A Parallel Pseudo-spectral Solver Tarang for Turbulence and Stability Simulations

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http://turbulence.phy.iitk.ac.in

Example:
Fluid solver

velocity field

Pressure

Ext. Force

$$\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{F}$$

kinematic viscosity

$$\nabla\cdot\mathbf{u} = 0$$

Incompressibility

Reynolds no = $\frac{UL}{\nu}$

Set of ODEs

$$\frac{du_i(\mathbf{k})}{dt} = -jk_m \widehat{u_m(\mathbf{r})u_i(\mathbf{r})} - jk_i p(\mathbf{k}) - \nu k^2 u_i(\mathbf{k})$$

Time advance (e.g., Euler's scheme)

$$u_i(\mathbf{k}, t+dt) = u_i(\mathbf{k}) + dt \times \mathrm{RHS}_i(\mathbf{k}, t)$$

Stiff equation for small viscosity ν (use exponential trick)

Nonlinear terms computation:

$\mathbf{u}(\mathbf{k}) \rightarrow \mathrm{IFT}(\mathbf{u}(\mathbf{r})) \rightarrow u_l(\mathbf{r}) u_i(\mathbf{r}) \rightarrow \mathrm{FT}(u_l(\mathbf{r}) u_i(\mathbf{r})) \rightarrow j\, k_l\, \mathrm{FT}(u_l(\mathbf{r}) u_i(\mathbf{r}))$

(pseudo-spectral)

Fourier transforms take around 80% of total time.

Code parallelization

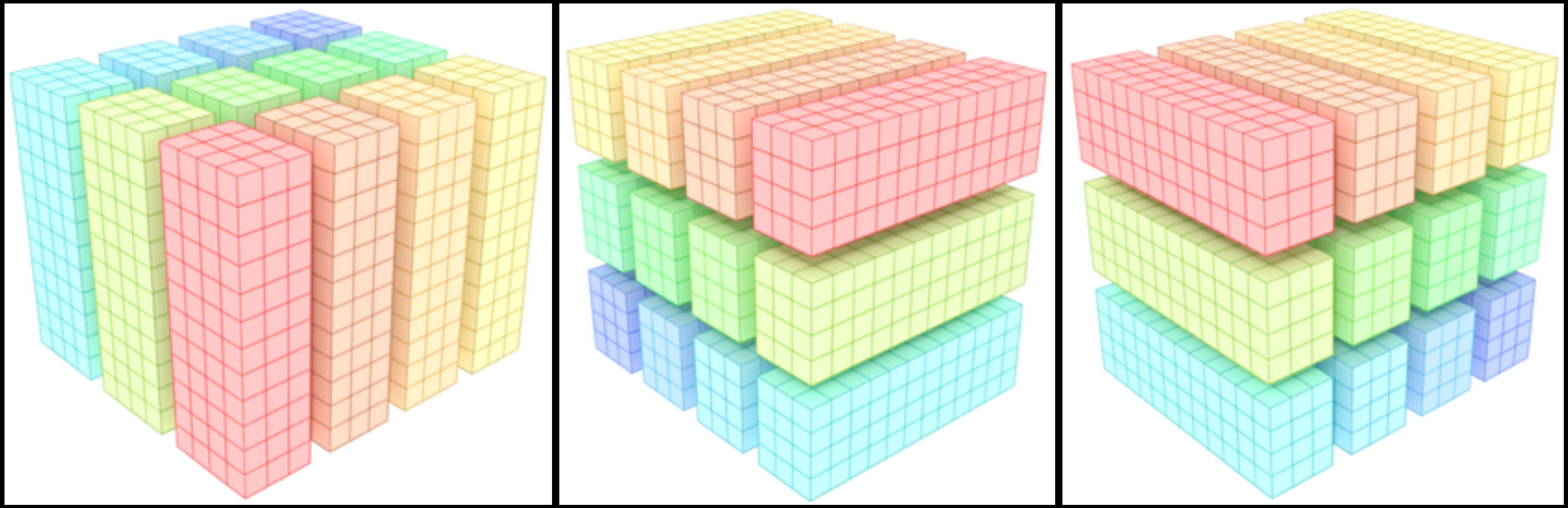
Spectral Transform
(FFT, SFT, Chebyshev)

Multiplication in real space

Input/Output
HDF5 lib

FFT Parallelization

Pencil Decomposition



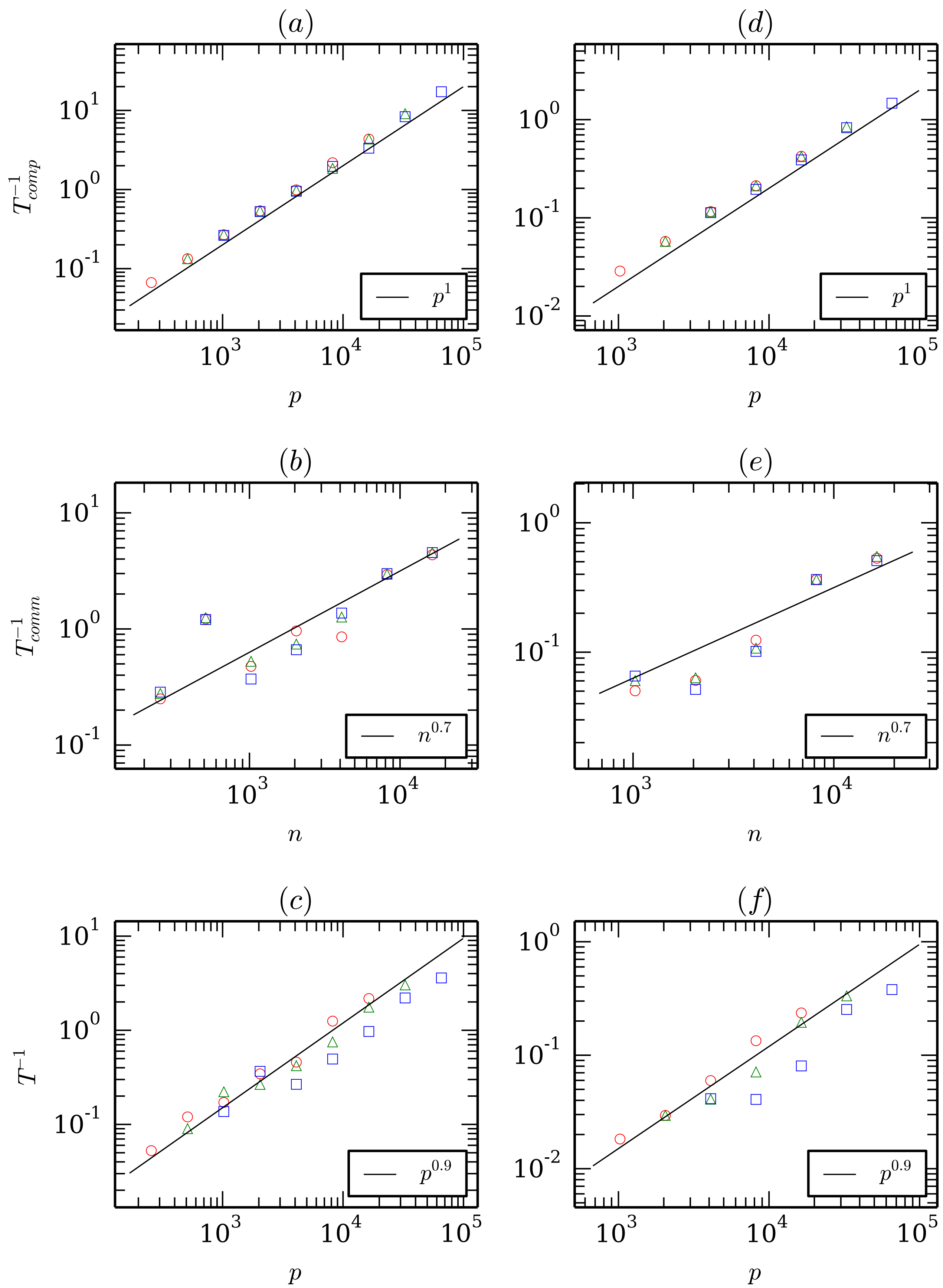
Average flop rating/core

0.6 GF
(~8%)

Overlap Communication & Computation

GPUs ??

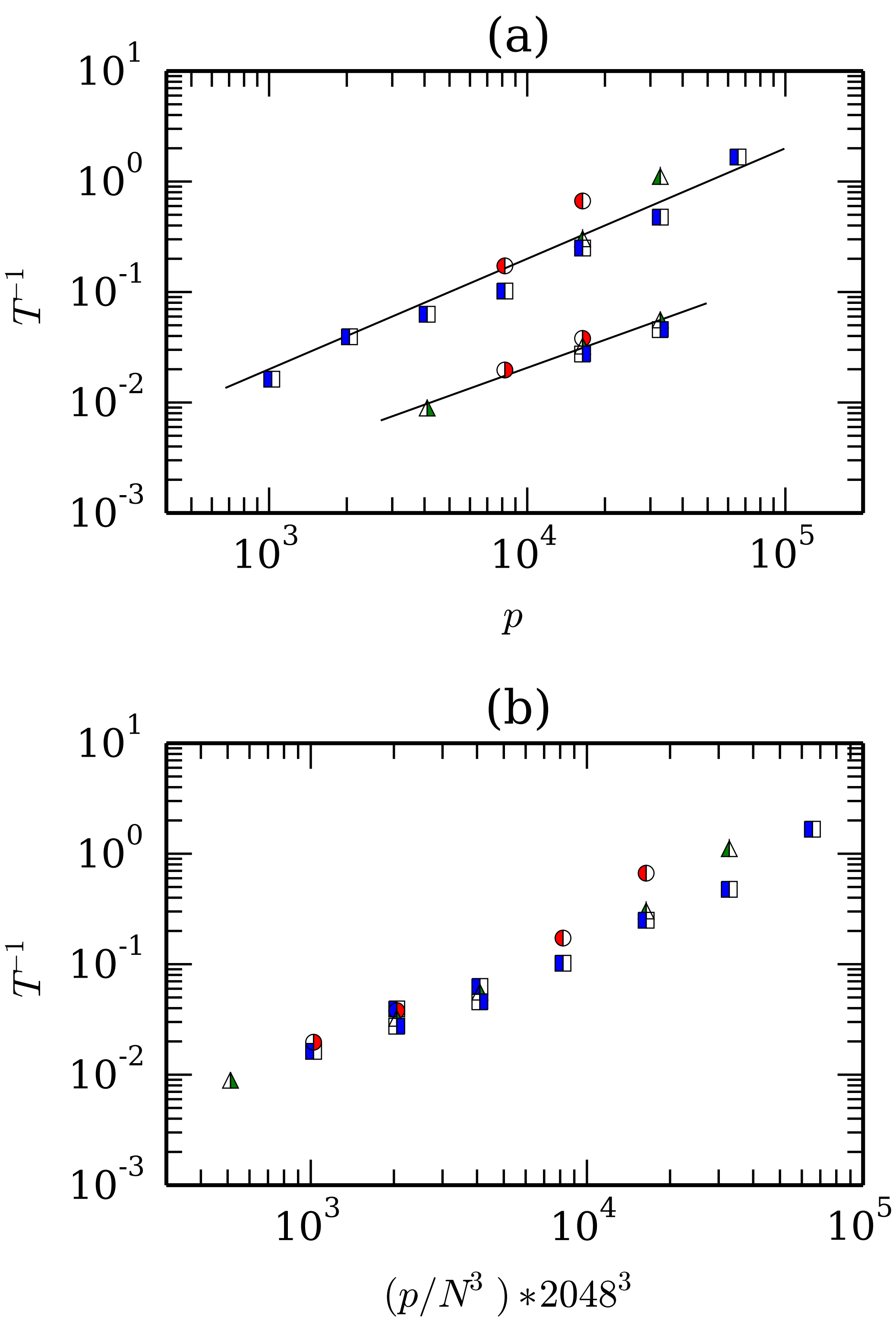
Xeon Phi ??



(a)
(b)
(c)
(d)
(e)
(f)
T^{-1}_{comp}
T^{-1}_{comm}
T^{-1}
p
n
p^1
$n^{0.7}$
$p^{0.9}$

Tarang scaling

On Shaheen at KAUST



(a)
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
T^{-1}
10^3
10^4
10^5
p
(b)
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
T^{-1}
10^3
10^4
10^5
$(p/N^3)*2048^3$

Tarang Design

Tarang = wave (Sanskrit)

Spectral code (Orszag)

One code to do many
turbulence & instabilities problems

VERY HIGH RESOLUTION (4096^3)

Opensource, download from
http://turbulence.phy.iitk.ac.in/downloads/

Verma et al., Pramana, 2013

Basis functions (FFF, SFF, SSF, SSS, ChFF)

Basis-independent universal function

e.g., compute_nlin $(u. \nabla)u$,
$(b. \nabla)u$, $(b. \nabla)b$, $(u. \nabla)T$.

General PDE solver

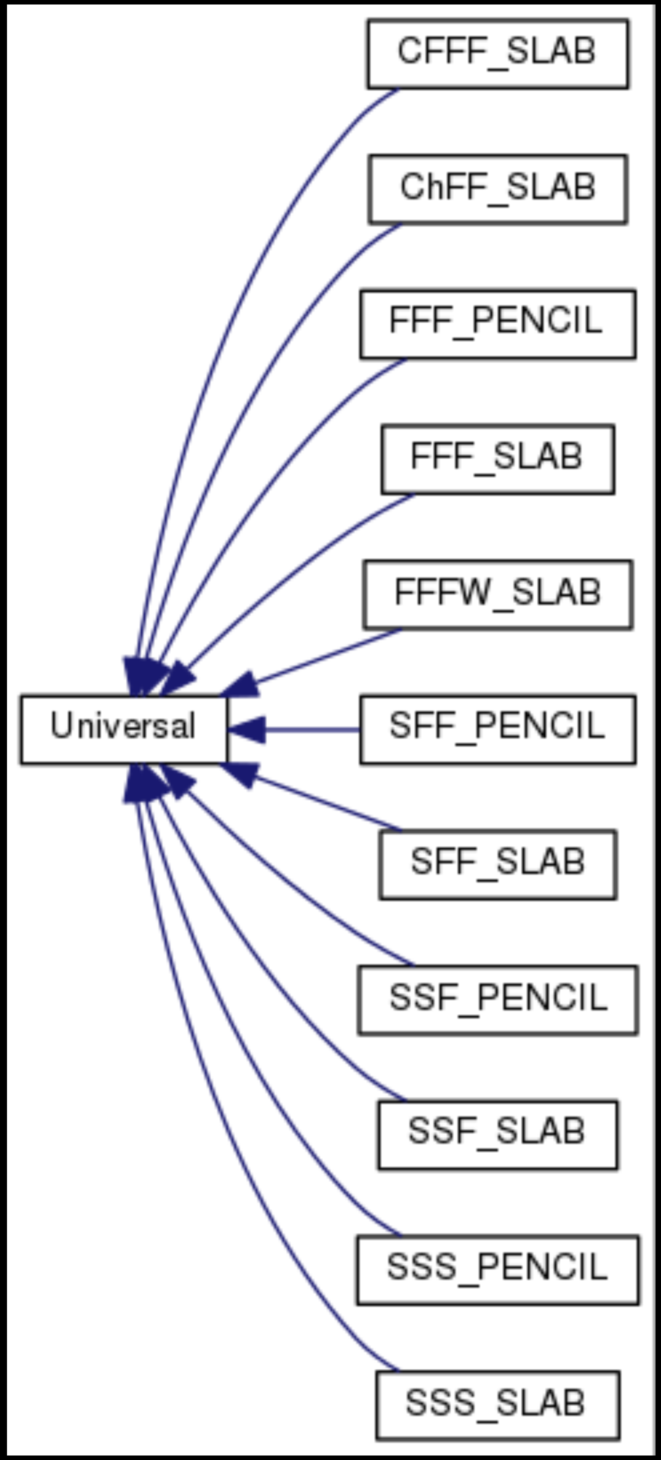
We can use these general functions to simulate
MHD, convection etc.

