Numerical Studies of Fluid Flows

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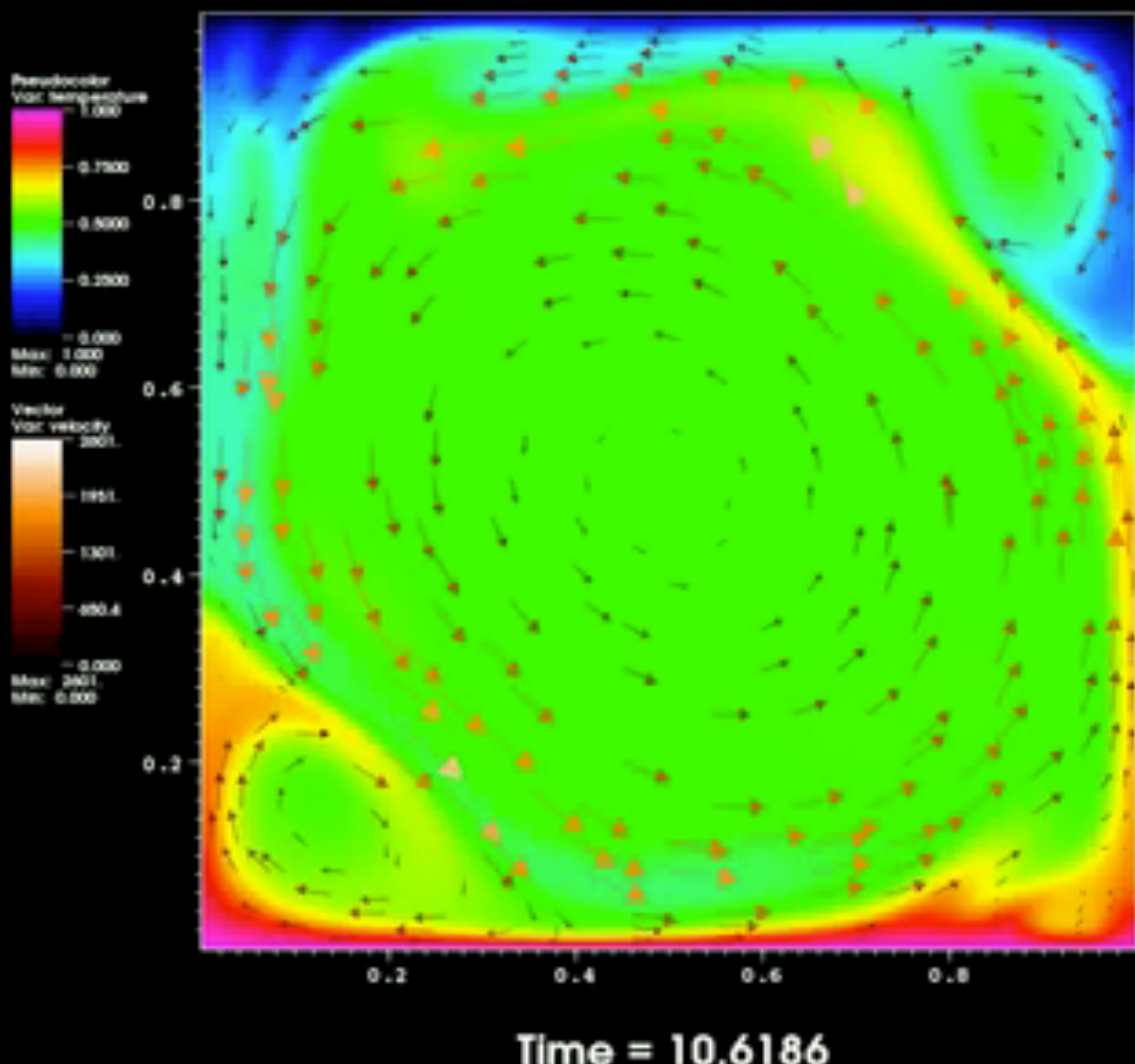
Field reversal

