, \quad \beta_2 = 1, \quad \beta_3 = 1/2$$

1st order

$$\alpha_1 = 0$$

$$\beta_1 = 1$$

Shock tube test



Vector potential

- **B**=curl**A**, advantage: div**B**=0
- **J**=curl**B**=curl(curl**A**) =curl2**A**
- Not a disadvantage: consider Alfven waves

B-formulation

$$\frac{\partial u}{\partial t} = B_0 \frac{\partial b}{\partial z}, \quad \text{and} \quad \frac{\partial b}{\partial t} = B_0 \frac{\partial u}{\partial z}$$

A-formulation

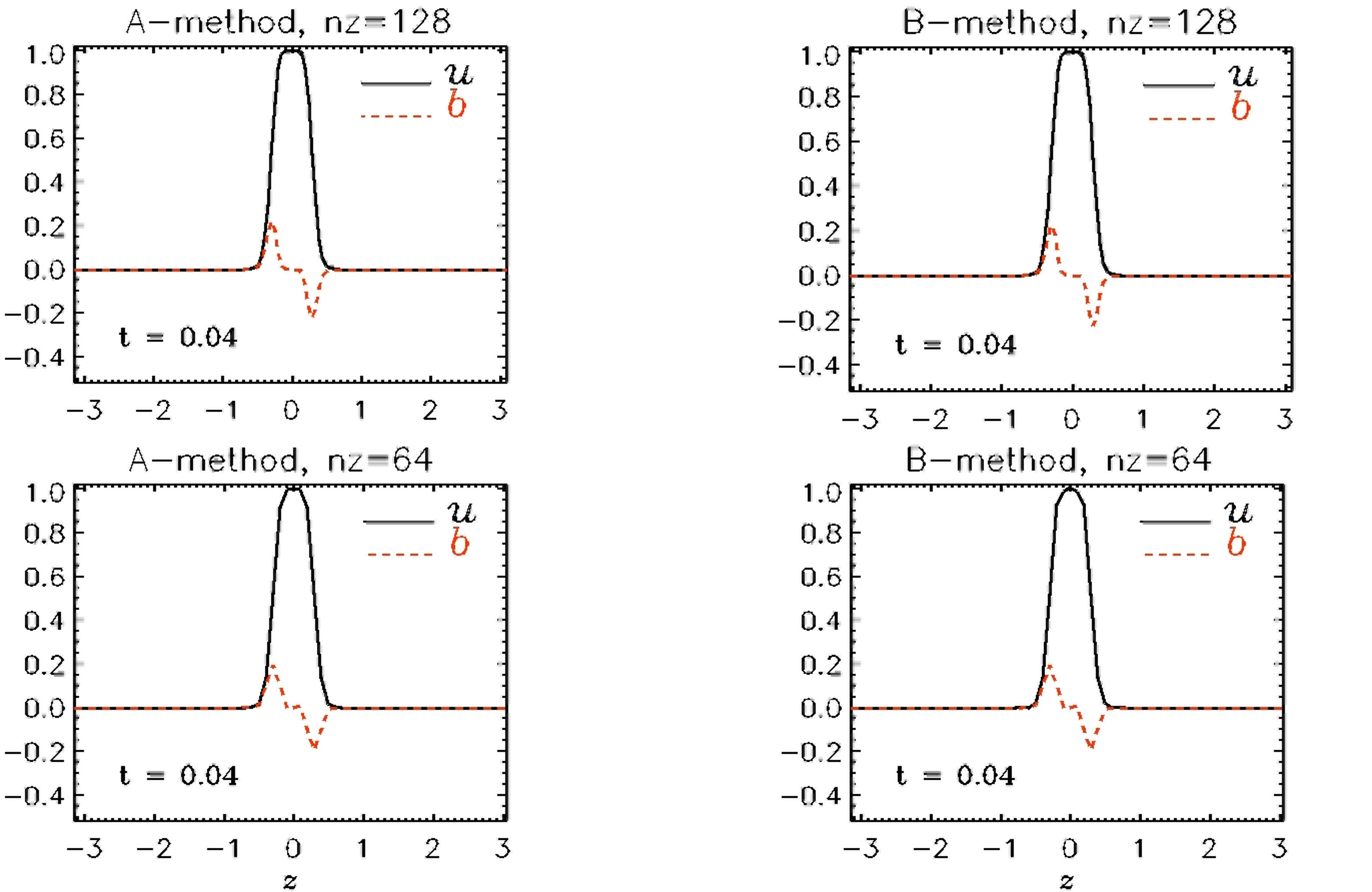
$$\frac{\partial u}{\partial t} = B_0 \frac{\partial^2 a}{\partial z^2}, \quad \text{and} \quad \frac{\partial a}{\partial t} = B_0 u$$