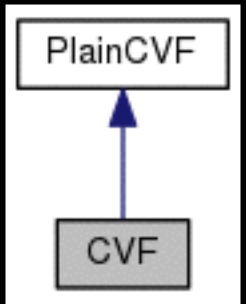
Fluid
MHD, Dynamo
Scalar
Rayleigh-Bénard convection
Stratified flows
Rayleigh-Taylor flow
Liquid metal flows
Rotating flow
Rotating convection

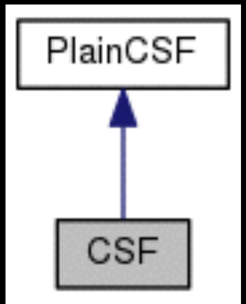
Instabilities
Chaos
Turbulence

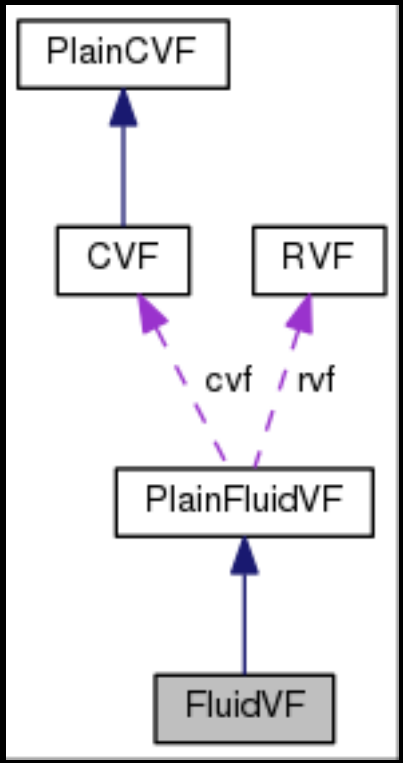
No-slip BC
Cylinder
sphere
Toroid
(in progress)

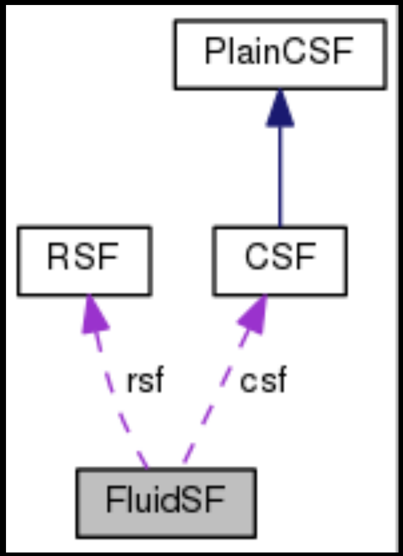
Periodic BC
Free-slip BC

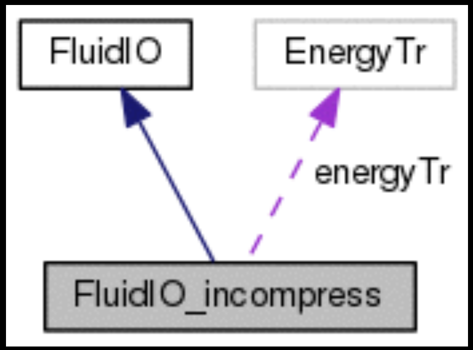

CFFF_SLAB
ChFF_SLAB
FFF_PENCIL
FFF_SLAB
FFFW_SLAB
Universal
SFF_PENCIL
SFF_SLAB
SSF_PENCIL
SSF_SLAB
SSS_PENCIL
SSS_SLAB

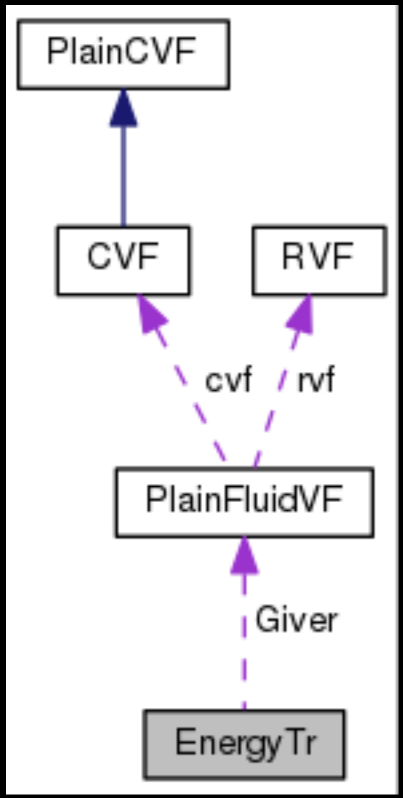

PlainCVF
CVF


PlainCSF
CSF


PlainCVF
CVF
RVF
cvf
rvf
PlainFluidVF
FluidVF


PlainCSF
RSF
CSF
rsf
csf
FluidSF


FluidIO
EnergyTr
energyTr
FluidIO_incompress


PlainCVF
CVF
RVF
cvf
rvf
PlainFluidVF
Giver
EnergyTr

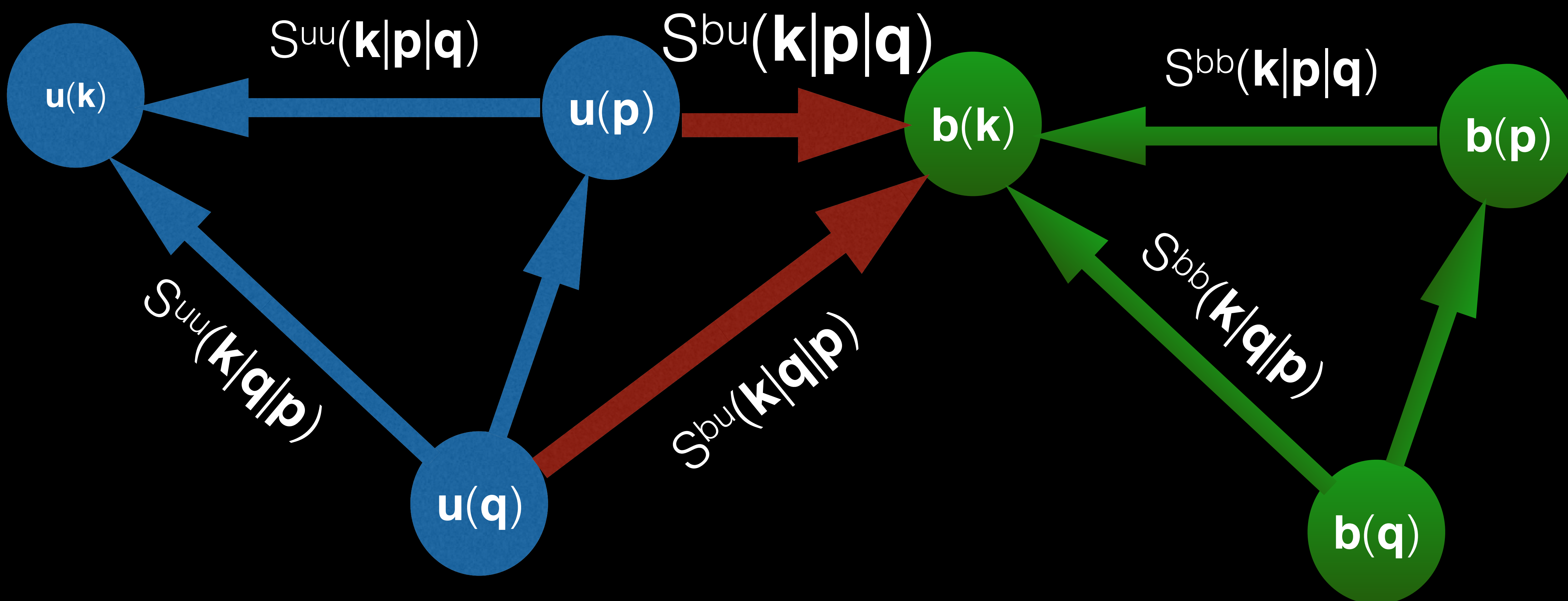
Rich libraries to compute
Spectrum
Fluxes
Shell-to-shell transfer
Structure functions

New things
Fourier modes
Real space probes
Ring-spectrum
Ring-to-ring transfer

Tested up to 4096^3 grids

Energy transfers
in MHD turbulence

ET in MHD



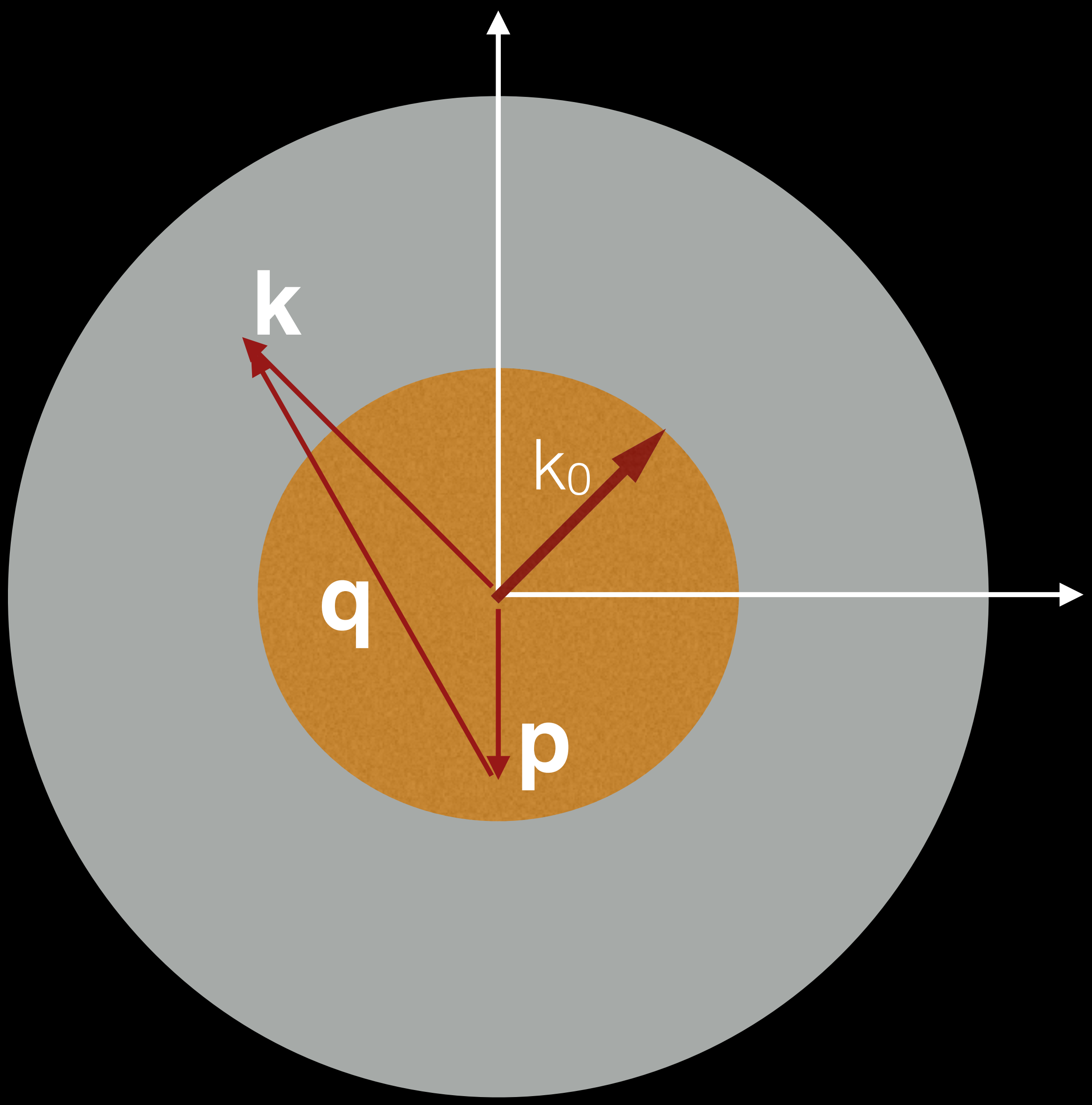
Helper Giver Receiver

$$S^{uu}(\mathbf{k}|\mathbf{p}|\mathbf{q}) = \mathrm{Im}\{[(\mathbf{k}\cdot\mathbf{u}(\mathbf{q})][(\mathbf{u}(\mathbf{p})\cdot\mathbf{u}^*(\mathbf{k})]\}$$

$$S^{bb}(\mathbf{k}|\mathbf{p}|\mathbf{q}) = \mathrm{Im}\{[(\mathbf{k}\cdot\mathbf{u}(\mathbf{q})][(\mathbf{b}(\mathbf{p})\cdot\mathbf{b}^*(\mathbf{k})]\}$$

$$S^{bu}(\mathbf{k}|\mathbf{p}|\mathbf{q}) = -\mathrm{Im}\{[(\mathbf{k}\cdot\mathbf{b}(\mathbf{q})][(\mathbf{u}(\mathbf{p})\cdot\mathbf{b}^*(\mathbf{k})]\}$$