with Mani Chandra

Glatzmaier
1994

Nek5000 (Spectral-element)
simulation



$(1,1) \rightarrow (2,2) \rightarrow (1,1)$

spectral-element code
Nek5000

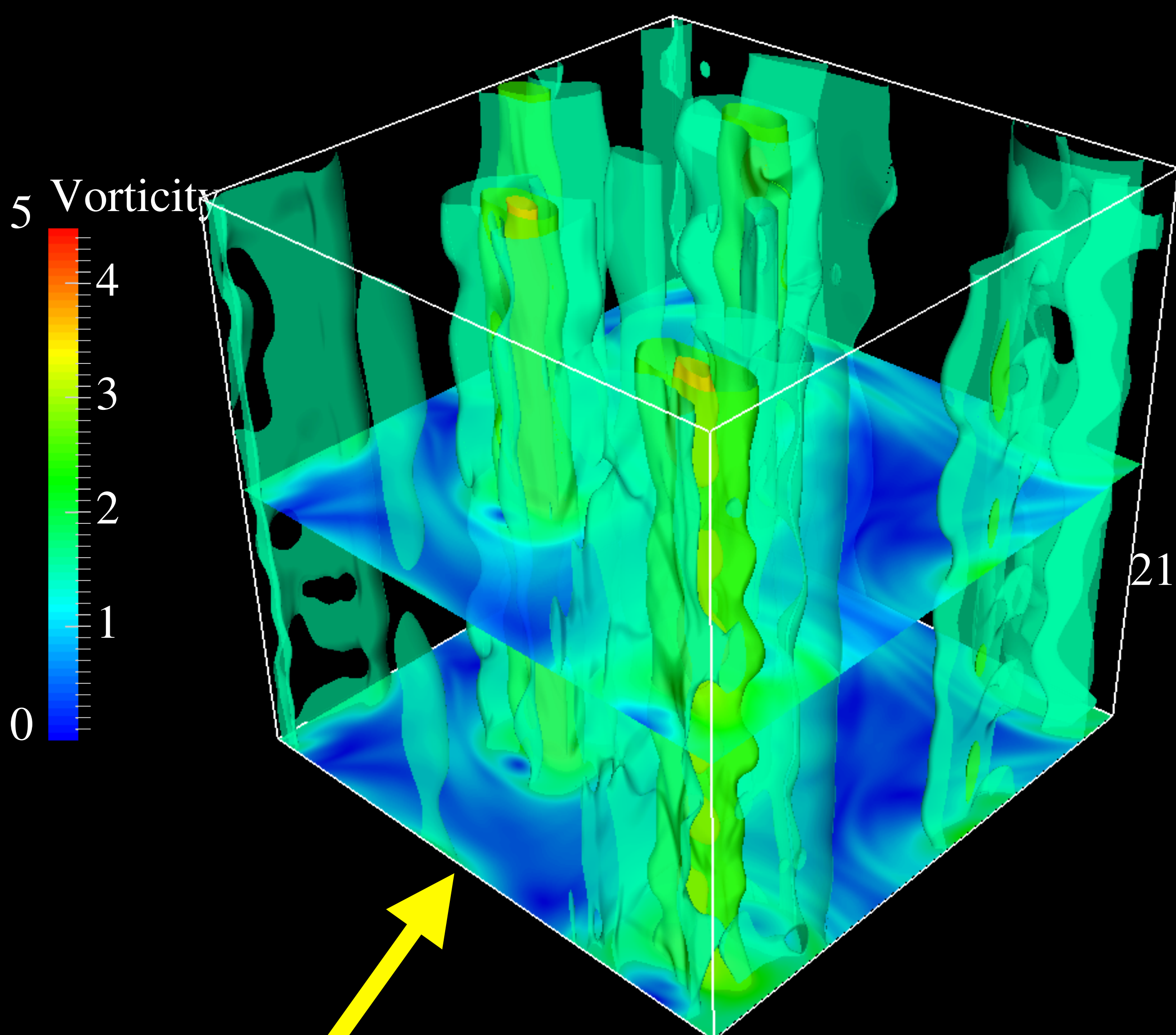
Chandra & Verma, PRE 2011, PRL 2013

Rotating Turbulence

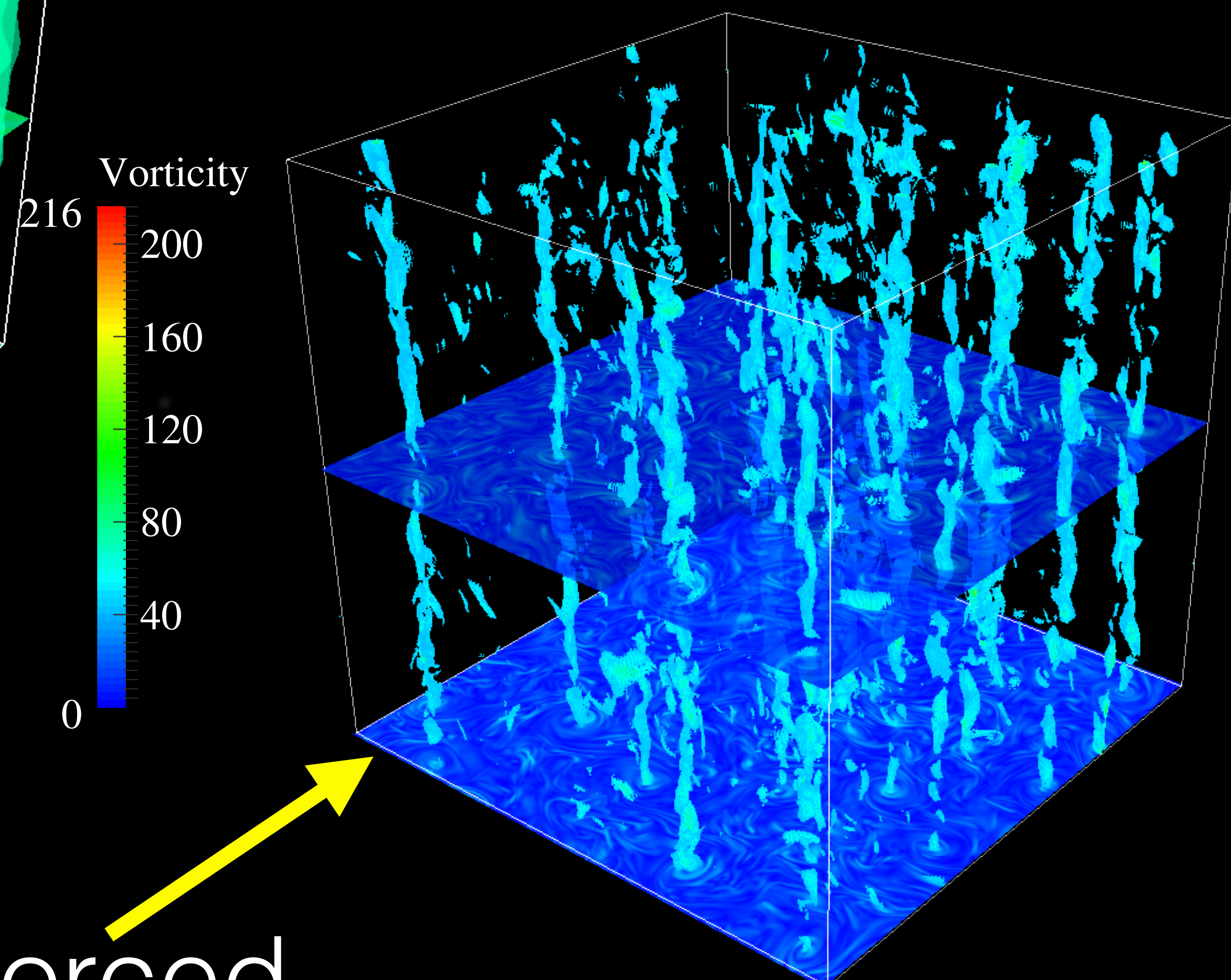
with Manohar Sharma, Sagar Chakraborty

Rotating Turbulence

Ro = 0.05



Decay



Forced

Spectral method (Tarang)
&
Spetral-element (Nek500)

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 = $\frac{UL}{\nu}$

Procedure

$$f(x) = \sum_{k_z} \hat{f}(k_x) \exp[i(k_x x)]$$

$$df(x)/dx = \sum_{k_z} [ik_x \hat{f}(k_x)] \exp[i(k_x x)]$$

Set of ODEs

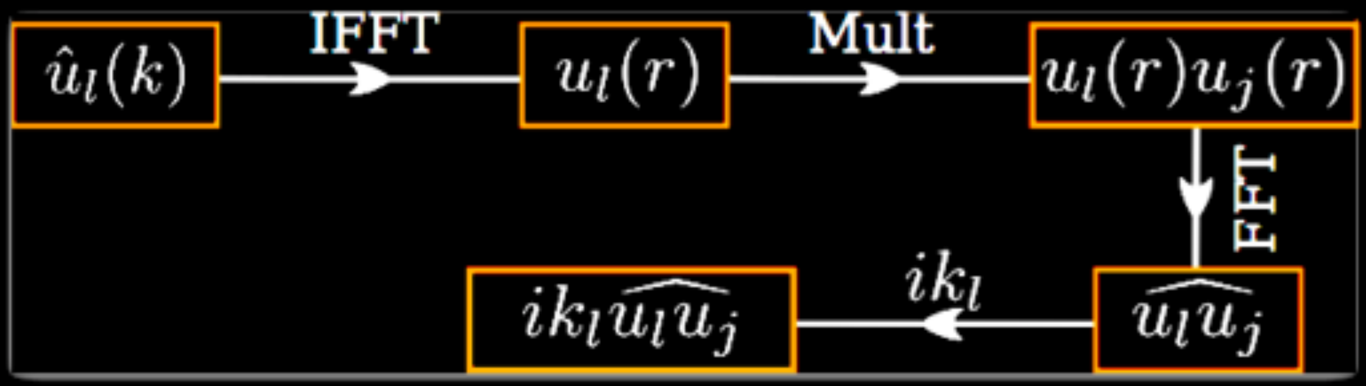