2nd der once
is better than
1st der twice!

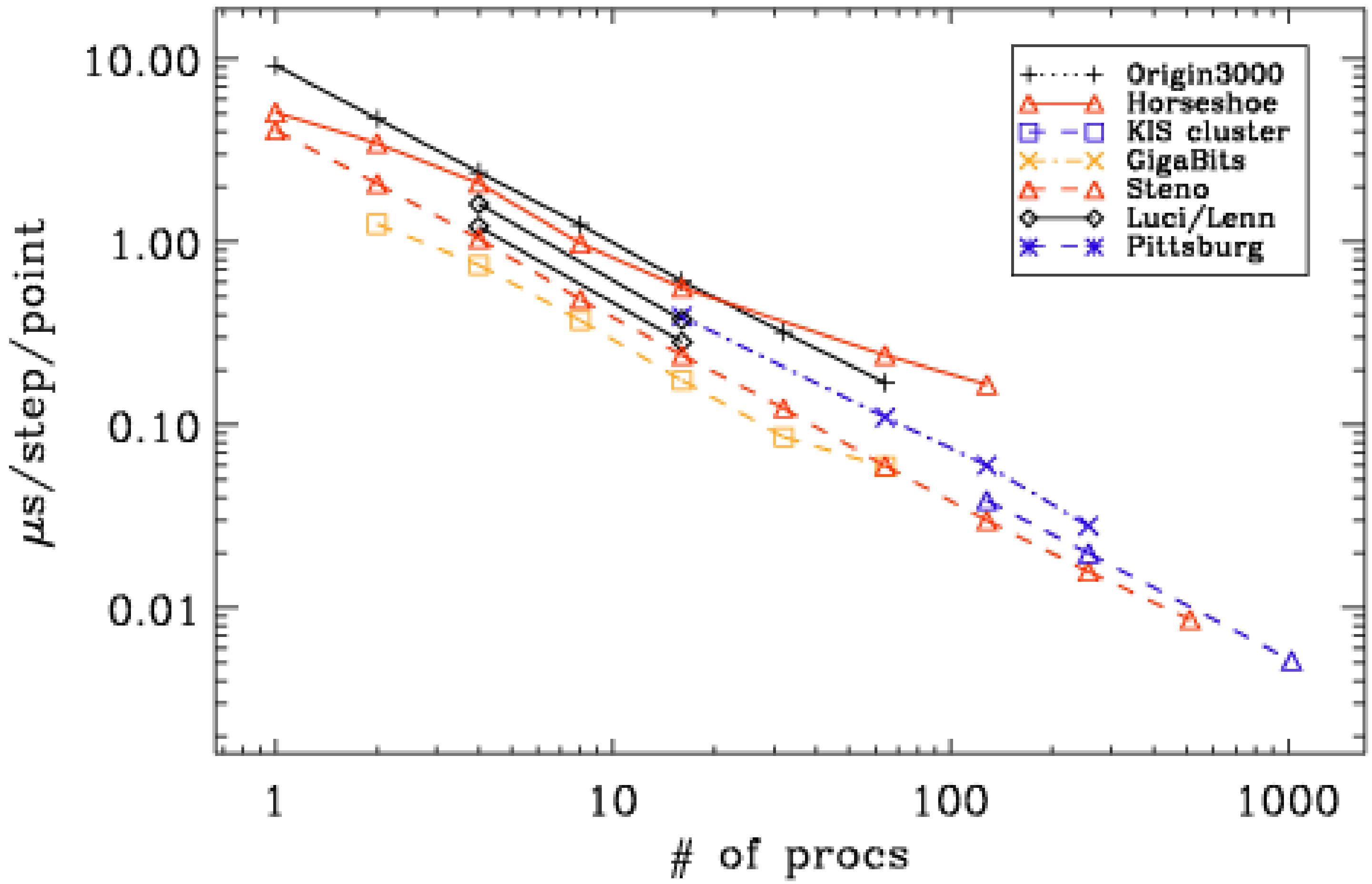
Comparison of A and B methods

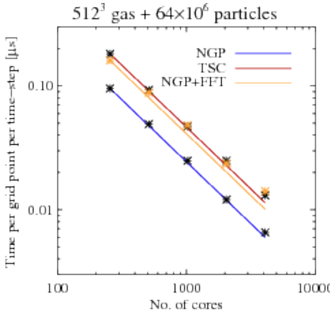
$$\frac{\partial u}{\partial t} = B_0 \frac{\partial^2 a}{\partial z^2} + \upsilon \frac{\partial^2 u}{\partial z^2}, \quad \text{and} \quad \frac{\partial a}{\partial t} = B_0 u + \eta \frac{\partial^2 a}{\partial z^2}$$

$$\frac{\partial u}{\partial t} = B_0 \frac{\partial b}{\partial z} + \upsilon \frac{\partial^2 u}{\partial z^2}, \quad \text{and} \quad \frac{\partial b}{\partial t} = B_0 \frac{\partial u}{\partial z} + \eta \frac{\partial^2 b}{\partial z^2}$$