Flux in MHD

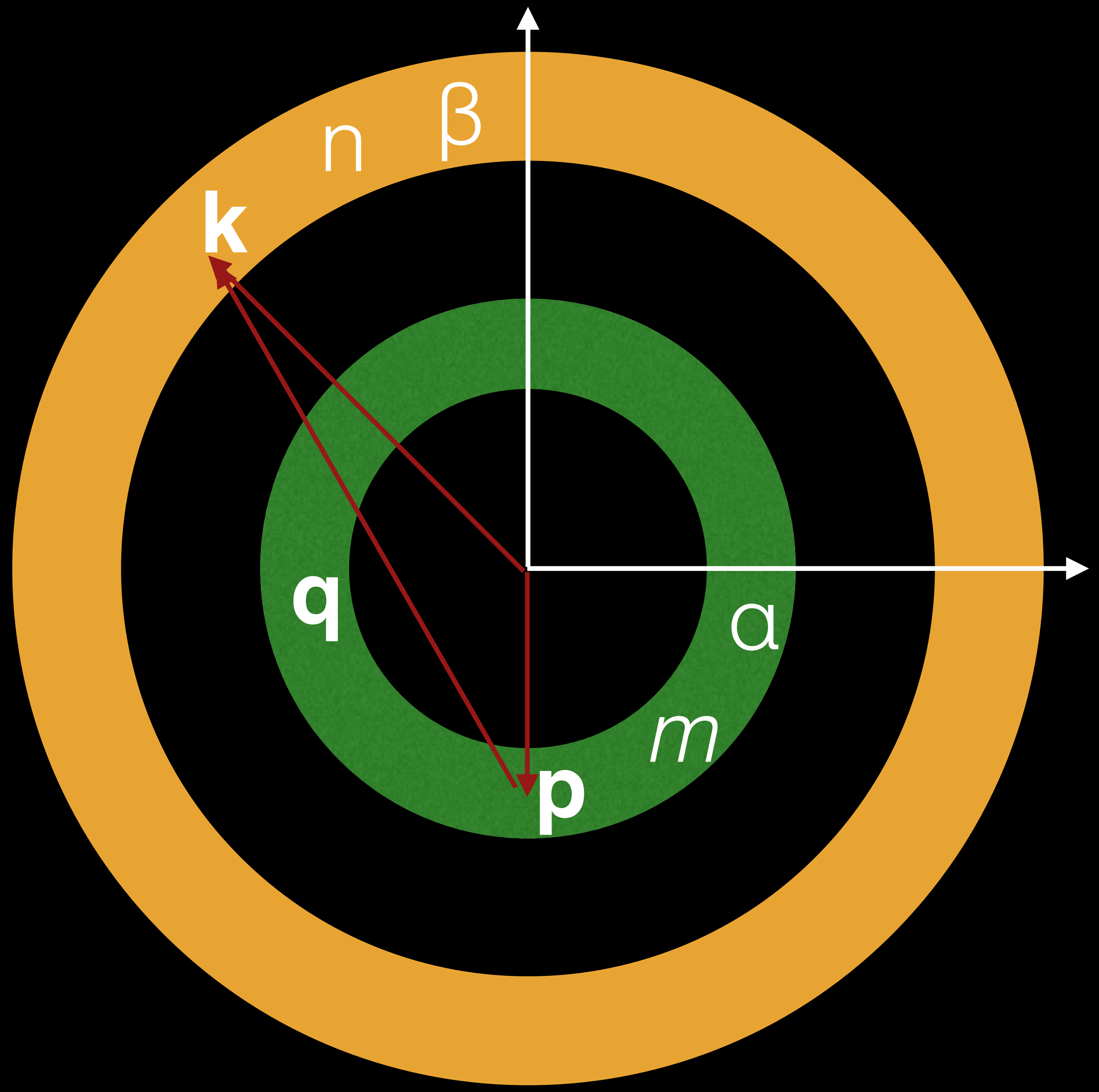


$$\Pi^{uu}(\mathbf{k}_0) = \sum_{p<k_0} \sum_{k>k_0} S^{uu}(\mathbf{k}\,|\,\mathbf{p}\,|\,\mathbf{q})$$

$$\Pi^{bb}(\mathbf{k}_0) = \sum_{p<k_0} \sum_{k>k_0} S^{bb}(\mathbf{k}\,|\,\mathbf{p}\,|\,\mathbf{q})$$

$$\Pi^{bu}(\mathbf{k}_0) = \sum_{p<k_0} \sum_{k>k_0} S^{bu}(\mathbf{k}\,|\,\mathbf{p}\,|\,\mathbf{q})$$

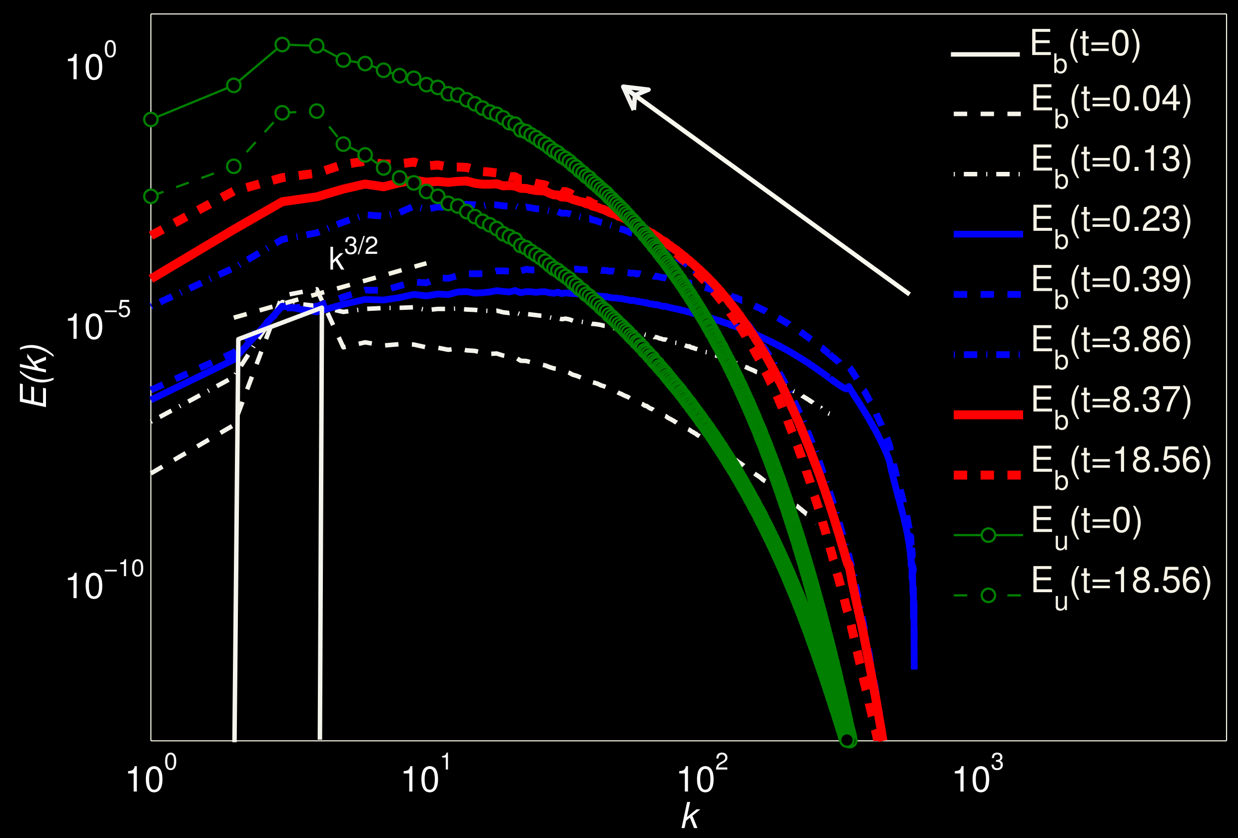
Shell-to-shell ET

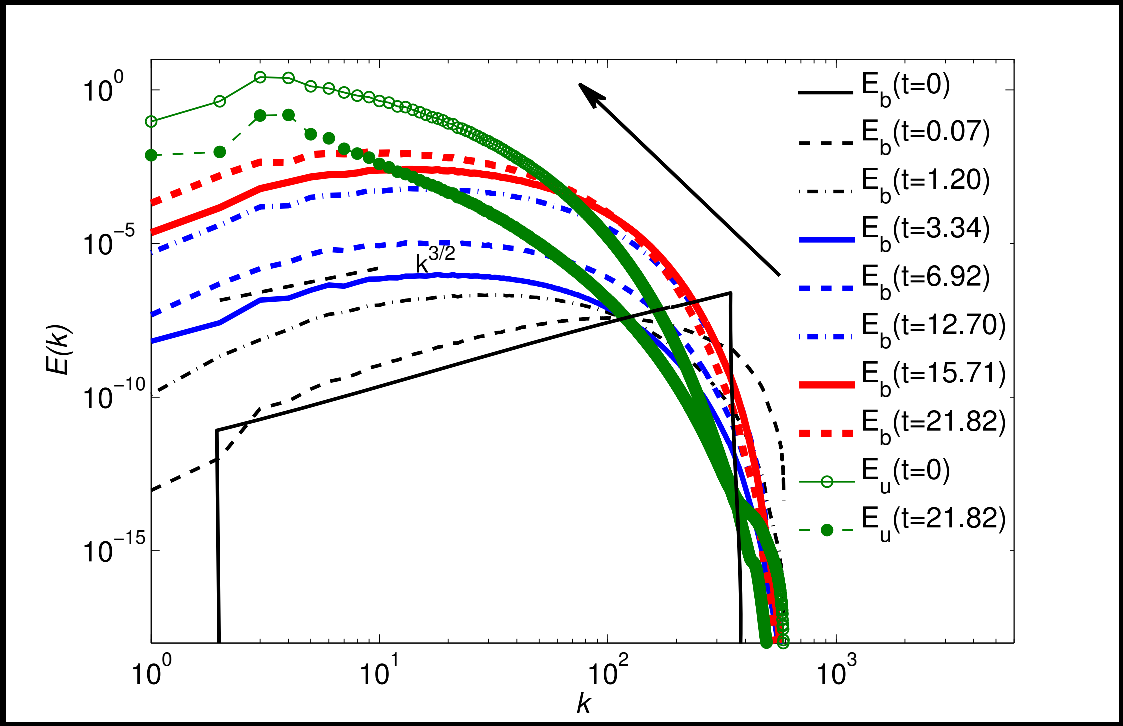


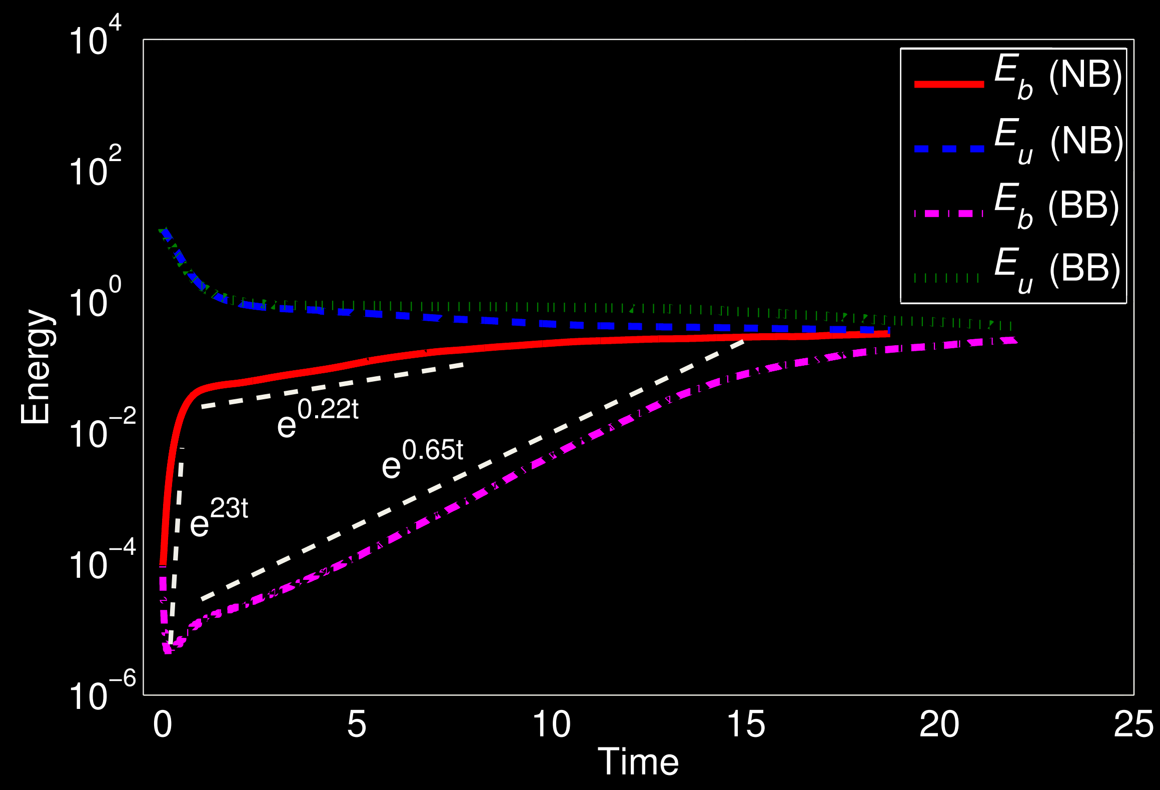
$$T_{\beta,n}^{\alpha,m} = \sum_{p \in m} \sum_{k \in n} S^{\beta\alpha}(\mathbf{k} \mid \mathbf{p} \mid \mathbf{q})$$

Narrow band (NB)

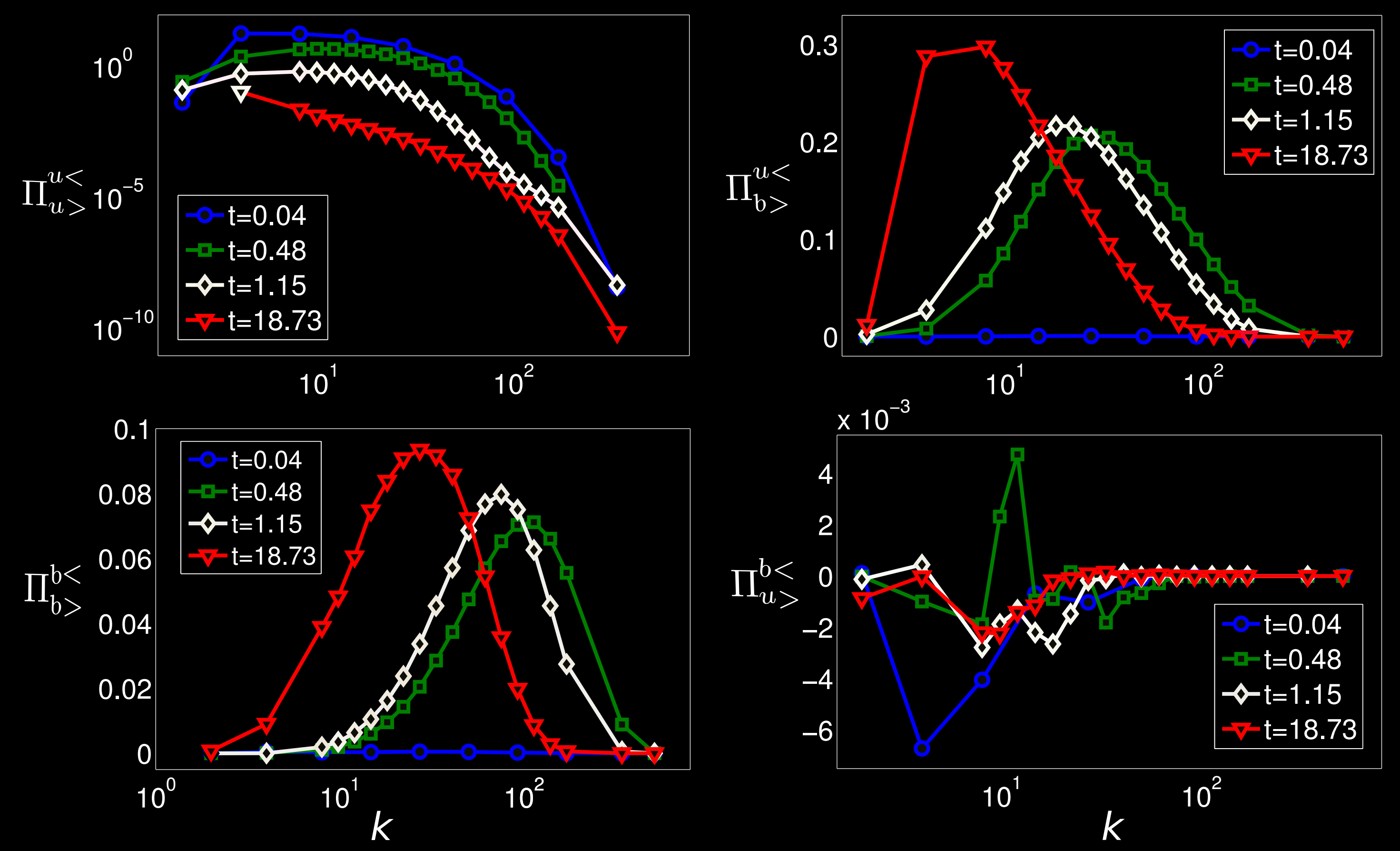
Broad band (NB)