$$\frac{du_i(\mathbf{k})}{dt} = -jk_m \widehat{u_m(\mathbf{r})u_i(\mathbf{r})} - jk_i p(\mathbf{k}) - \nu k^2 u_i(\mathbf{k})$$

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:



(pseudo-spectral)

Fourier transforms take around 80% of total time.

Tarang = wave (Sanskrit)

Spectral code (Orszag)

One code to do many
turbulence & instabilities problems

VERY HIGH RESOLUTION (6144^3)

Cores: 196692 of Shaheen II

Opensource, download from
http://turbulencehub.org

Verma et al., Pramana, 2013
Submitted to SC16

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

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 6144^3 grids

Object-oriented design

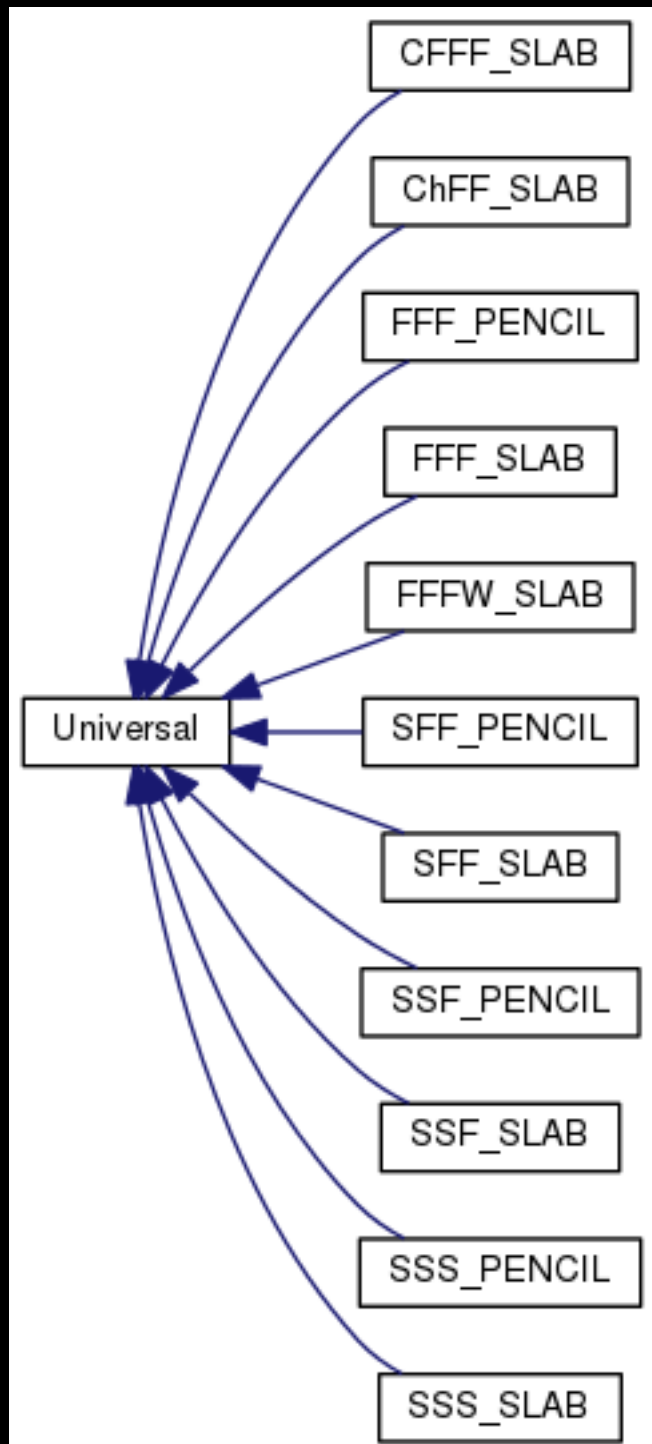
Basis functions (FFF, SFF, SSF, SSS, ChFF)

