

Solving PDEs by Pseudo Spectral Method

Basic Principle and Examples

Rupak Mukherjee

`rupakmukherjee06@gmail.com`

June 27, 2020

Basic Principle

$$u \approx U = \sum_k a_k \phi_k$$

$u \rightarrow$ exact, $U \rightarrow$ approximate.

a_k = Degrees of Freedom (dof) (Galerkin, Collocation, Continuous Galerkin (CG), Discontinuous Galerkin (DG), Penalty, Staggered Grid, Tau)

ϕ_k = Orthogonal Polynomial (Fourier, Legendre, Chebyshev)

Why, Where

WHY

- 1 Higher accuracy, fast convergence
- 2 Low # of dof for given accuracy
- 3 Low phase / dispersion error
- 4 Low dissipation error
- 5 Easy implementation of Boundary Condition (BC)
- 6 Efficient Parallalisation

WHERE

- 1 Detailed physics is needed (e.g. Turbulence)
- 2 Long time integration (dispersion and dissipation)

Model Problem

$$u_t + cu_x = 0, \quad x \in [0, 2\pi], \quad t > 0$$

Def:

Inner Product:

$$(u, v) = \int_0^{2\pi} uv^* dx$$

Fourier Galerkin (FG)

$$u = \sum_{k=-\infty}^{\infty} \hat{u}_k e^{ikx} \approx U = \sum_{k=-N/2}^{N/2} a_k e^{ikx}$$

$$\Rightarrow \sum_{k=-N/2}^{N/2} (\dot{a}_k + ikca_k) e^{ikx} = R$$

Project

$$\Rightarrow \left(\sum_{k=-N/2}^{N/2} (\dot{a}_k + ikca_k) e^{ikx}, e^{imx} \right) = (R, e^{imx})$$

$$\Rightarrow (\dot{a}_m + imca_m) 2\pi = (R, e^{imx}) = 0, \quad m = -N/2, \dots, N/2 \quad (\text{Galerkin})$$

$$\Rightarrow \dot{a}_k + ikca_k = 0 \quad \& \quad a_k(0) = \hat{u}_k(0)$$

RK4 / Leap Frog

Accuracy

Example: $u_0(x) = \sin(\pi(\cos(x)))$

N	FD-2	FD-4	FG
8	1.11	9.62×10^{-1}	9.87×10^{-2}
16	6.13×10^{-1}	2.36×10^{-1}	2.55×10^{-4}
32	1.99×10^{-1}	2.67×10^{-2}	1.05×10^{-11}
64	5.42×10^{-2}	1.85×10^{-2}	6.22×10^{-13}

Galerkin

Basis

$$\phi = \sum_{k=-N/2}^{N/2} c_k e^{ikx} \in \mathcal{P}_p^{N/2}$$

$\mathcal{P}_p^{N/2}$: Fourier Polynomial of Degree $N/2$

Galerkin

$$(U_t + cU_x, \phi) = 0; \quad \forall \phi \in \mathcal{P}_p^{N/2}$$

- Non-Linear Problems are tricky!

Variable Coefficient PDE

$$u_t + uu_x = \nu u_{xx}$$

- Will mix modes.
- Aliasing Error appears.
- Use Pseudospectral Method (Derivative in spectral space & multiplication in real space)
- For de-aliasing use $\frac{3}{2}$ padding instead of $\frac{2}{3}$ truncation.
- In fully developed turbulence, high frequencies; pump energy into low frequencies. Hence aliasing error changes physics.
- For smooth looking solution, use of cosmetic filtering is permitted.