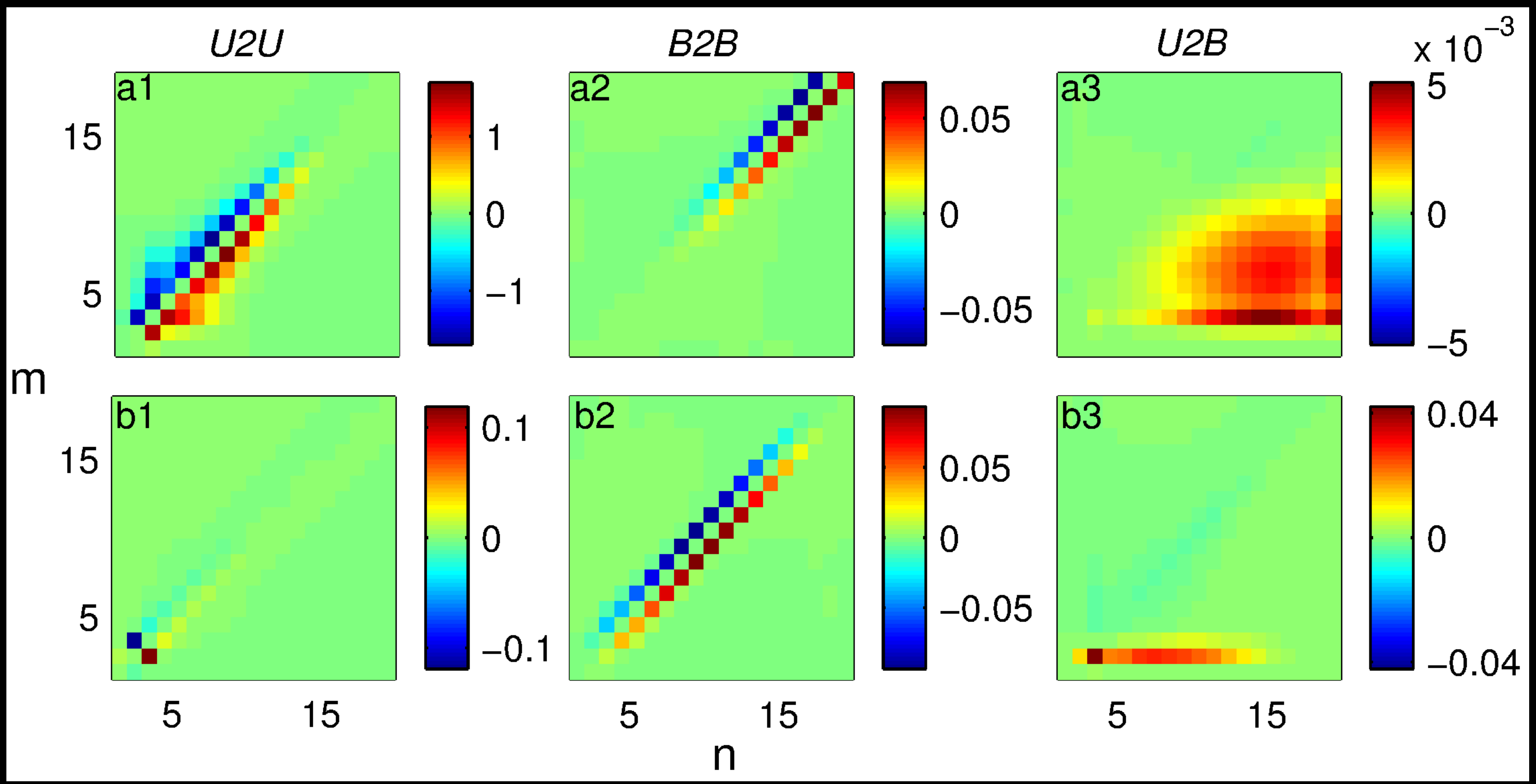




Flux



Shell-to-shell transfer



Tarang team

Anando Chatterjee

Abhishek Kumar

Ravi Samtaney

Mainak Chaudhuri

Ex members:

Supriyo Paul

Mani Chandra

Rakesh Yadav

Sandeep Reddy

Pankaj Mishra

Vijay

Sumit Kumar

Examples

Energy spectrum of stably-stratified flows and Rayleigh Benard convection

Kumar, Chatterjee, Verma, PRE 2014

Stably stratified flows
Simulation results

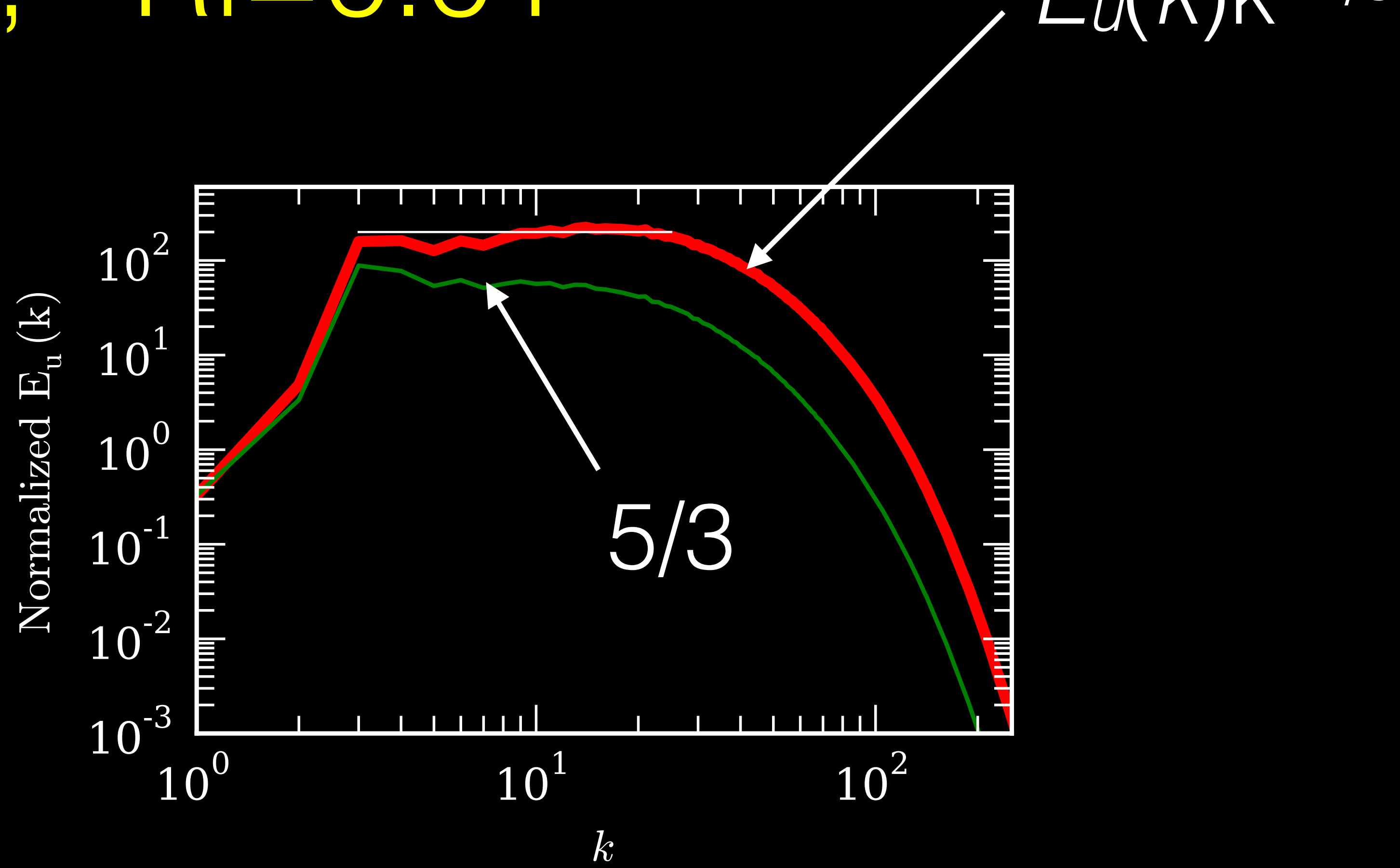
Pr=1

Forcing the VELOCITY field
(Random)