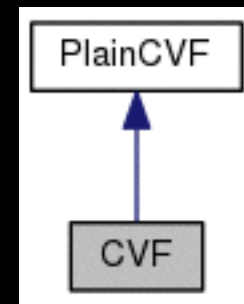
Basis-independent universal function

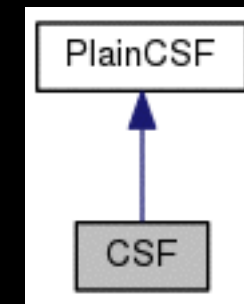
e.g., compute_nlin $(u. \nabla)u$,
$(b. \nabla)u$, $(b. \nabla)b$, $(u. \nabla)T$.

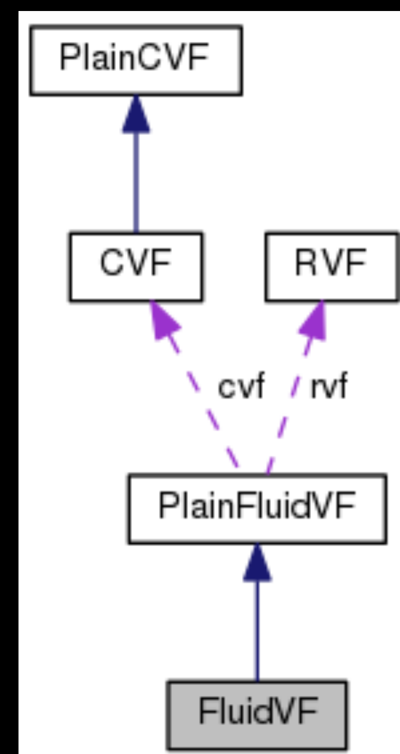
General PDE solver

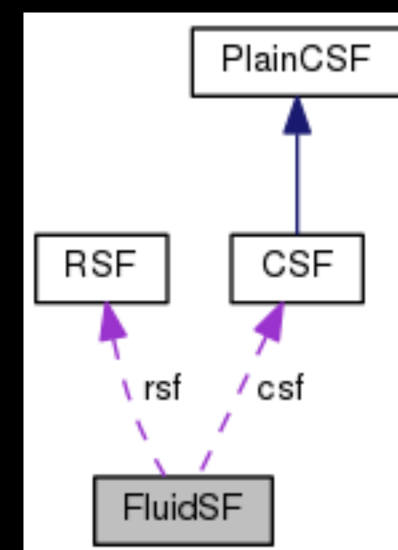
We can use these general functions to simulate
MHD, convection etc.



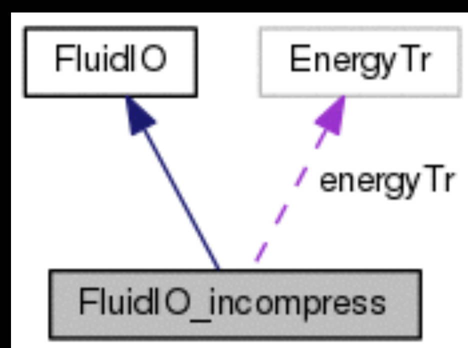


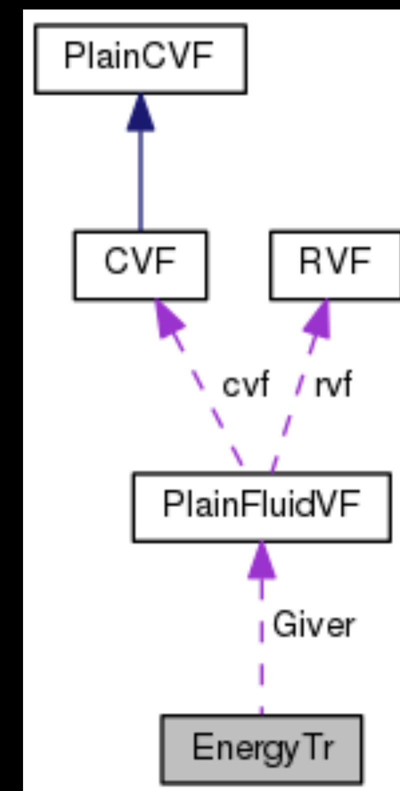






Generated by Doxygen


FluidIO
EnergyTr
energyTr
FluidIO_incompress


PlainCVF
CVF
RVF
cvf
rvf
PlainFluidVF
Giver
EnergyTr

Spectral Transform
(FFT, SFT, Chebyshev)