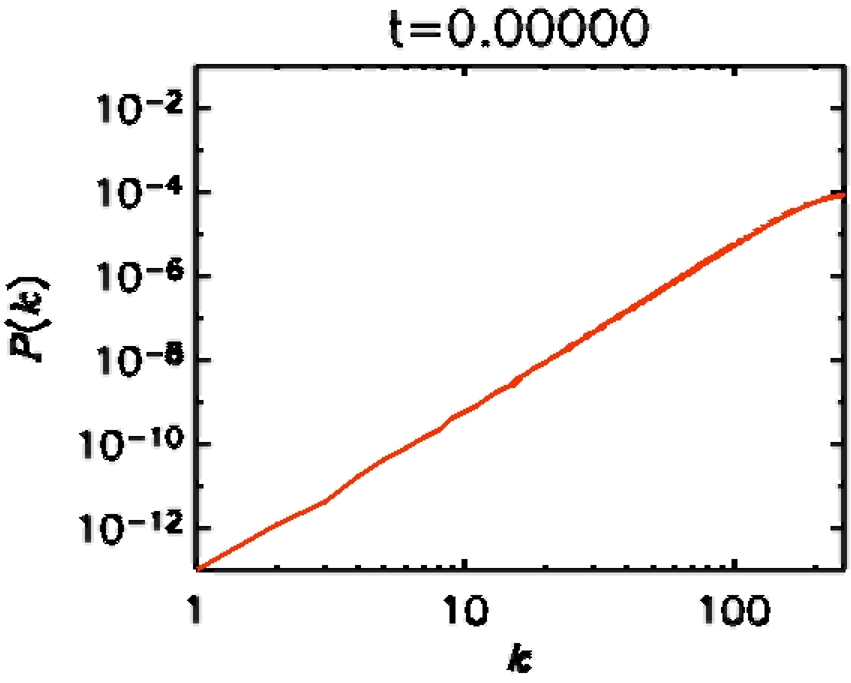


Faster and bigger machines

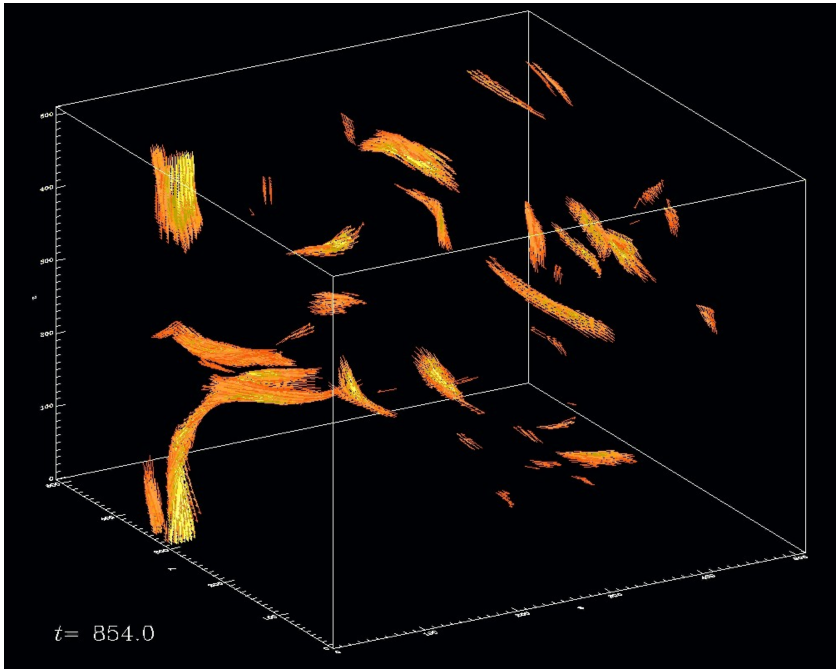




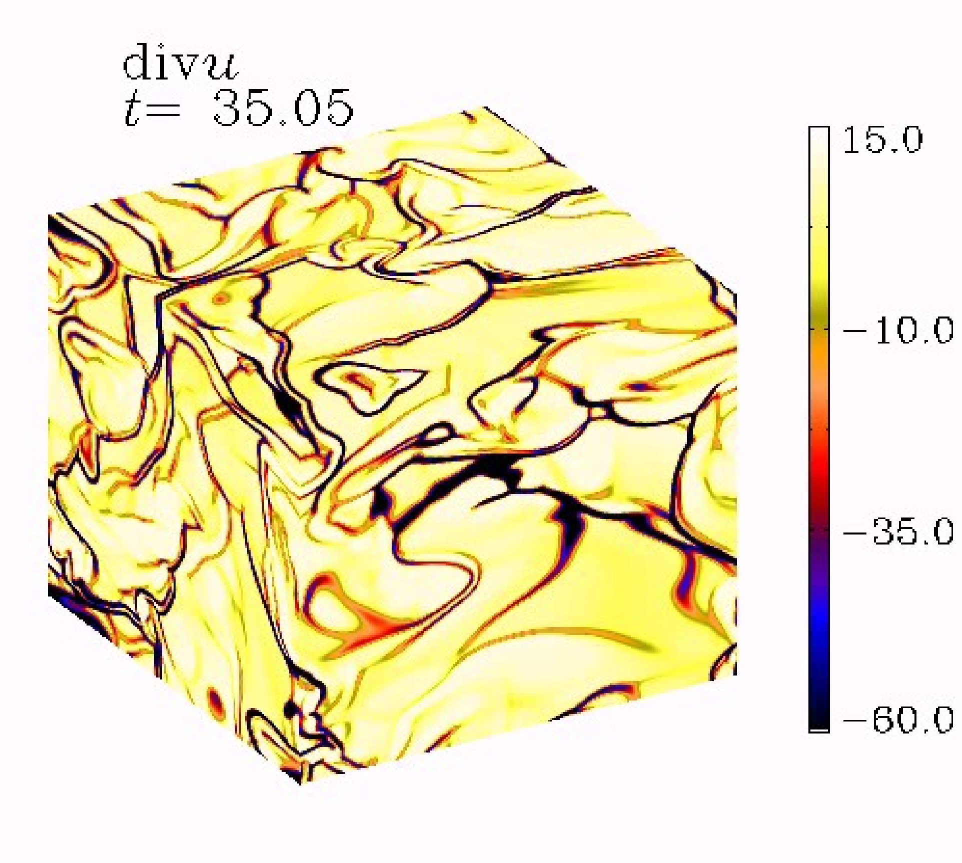
Online data reduction and visualization