Periodic BC $(\mathbf{u},\theta)$

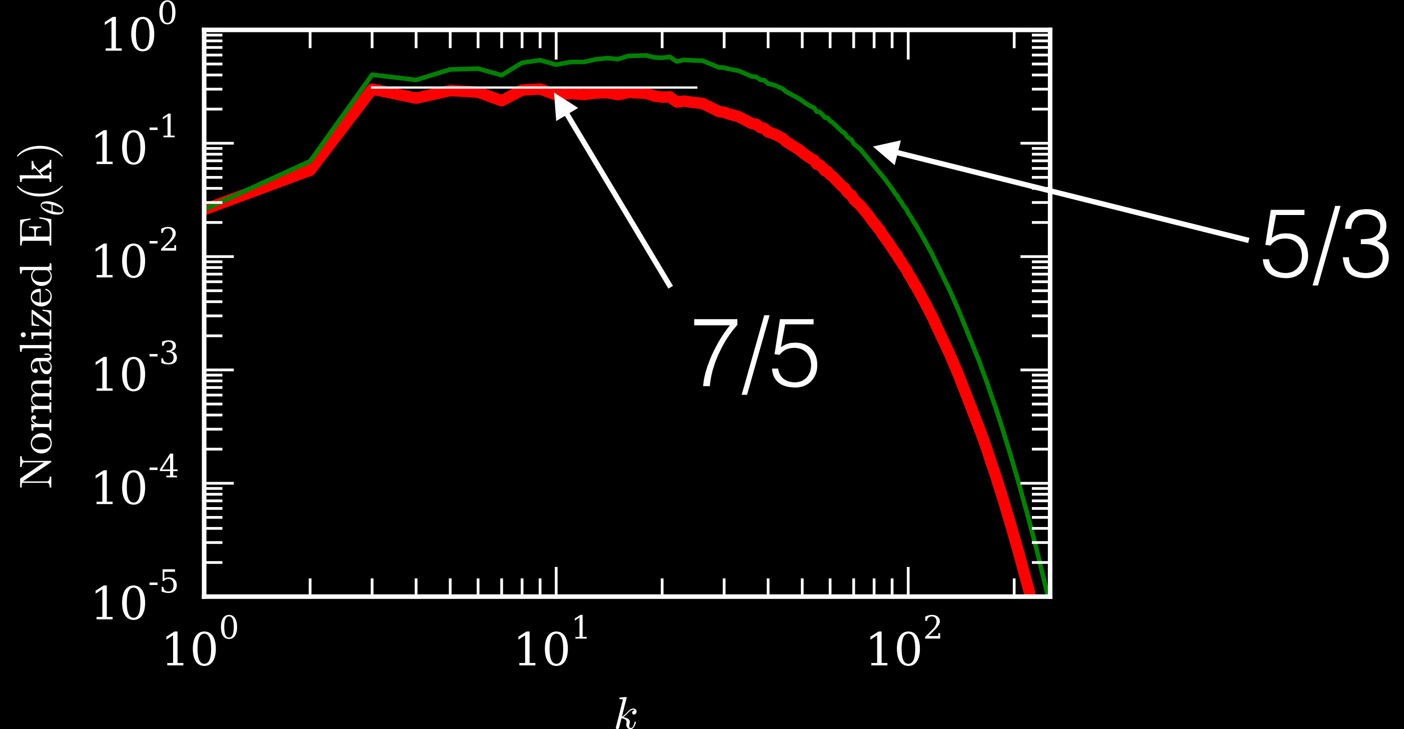
Fr=10; Ri=0.01

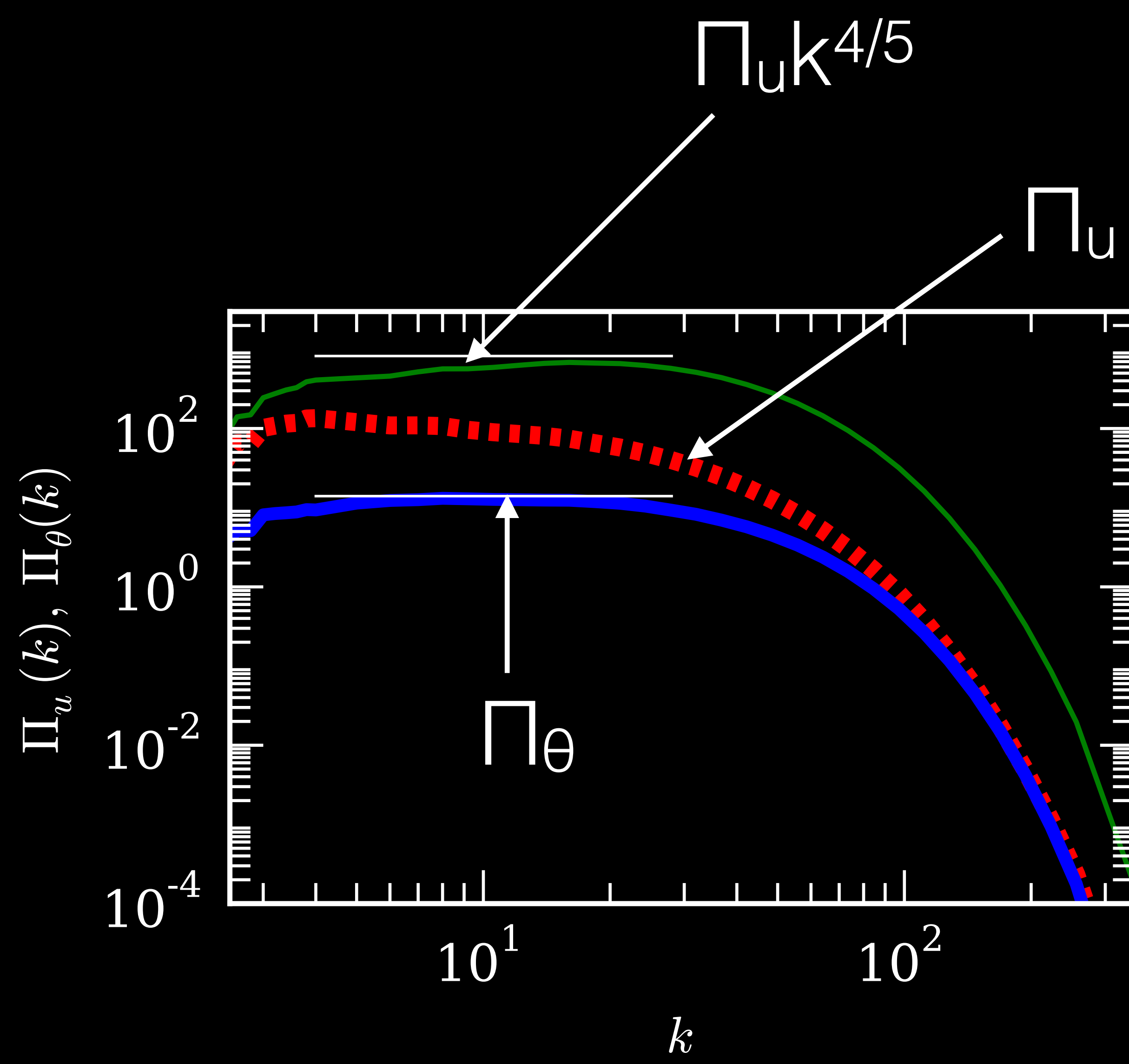
$E_u(k)$



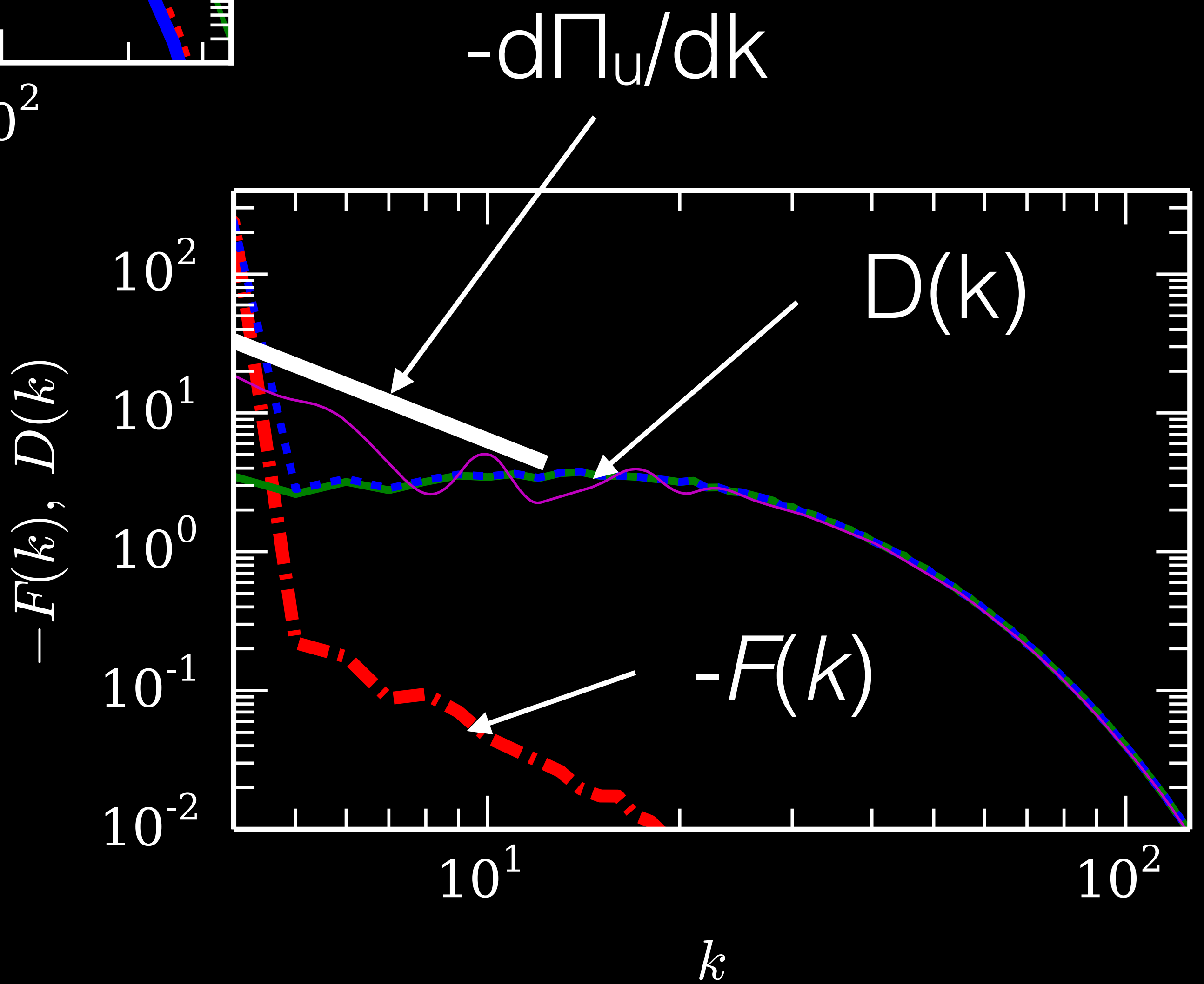
BO fits BETTER

$E_\theta(k)$





$\Pi_u k^{4/5}$
Π_u
Π_θ
10^2
10^0
10^{-2}
10^{-4}
10^1
10^2
k
$\Pi_u(k),\ \Pi_\theta(k)$



$-d\Pi_u/dk$
D(k)
$-F(k)$
10^2
10^1
10^0
10^{-1}
10^{-2}
10^1
10^2
k
$-F(k),\ D(k)$

RBC
Simulation results

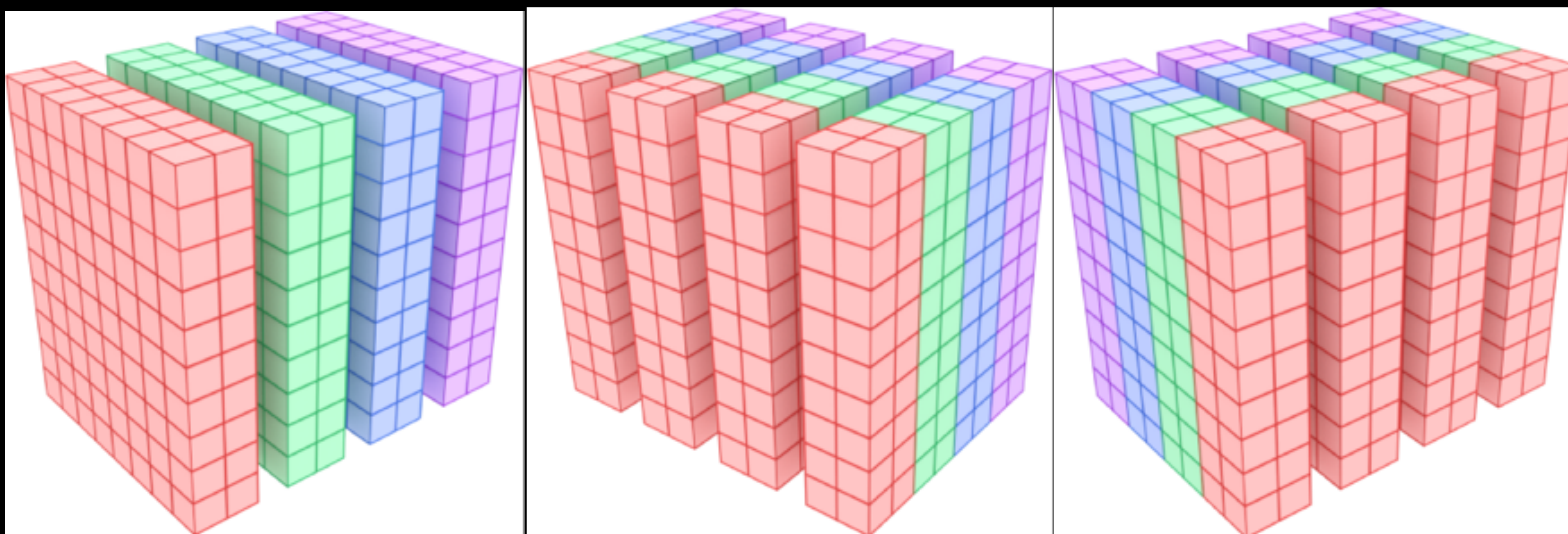
Pr=1

Free-slip BC

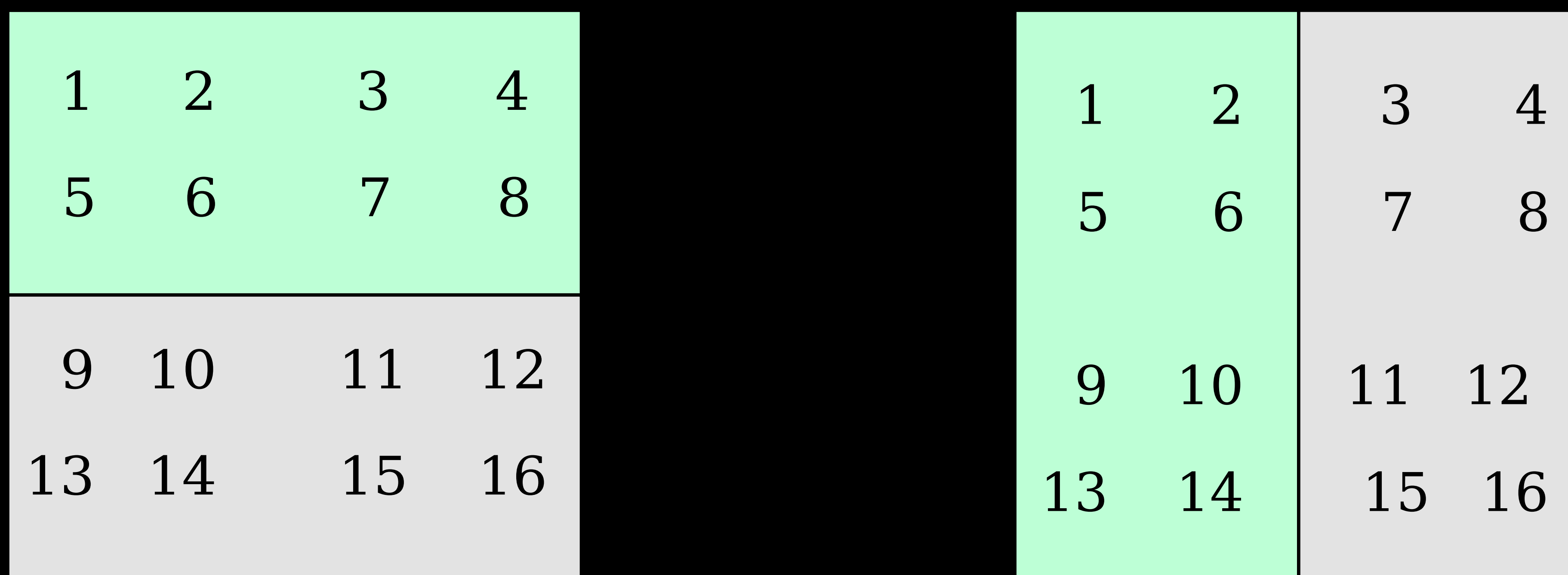
$$u_z = 0$$
$$\partial_z u_x = \partial_z u_y = 0$$