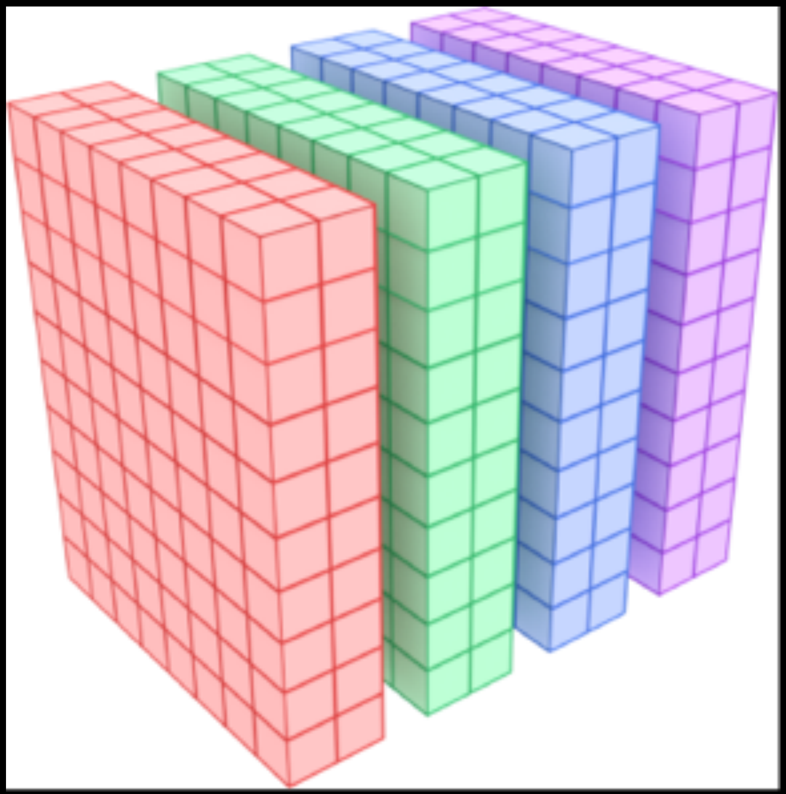
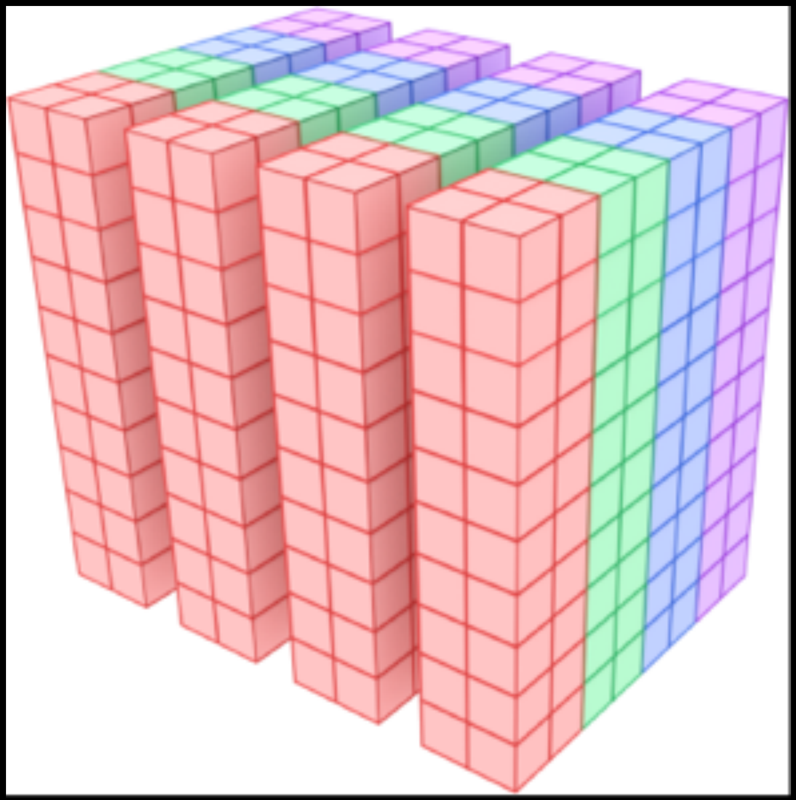
Multiplication in real space