non-helically forced turbulence

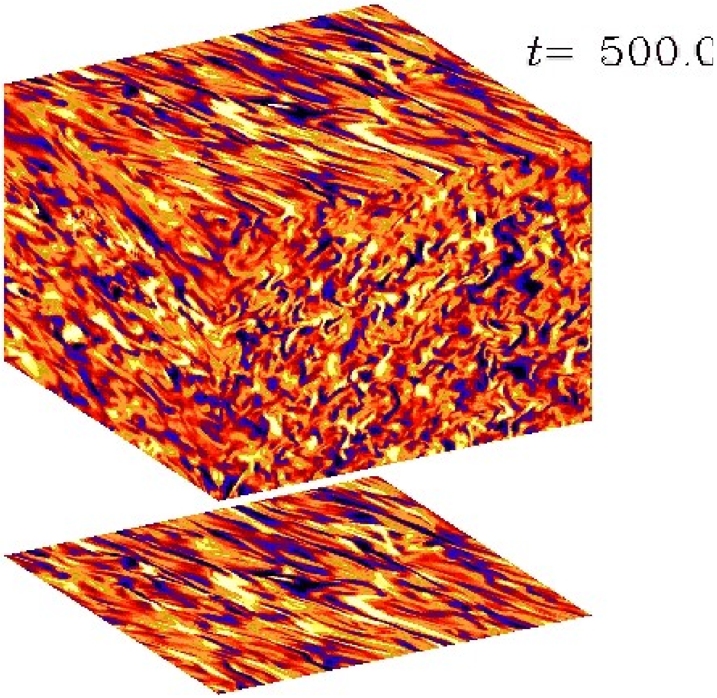


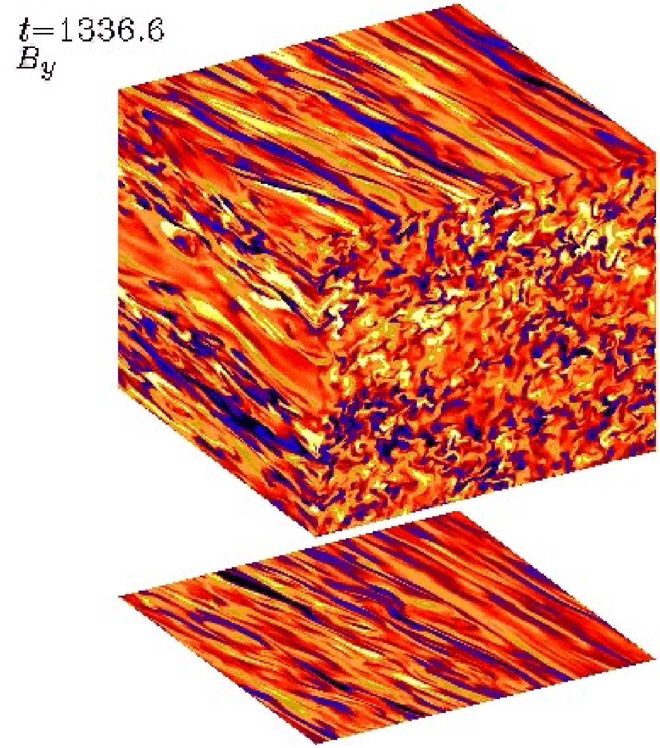
Scalars on periphery of the box



MRI turbulence

MRI = magnetorotational instability