Conducting plates $\theta = 0$

Slab decomposition

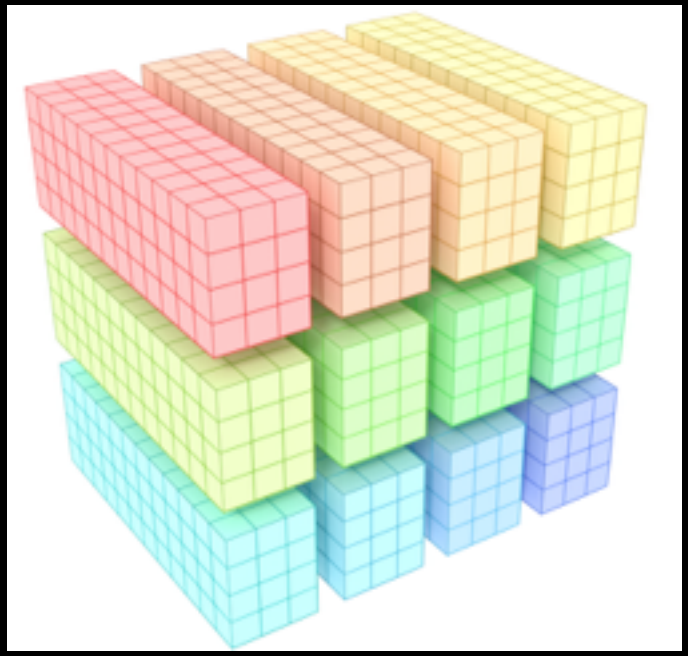


Transpose-free FFT

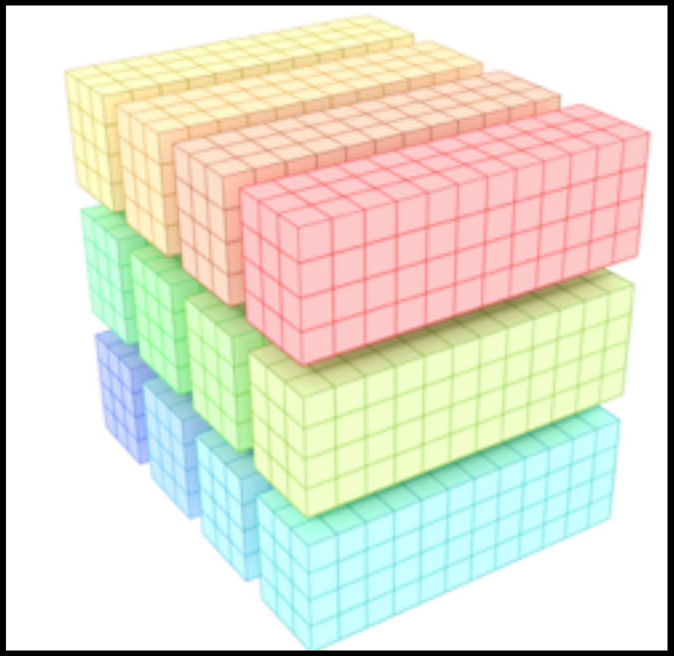


12-15% faster compared to FFTW

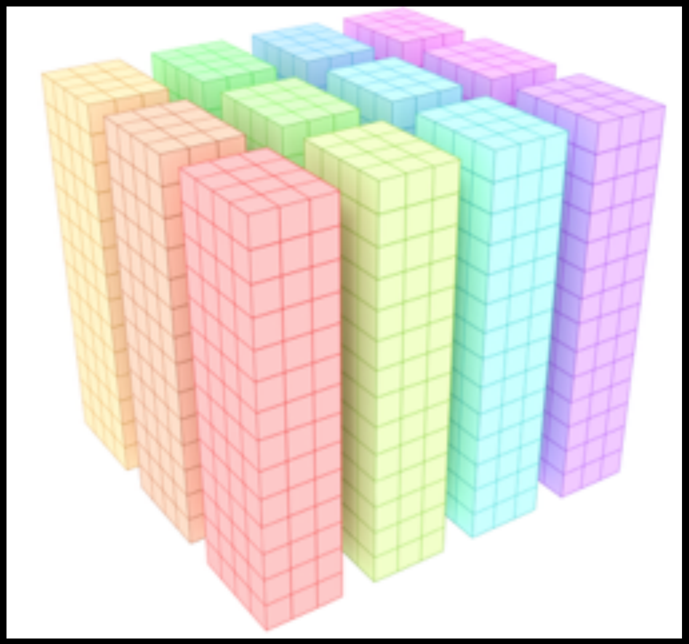
Pencil decomposition



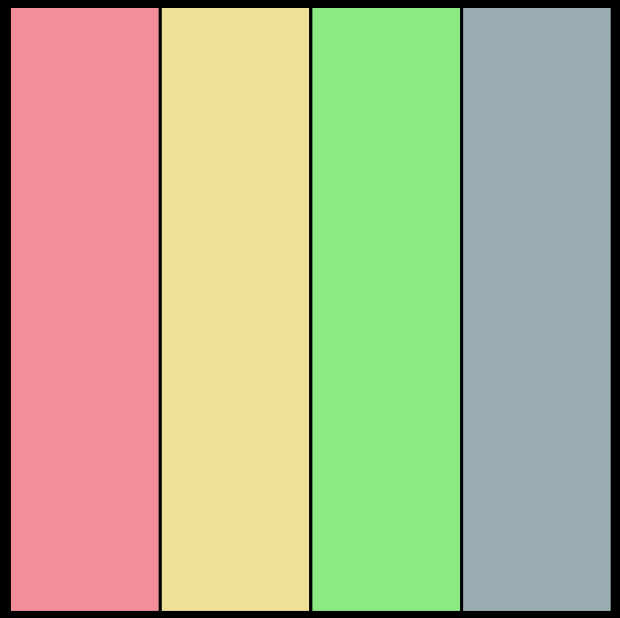
along x



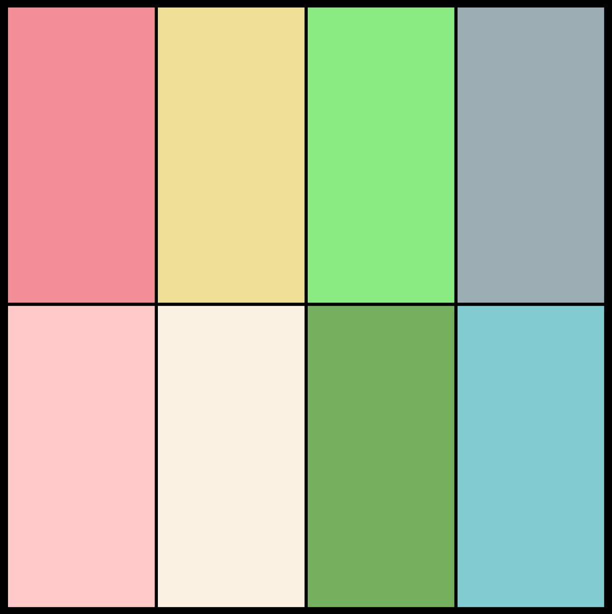
along y



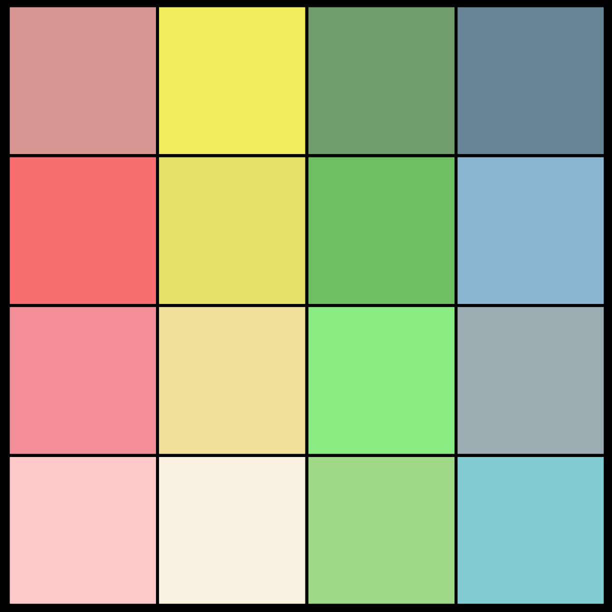
along z



px1 procs



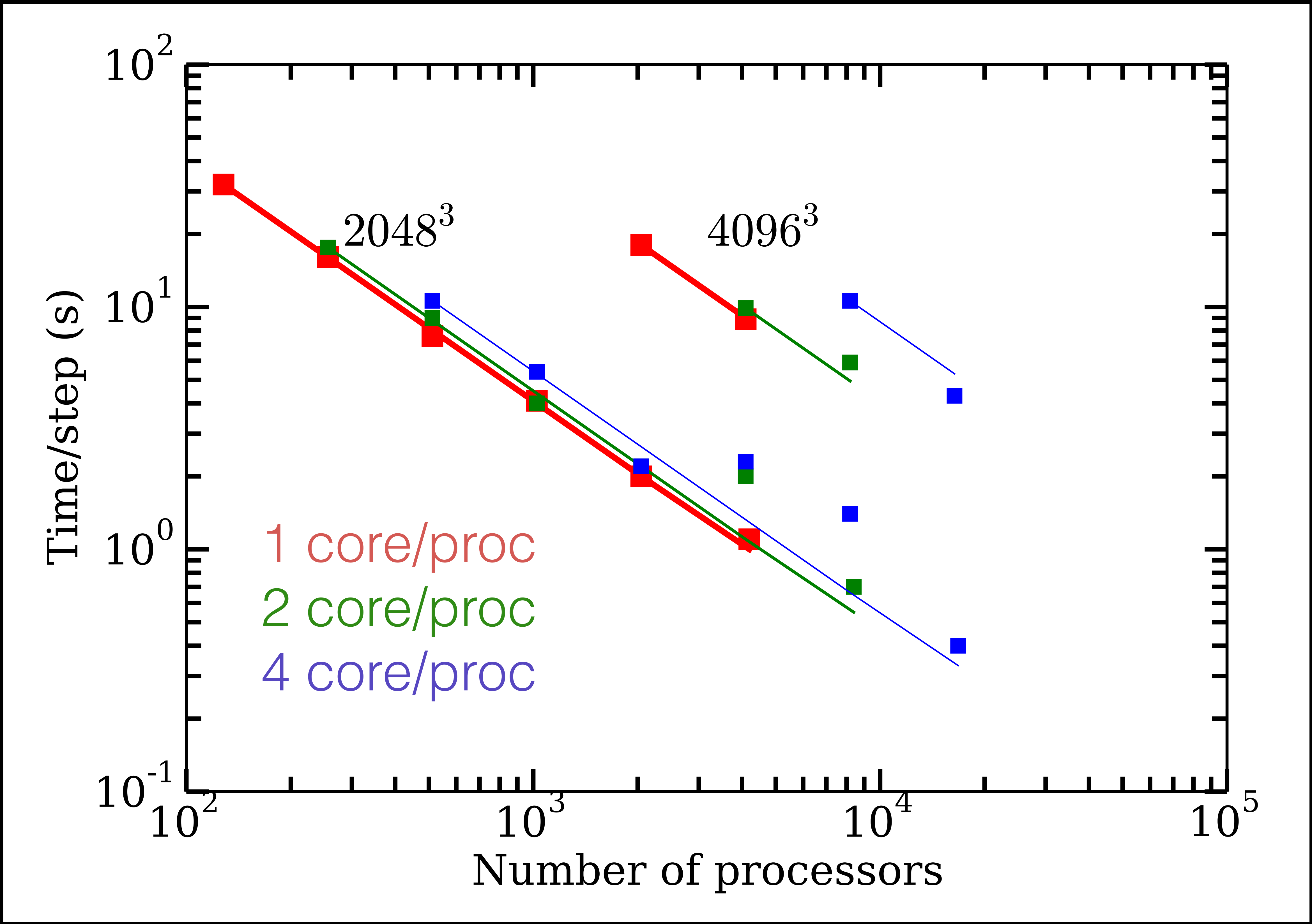
px2 procs



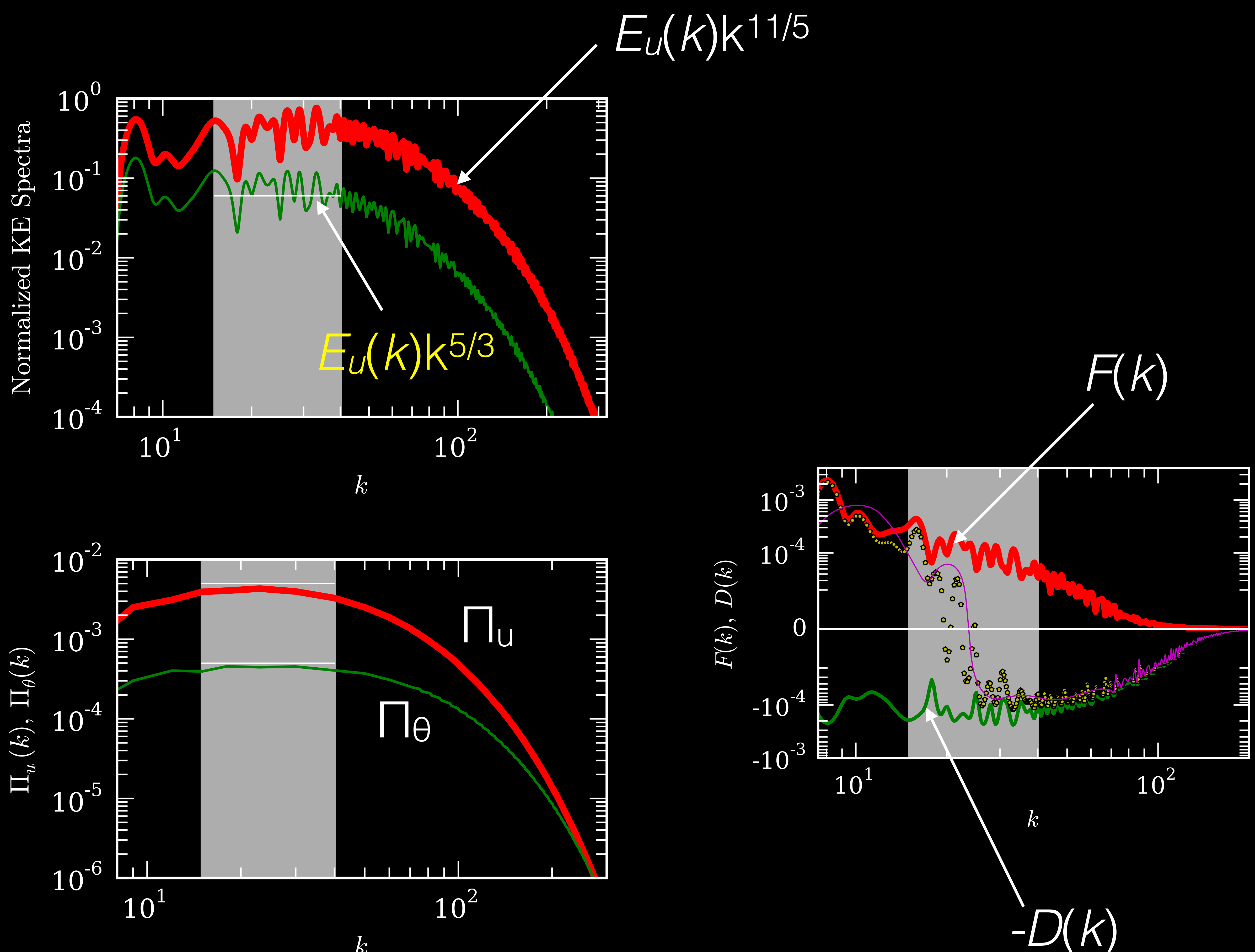
px4 procs

FFT scaling

On Shaheen at KAUST

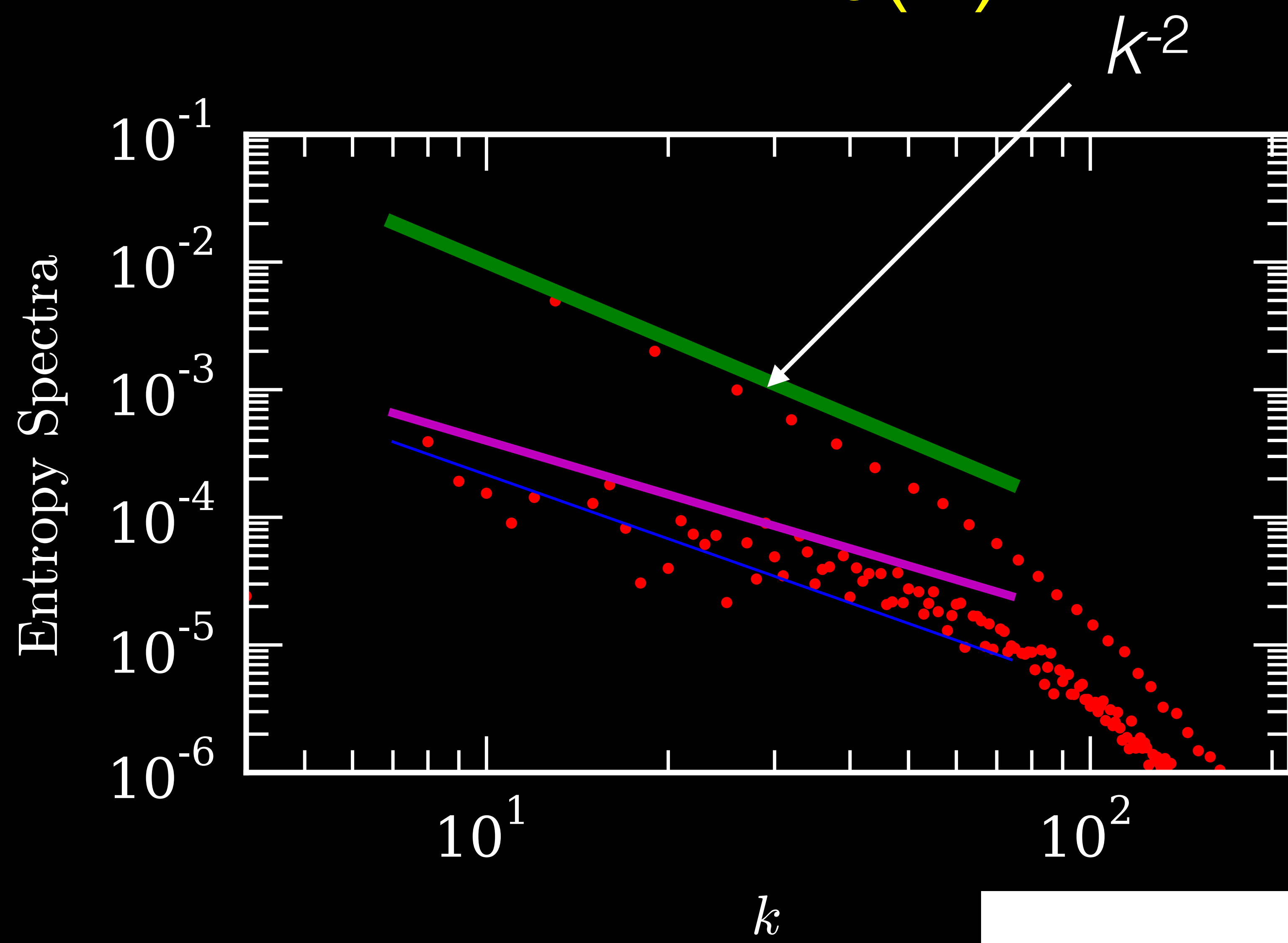


Time/step (s)
Number of processors
10^2
10^1
10^0
10^{-1}
10^2
10^3
10^4
10^5
2048^3
4096^3
1 core/proc
2 core/proc
4 core/proc