Input/Output
HDF5 lib

FFT Parallelization

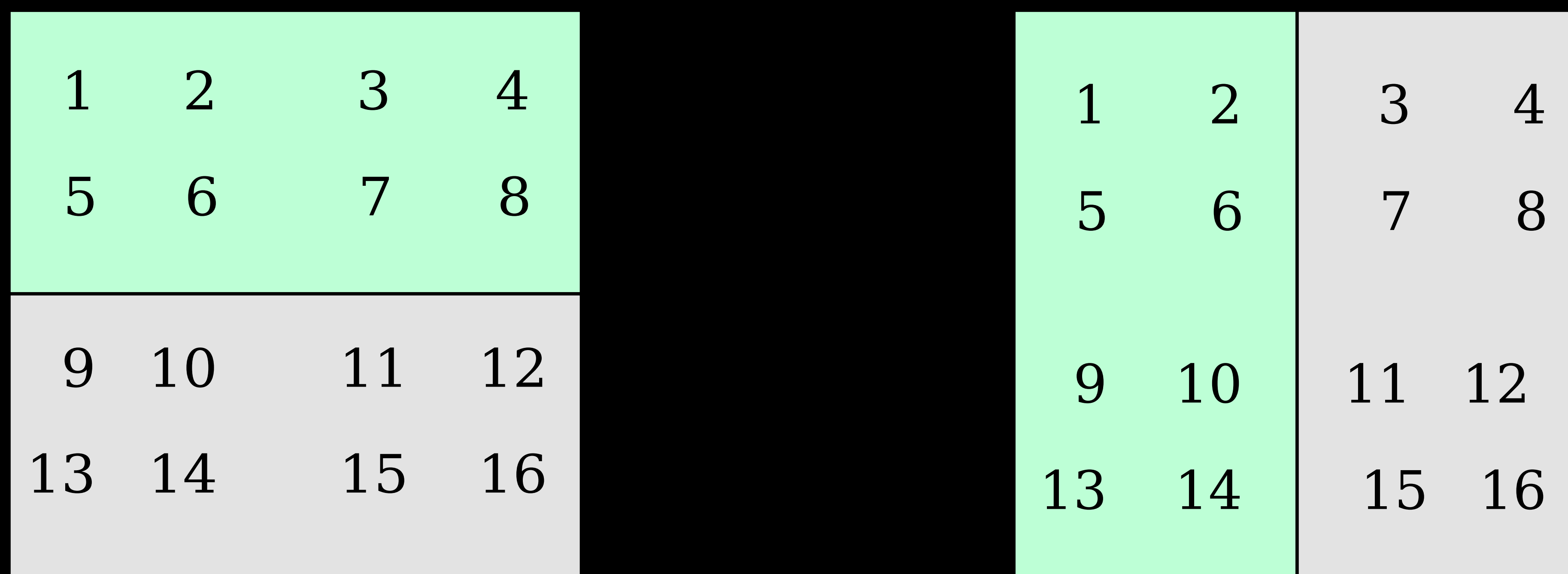
$$f(x,y,z) = \sum_{k_x} \sum_{k_y} \sum_{k_z} \hat{f}(k_x, k_y, k_z) \exp[i(k_x x + k_y y + k_z z)]$$