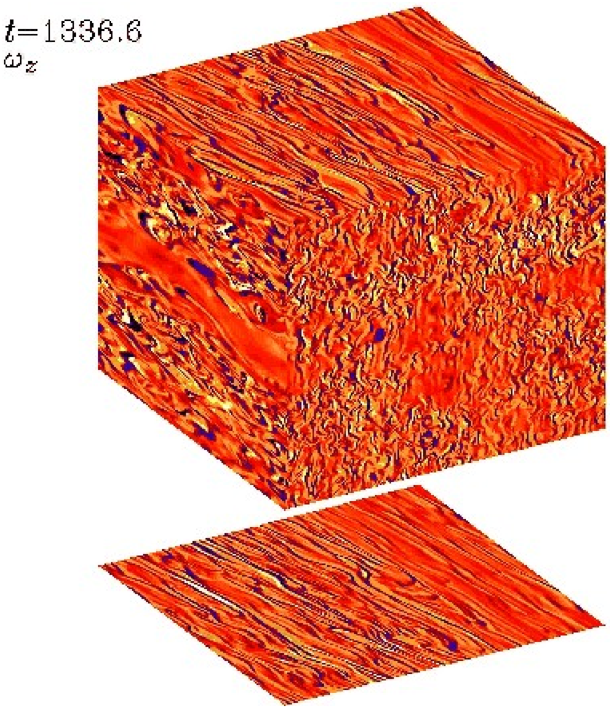


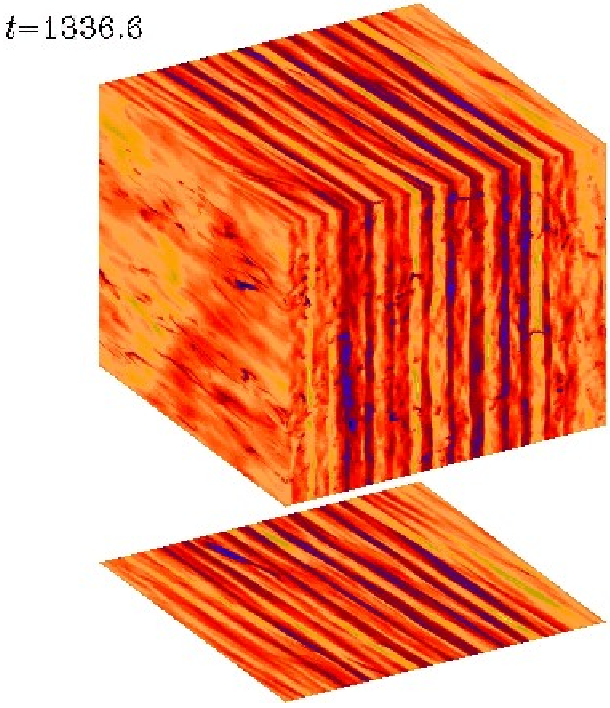


256^3
w/o hypervisc.
t = 600 = 20 orbits

512^3
w/o hypervisc.
Δt = 60 = 2 orbits

Vorticity and Density