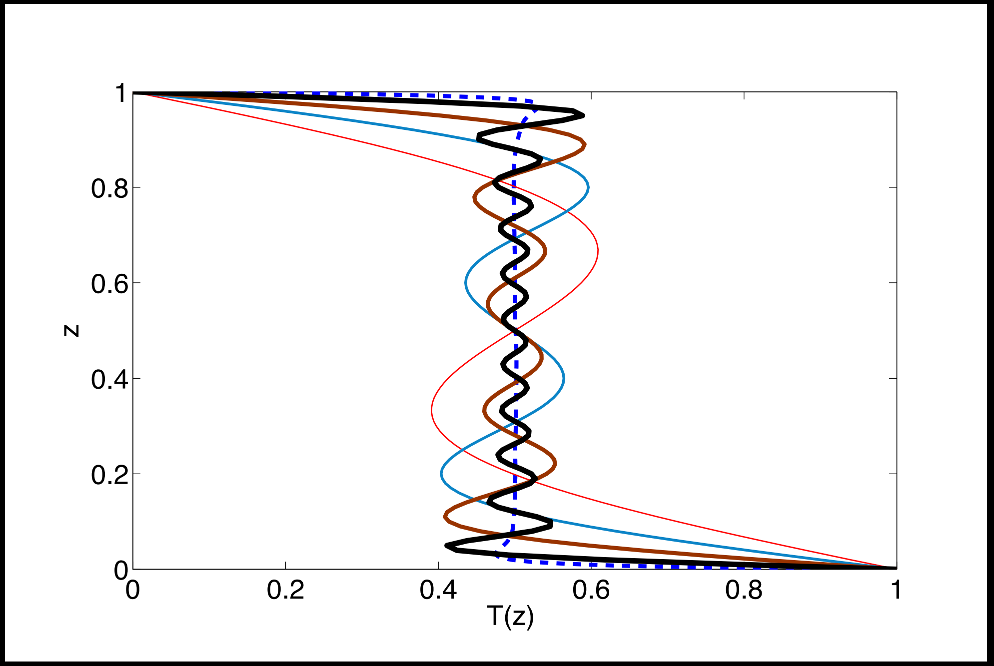


Kumar, Chatterjee, Verma, PRE 2014

$E_\theta(k)$

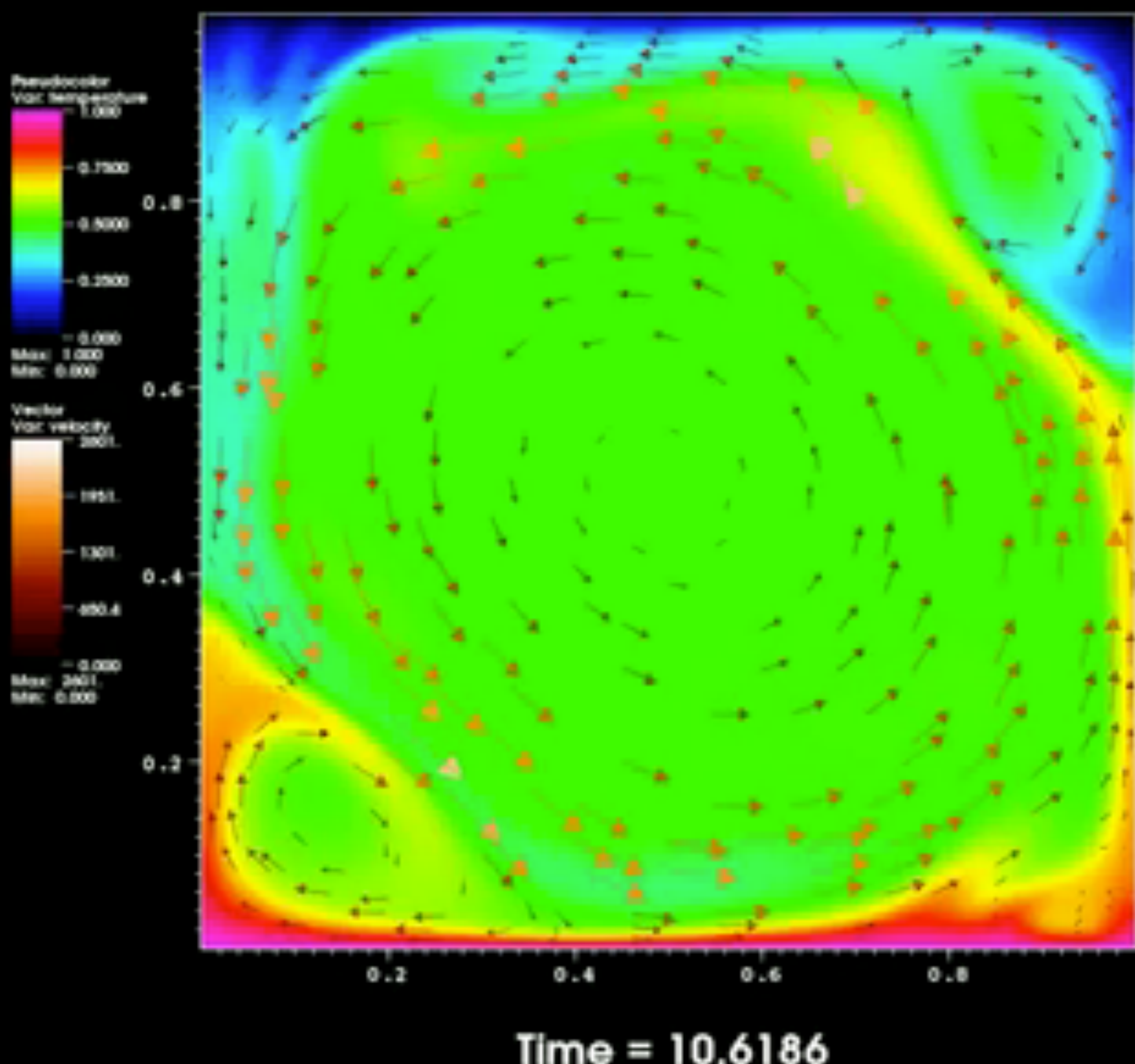


$\theta_K \approx -1/(2n\pi)$



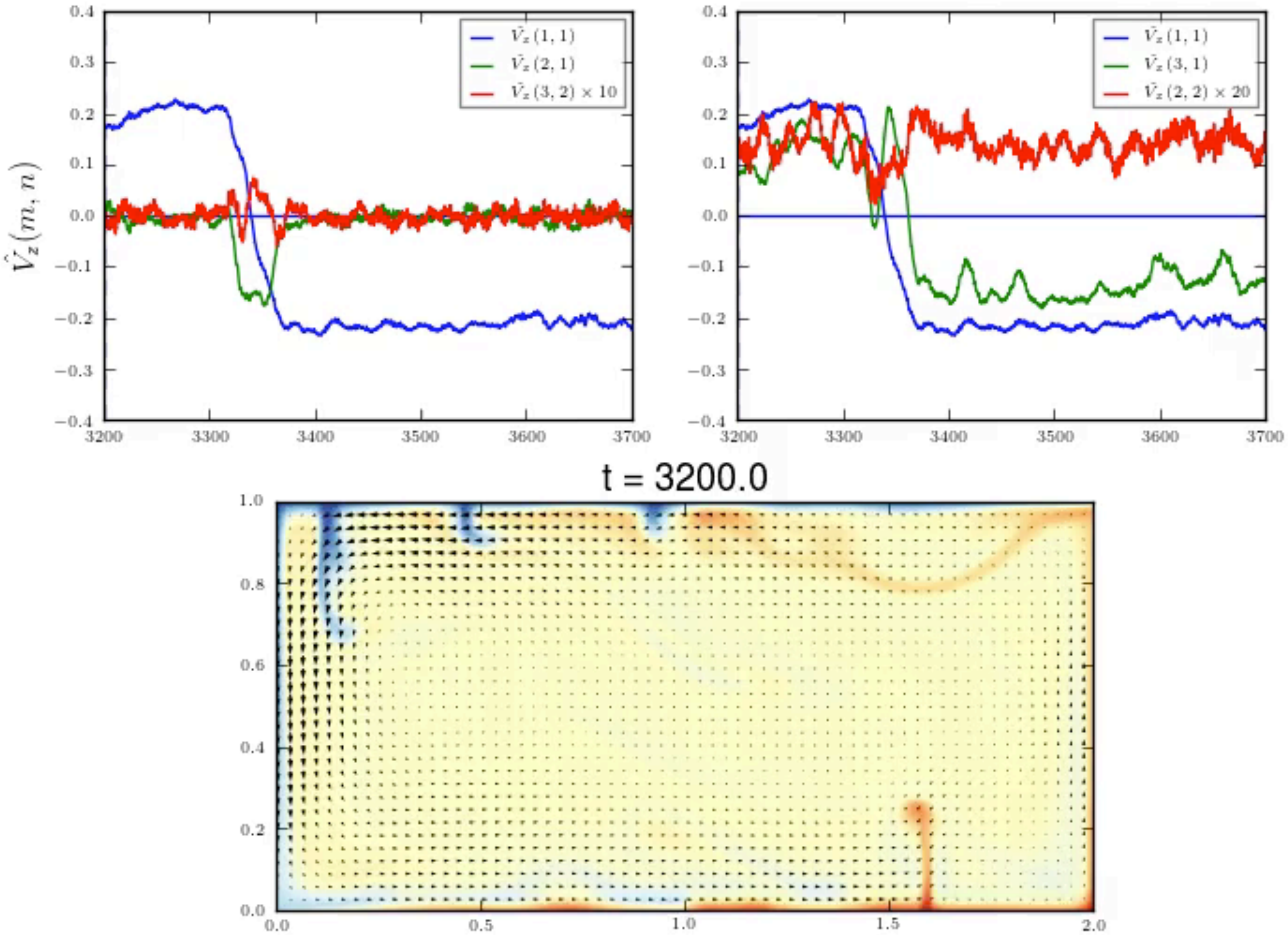
Flow reversal

Nek5000 (Spectral-element) simulation



(1,1)→(2,2) →(1,1)