Slab decomposition

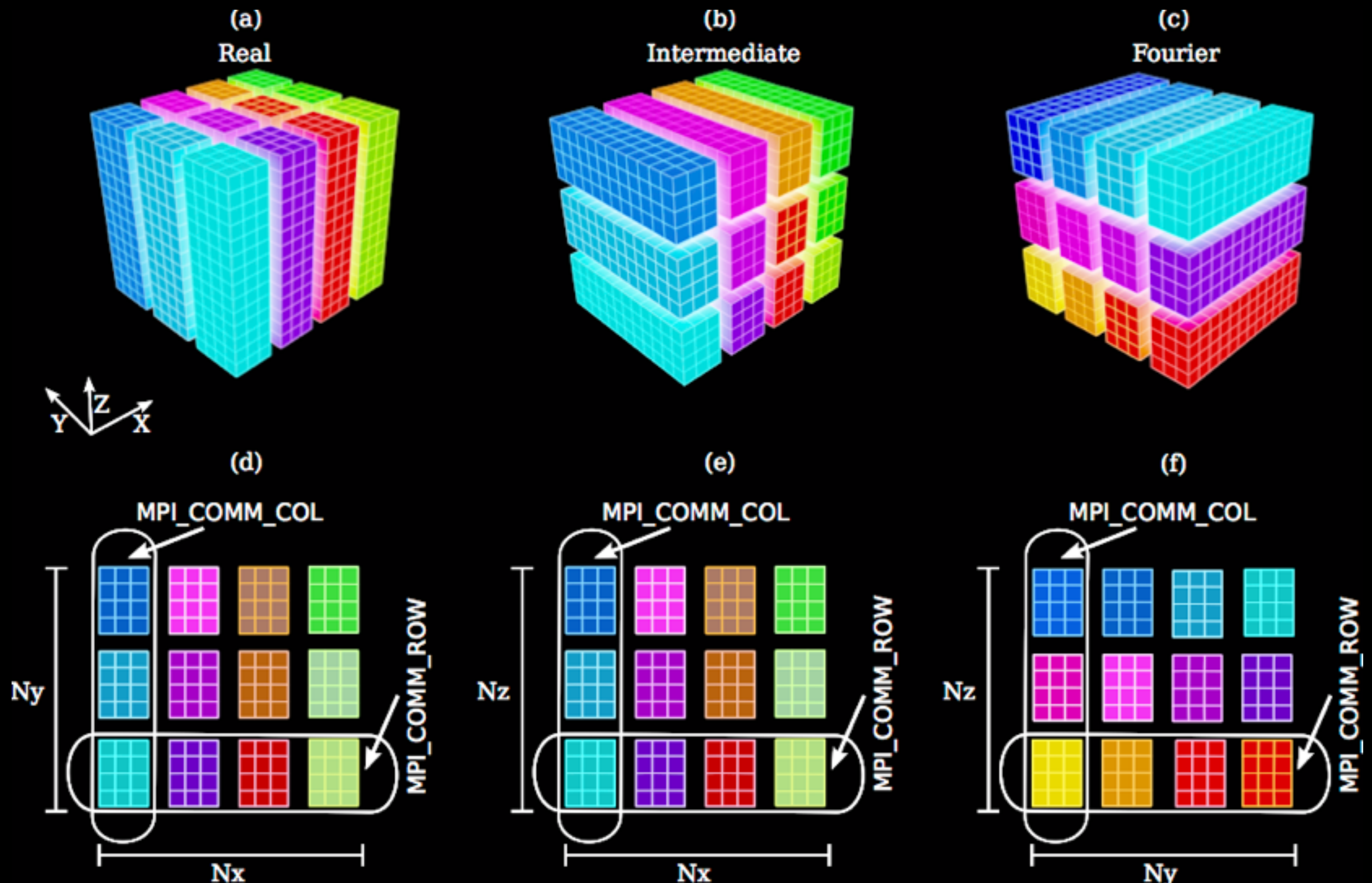
Data divided among 4 procs

Transpose-free FFT



12-15% faster compared to FFTW

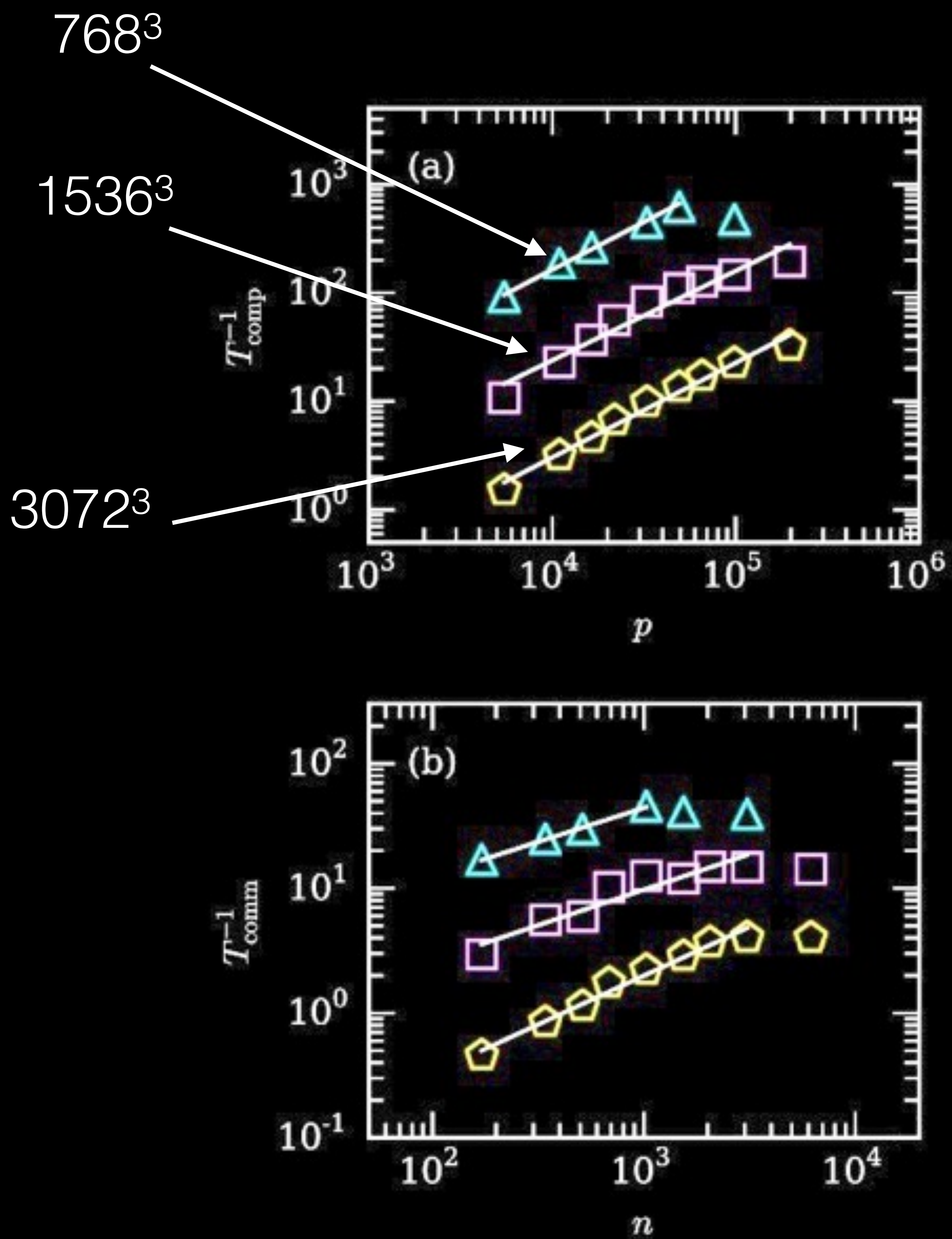
Pencil decomposition

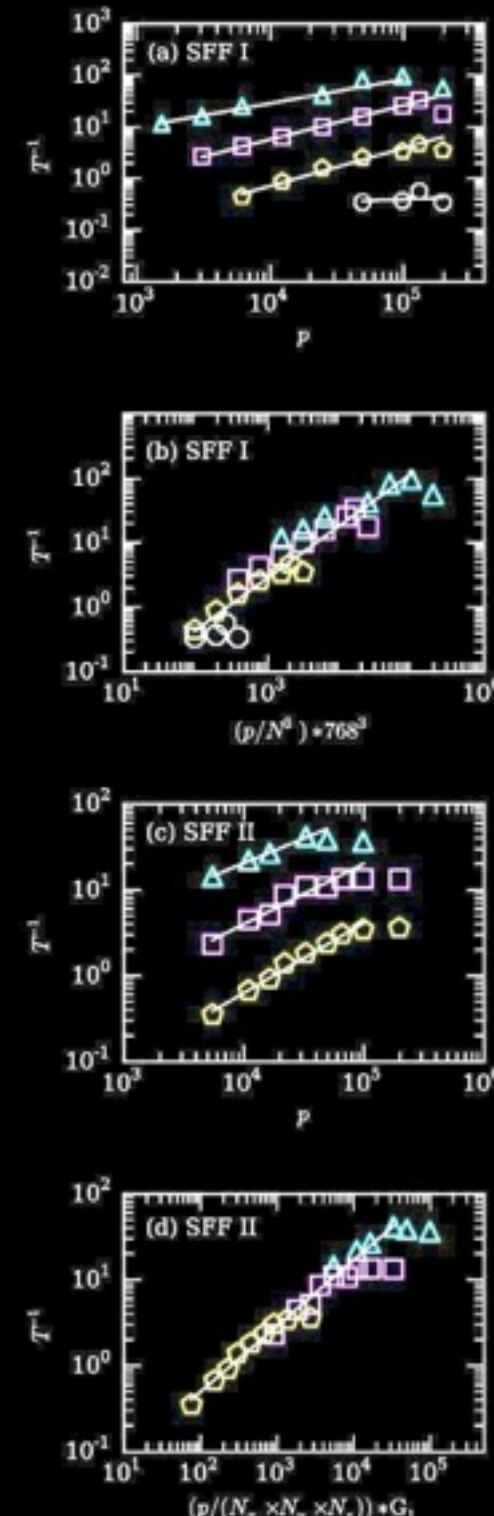


FFT scaling

On Shaheen at KAUST