See poster by Tobi Heinemann on density wave excitation!

Transfer equation & parallelization

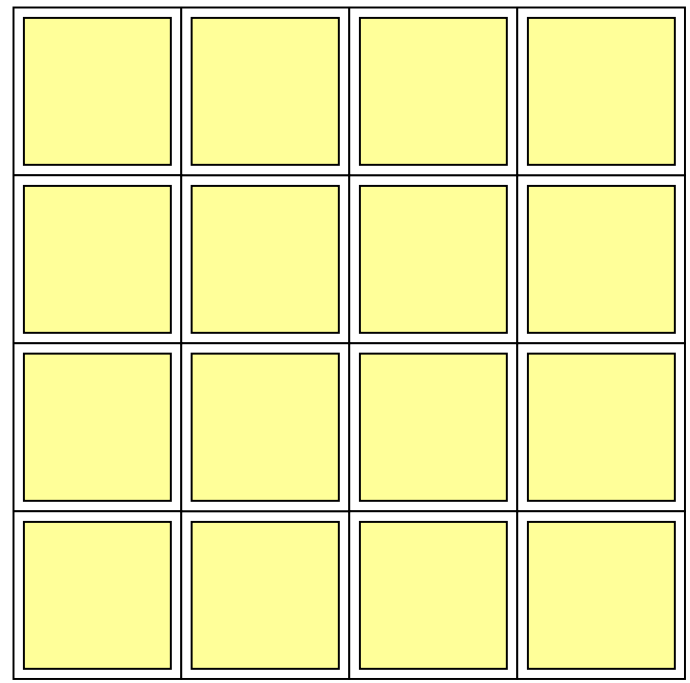
$$\frac{\mathrm{d}I}{\mathrm{d}\tau} = I - S$$