Chandra & Verma, PRE 2011, PRL 2013

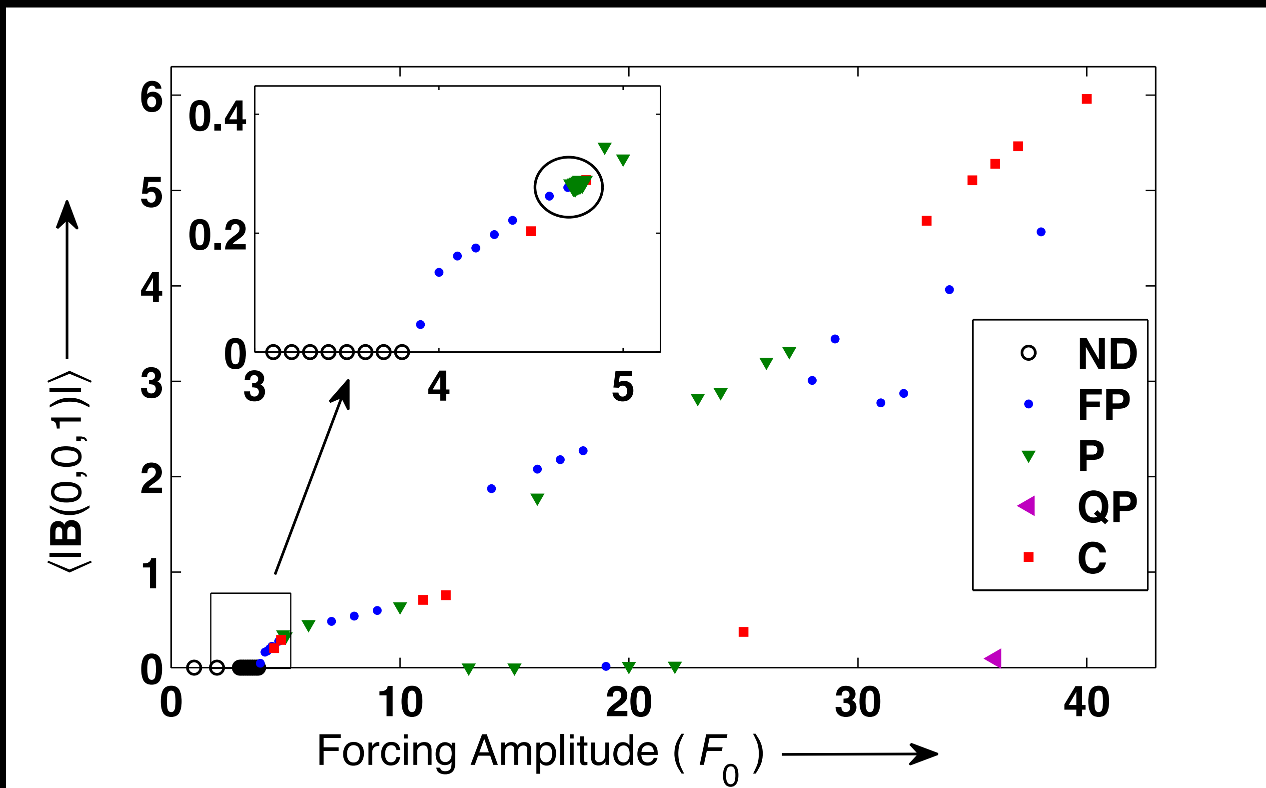


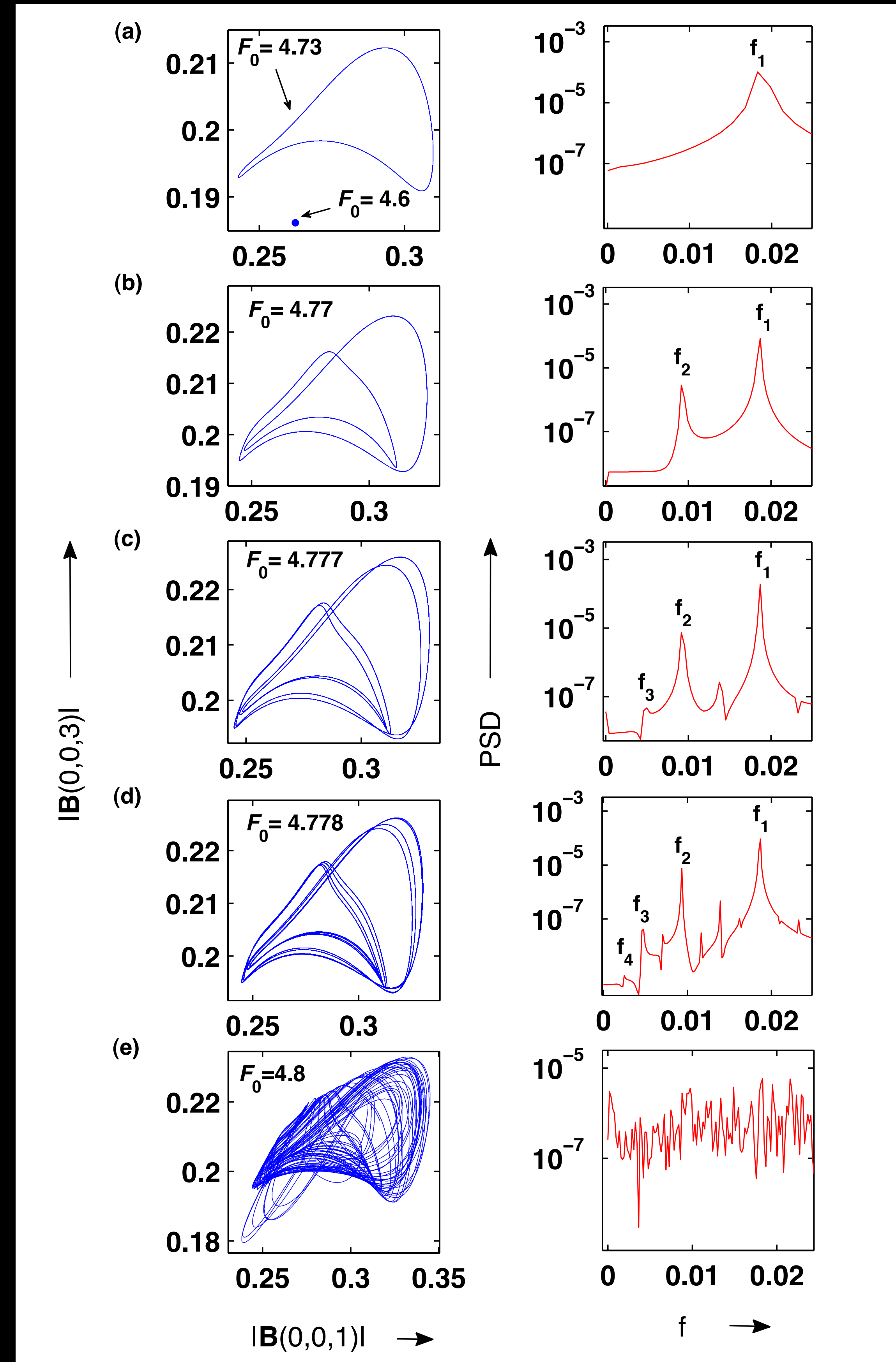
MKV, S. Ambhire, A. Pande, submitted to Phys. Fluids

Dynamo simulation

Yadav et al., EPL 2010; PRE, 2012

64^3 128^3


⟨|B(0,0,1)|⟩
Forcing Amplitude (F_0)
ND
FP
P
QP
C


(a)
F_0= 4.73
F_0= 4.6
(b)
F_0= 4.77
(c)
F_0= 4.777
(d)
F_0= 4.778
(e)
F_0=4.8
|B(0,0,3)|
|B(0,0,1)|
PSD
f
f_1
f_2
f_3
f_4

Instability analysis

Prandtl No Pr =0

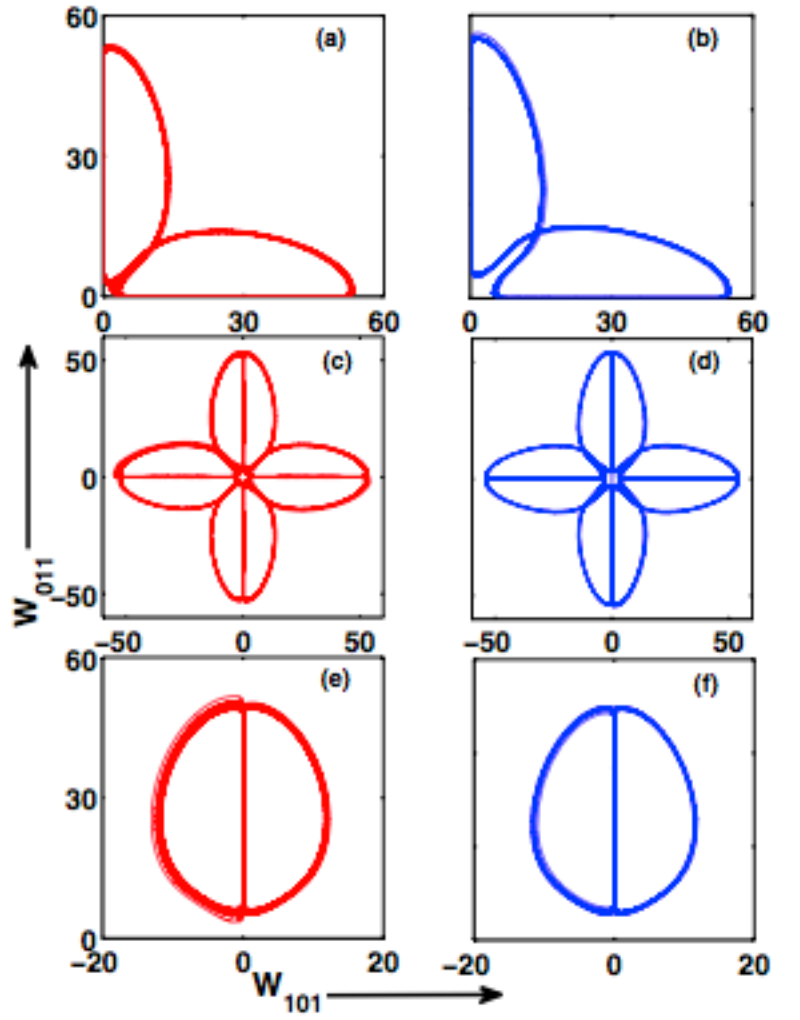
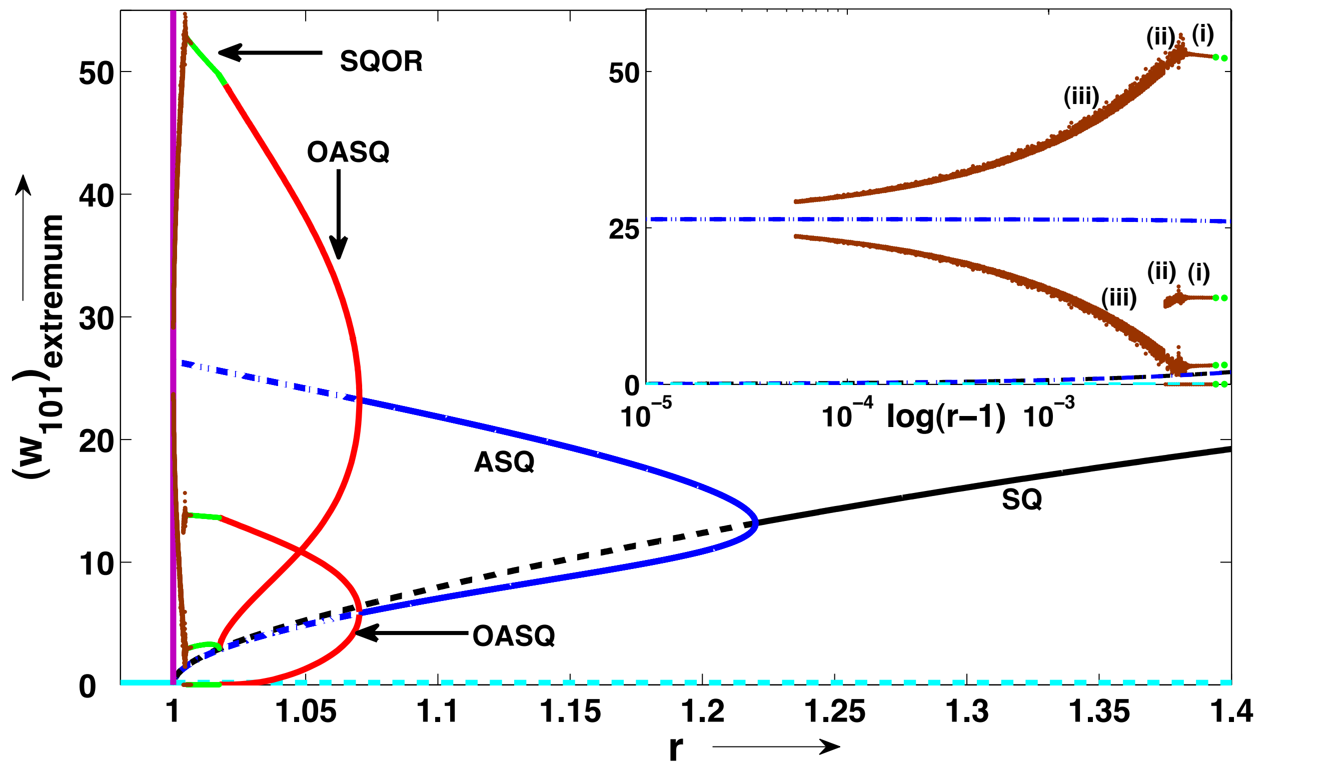
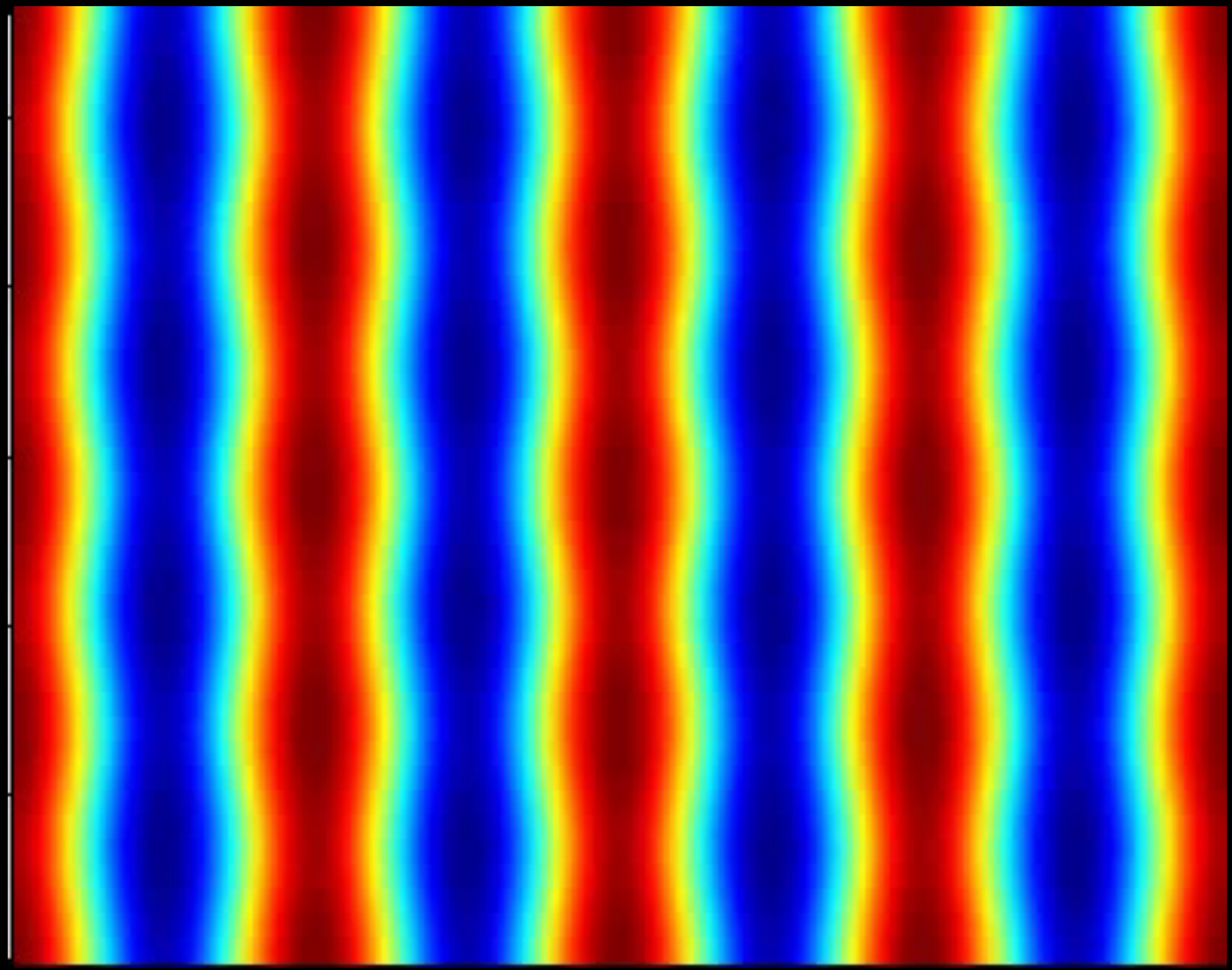


Fig. 5: (Colour on-line) The three different chaotic solutions observed near $r = 1$: Ch1 at $r = 1.0041$ for the model (a) and at $r = 1.0045$ in DNS (b); Ch2 at $r = 1.0038$ for the model (c) and at $r = 1.0030$ in DNS (d); Ch3 at $r = 1.0030$ for the model (e) and at $r = 1.0023$ in DNS (f). These solutions belong to (i), (ii), and (iii) regimes in the bifurcation diagram (fig. 2).



Pal et al., EPL 2009;
Mishra et al., EPL 2010



Invite collaborations

- ★ Code development
- ★ Module development
- ★ Optimization
- ★ Porting to large number of processors
- ★ GPU/Xeon-Phi Porting
- ★ Testing
- ★ Feel free to use the code.

Ported to:

PARAM, CDAC

Shaheen, KAUST

HPC system IITK

Funding

Dept of Science and Tech., India

Dept of Atomic Energy, India

KAUST (computer time)