Navier-Stokes Equation

Burgers Equation

$$\frac{\partial u(x, t)}{\partial t} + u(x, t) \frac{\partial u(x, t)}{\partial x} = \nu \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t)$$

- Initial Condition : $u(x, 0) = \sin(x)$, $\nu = 0 = f$
- $\nu \neq 0 \Rightarrow$ No Gibbs Oscillation
- $f \neq 0 \Rightarrow$ Intermittency

Simulation Method : Pseudo-Spectral

$$u(x, t)$$

$\downarrow FFT$

$$\widehat{u}_k(k, t) \xrightarrow{\text{Multiply}} ik * \widehat{u}_k(k, t) \xrightarrow{IFFT} \frac{du(x, t)}{dx} \rightarrow$$

$$\xrightarrow{\text{Multiply}} u(x, t) * \frac{du(x, t)}{dx} \xrightarrow{RK4} u(x, t + 1)$$

Burgers Equation with $\nu = 0$

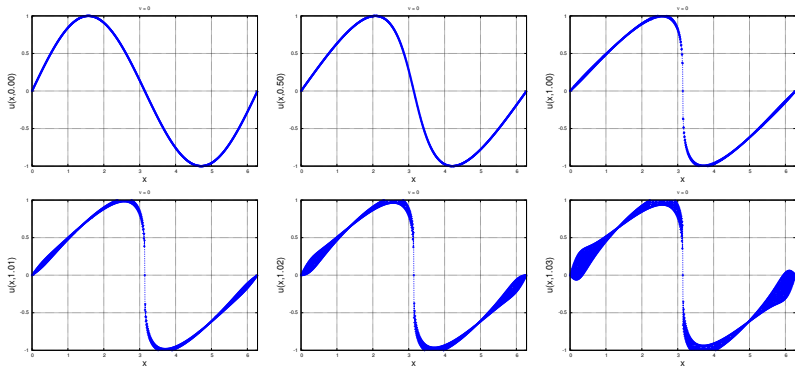


Figure: Compare with: Fig 1, PRE, 84, 016301, Fig 1, PNAS, 97, 12413

- Can be simulated better with WENO schemes!
- "Tygers" are the artificial effect of Galerkin truncation. Hence will not appear in any FD based scheme!

Burgers Equation with $\nu = 0$

Parameters: $N = 2^{14}$, $L = 2\pi$, $dt = 10^{-6}$, $\nu = 0$

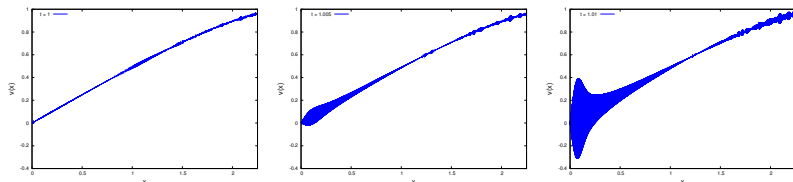


Figure: The occurrence of “tiger” after the generation of shock at time (a) $t = t^* = \frac{1}{\max|\frac{du_x}{dx}|_{t=0}} = 1$, (b) $t = 1.005$ and at (c) $t = 1.01$.