Analytic Solution:

$$I(\tau) = I_0 e^{\tau_0 - \tau} + \boxed{\int_{\tau_0}^{\tau} e^{\tau' - \tau} S(\tau') d\tau'}$$

Intrinsic Calculation

Processors



Ray direction

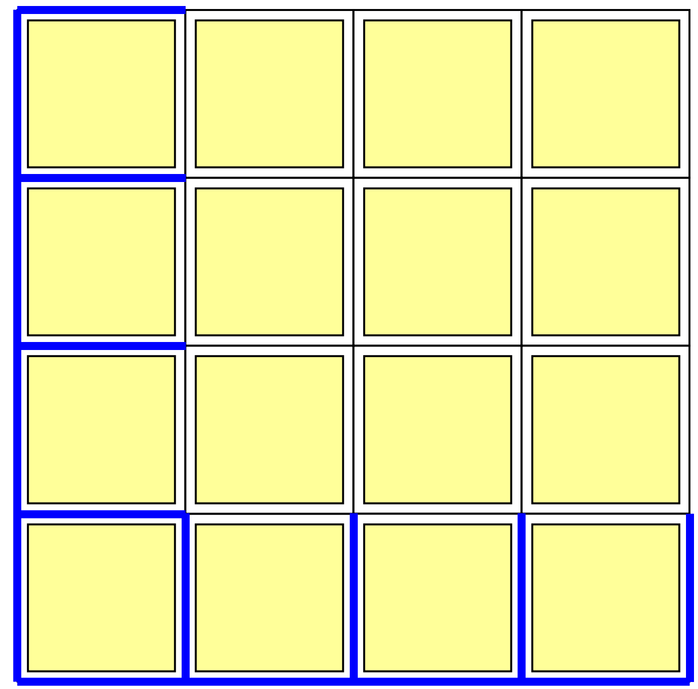
The Transfer Equation & Parallelization

Analytic Solution:

$$I(\tau) = \boxed{I_0 e^{\tau_0-\tau}} + \boxed{\int_{\tau_0}^{\tau} e^{\tau'-\tau} S(\tau')\,d\tau'}$$

Communication

Processors



Ray direction

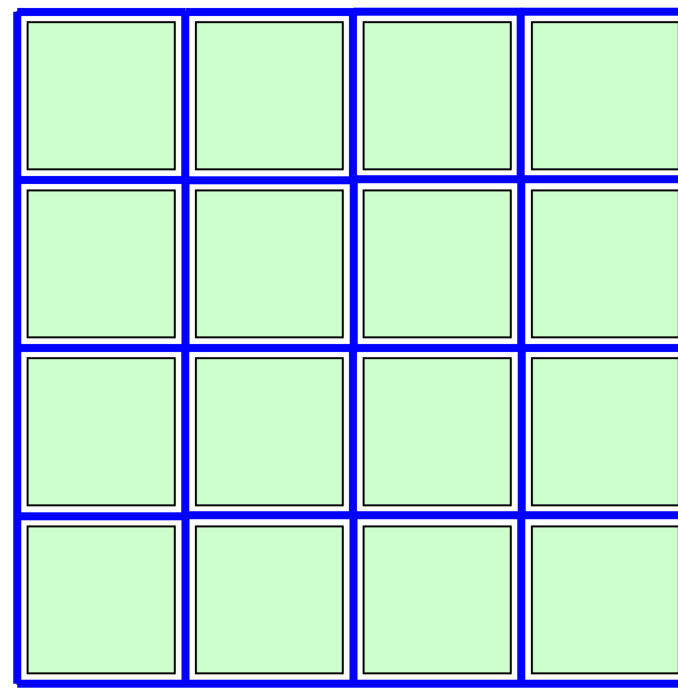
The Transfer Equation & Parallelization

Analytic Solution:

$$I(\tau) = \boxed{I_0 e^{\tau_0 - \tau} + \int_{\tau_0}^{\tau} e^{\tau' - \tau} S(\tau') d\tau'}$$

Intrinsic Calculation

Processors



Ray direction

Conclusions

- Advantage of high order
- Bottleneck real
- Boundary conditions easy to implement
- Online data analysis