Burgers Equation with $\nu \neq 0$

Compare with: Fig 11, Pramana, 73, 1, 2009

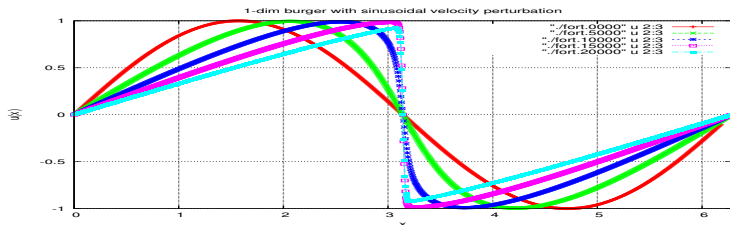


Figure: Parameters: $N = 2^{10}$, $L = 2\pi$, $dt = 10^{-3}$, $\nu = 10^{-2}$

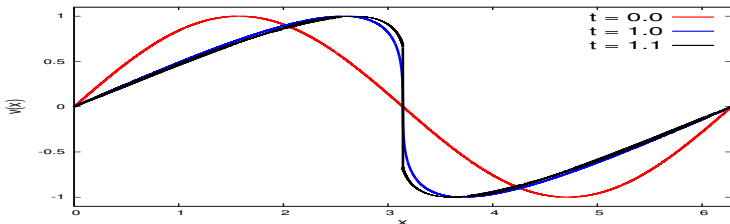


Figure: Parameters: $N = 2^{14}$, $L = 2\pi$, $dt = 10^{-6}$, $\nu = 10^{-6}$

Burgers Equation with $\nu \neq 0$

- Energy Spectra should follow a power law with slope $\frac{1}{k^2}$

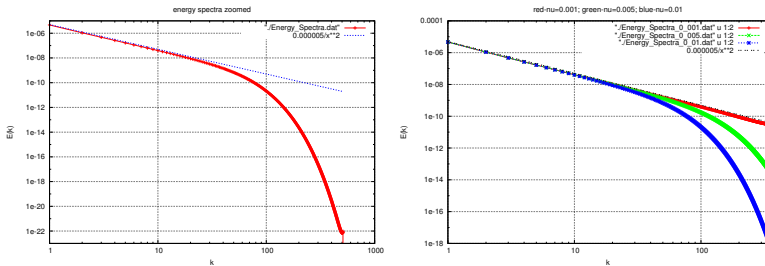


Figure: a. with zero viscosity, b. with different viscosity, Fig 12, Pramana, 73, 1, 2009

- Viscosity acts on higher modes of wavenumber i.e. in small scales.

Homework - 1 [Structure Factor]

Order-P Velocity Correlation Function

$$S_p(\ell) = \langle [v(x + \ell) - v(x)]^p \rangle$$

where $v(x)$ is the velocity at the point x and the angular brackets denote and average over the statistical steady state of the turbulent fluid.

For ℓ in inertial range, $S_p(\ell) \sim \ell^{\xi_p}$
for small Δx ,

$$S_p(\Delta x, t) \sim C_p |\Delta x|^p + C'_p |\Delta x|$$

For $p < 1$, the first term dominates and for $p > 1$ the second term.

Reference: "Burgulence", Uriel Frisch, Jeremie Bec, arXiv: nlin/0012033v2 (2001)

Homework - 1 [Structure Factor]

Order-P Velocity Correlation Function

Parameters: $N = 2^{14}$, $L = 2\pi$, $dt = 10^{-6}$, $\nu = 10^{-6}$

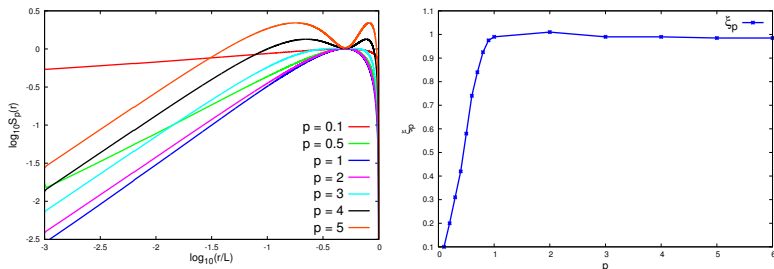
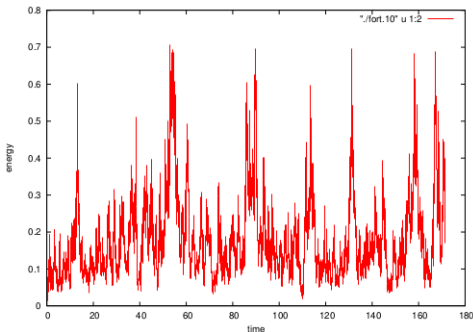


Figure: Compare with: Fig 1(b), 2(a), PRL, 94, 194501

Homework - 2 [Burgers Equation with $f \neq 0$]

- Forcing :: Gaussian random noise with zero mean and Fourier-space Spectrum $\sim \frac{1}{k}$
- One should observe intermittency.



Homework - 2 [Burgers Equation with $f \neq 0$]

The order- p velocity structure function looks like,
(Parameters: $N = 2^{10}$, $L = 2\pi$, $\nu = 10^{-2}$)

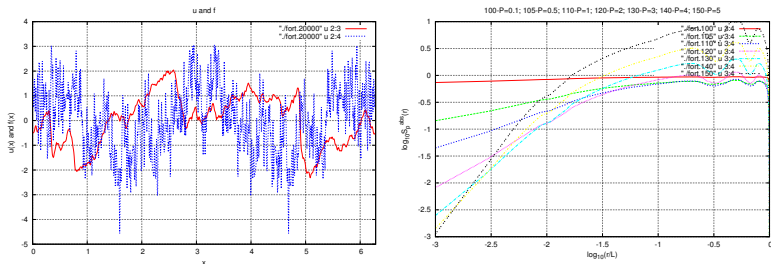


Figure: Compare with: Fig 1(a), (c), PRL, 94, 194501

A nuclear fusion meme by Shawn Zamperini.

1D modellers when they're
forced to use 2D codes



Incompressible Navier-Stokes Equation

Basic Equations

$$\frac{\partial \vec{\omega}}{\partial t} + \vec{u} \cdot \vec{\nabla} \vec{\omega} = \nu \nabla^2 \vec{\omega}$$
$$\vec{\omega} = \vec{\nabla} \times \vec{u}$$

In Two dimensions

$$\vec{\omega} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \times (u_x, u_y, 0) = \left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \right) \vec{z}$$

Simulation Method

Pseudocode : Pseudo-Spectral Method

$$\omega(x, y) \xrightarrow{\text{FFT}} \hat{\omega}(k_x, k_y) \text{ [at time = } t]$$

\Downarrow

$$\hat{\psi} = \frac{\hat{\omega}}{k_x^2 + k_y^2}$$

$$\hat{u}_x = ik_y \hat{\psi}, \hat{u}_y = -ik_x \hat{\psi}$$

$$ik_x \hat{\omega}, ik_y \hat{\omega}$$

\Downarrow IFFT

$$u_x, u_y$$

$$\frac{\partial \omega}{\partial x} = \mathcal{IF}[ik_x \hat{\omega}]$$

$$\frac{\partial \omega}{\partial y} = \mathcal{IF}[ik_y \hat{\omega}]$$

\Downarrow

$$u_x \cdot \frac{\partial \omega}{\partial x}, u_y \cdot \frac{\partial \omega}{\partial y}$$

\Downarrow FFT

Simulation Method cont.

Pseudocode : Pseudo-Spectral Method

$$\begin{aligned} & \Downarrow \text{FFT} \\ NLkx &= \widehat{u_x \cdot \frac{\partial \omega}{\partial x}}, NLky = \widehat{u_y \cdot \frac{\partial \omega}{\partial y}} \\ & \Downarrow \text{De-Aliased (2/3 rule)} \\ NLk &= NLkx + NLky + \nu \cdot (k_x^2 + k_y^2) \hat{\omega} \\ & \Downarrow \\ \frac{\partial \hat{\omega}}{\partial t} &= -NLk \\ & \Downarrow \text{RK(4)} \\ \hat{\omega}(k_x, k_y) & \text{ [at time = } t+dt] \end{aligned}$$

A quick visual

Initial Condition

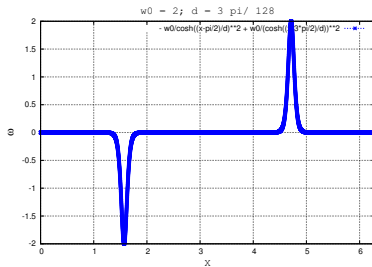
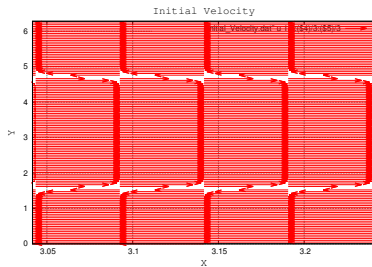


Figure: Vorticity



Velocity

- $\nu = 0.0001$

Movie in the weekend?

KH Instability

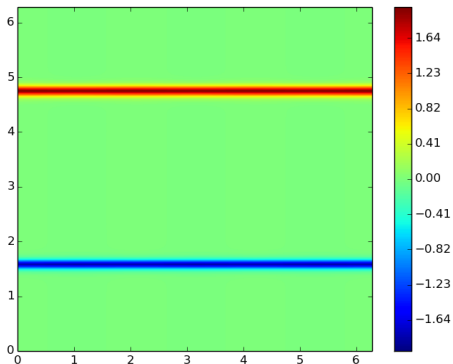
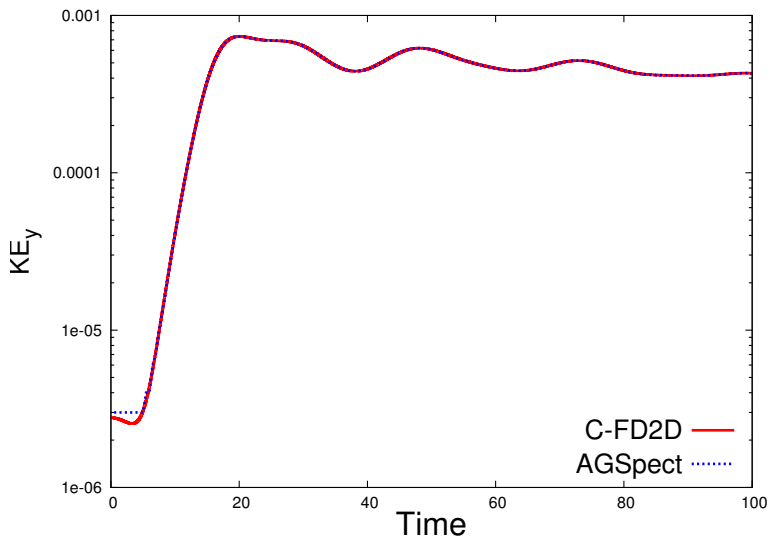


Figure: KH Instability for Incompressible Flow

KH Instability and its nonlinear saturation

Growth Rate Comparison; $k = 3$



Homework - 3

Analytical Growth Rate for a Broken Jet

P G Drazin, Journal of Fluid Mechanics, **10**, 579 (1961): *Eqn: 43*

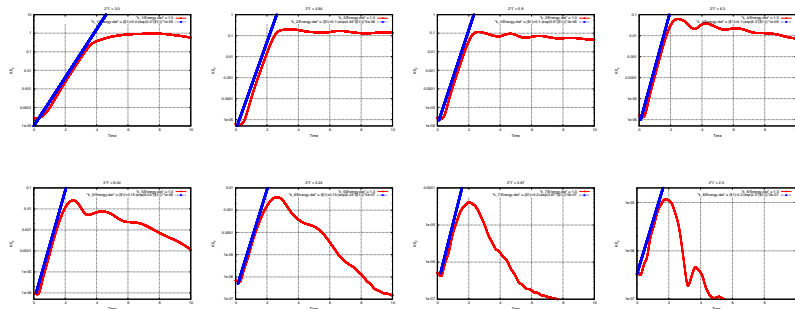
$$\gamma = \frac{k_x U_0}{3} \left[\sqrt{3} - 2 \frac{k_x}{R_E} - 2 \left\{ \left(\frac{k_x}{R_E} \right)^2 + 2\sqrt{3} \frac{k_x}{R_E} \right\}^{\frac{1}{2}} \right]$$

$$R_E = \frac{U_0 d}{\nu}$$

d = Shearing Length

Homework - 3

Numerical Growth Rate - How do you fit these curves?



- $L_x = L_y = 2\pi$; $\omega_0 = 25$; $d = \frac{3\pi}{128}$; $\nu = 0.0015$

Homework - 3

Compare the Growth Rates!