with Anando Chatterjee, Abhishek Kumar,
Ravi Samtaney, Bilel Hadri, Rooh Khurram

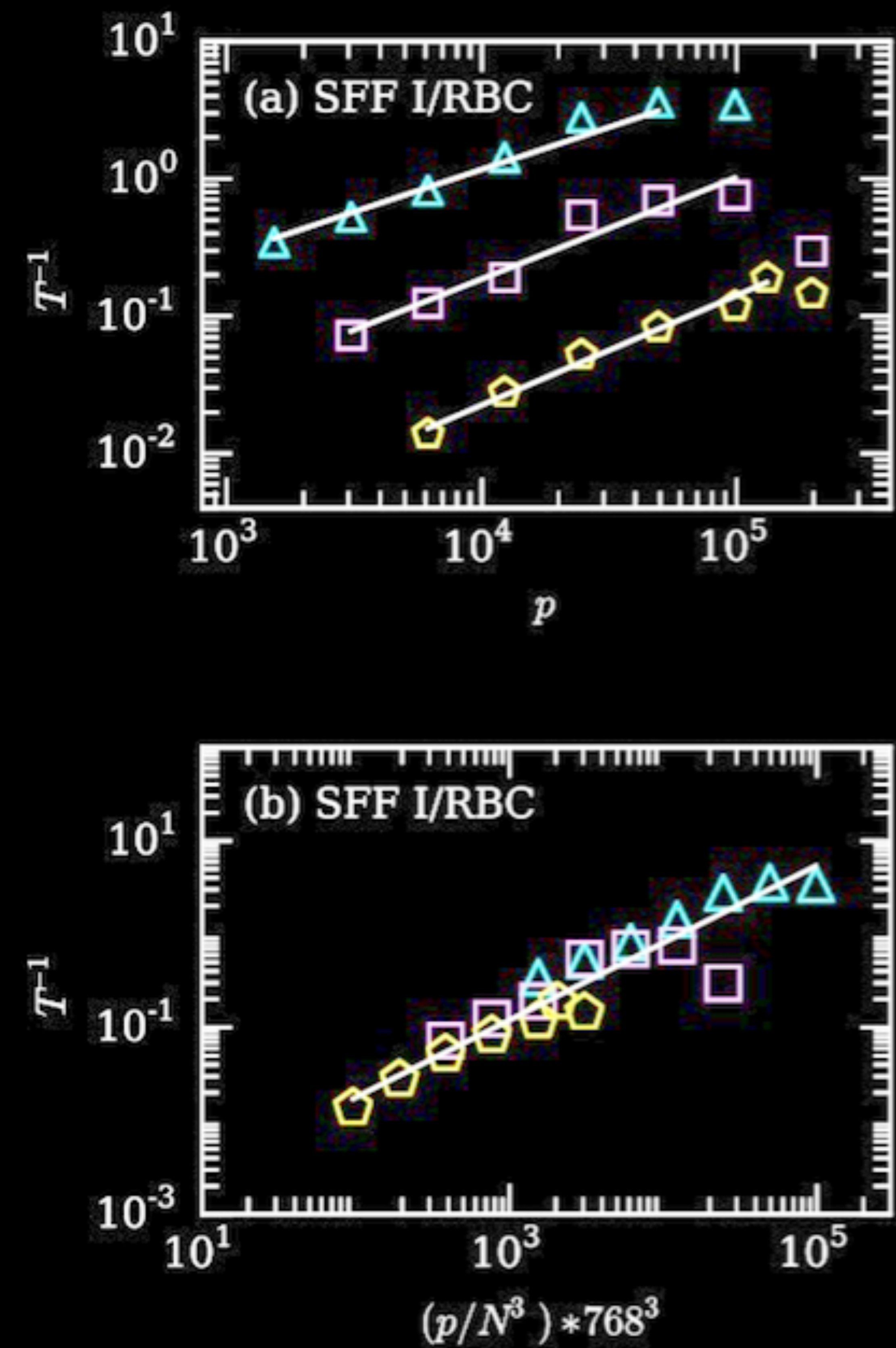
Cray XC40
ranked 9th in top500


768^3
1536^3
3072^3
(a)
T^{-1}_{comp}
p
(b)
T^{-1}_{comm}
n


(a) SFF I
(b) SFF I
(c) SFF II
(d) SFF II
T^{-1}
p
$(p/N^3)*768^3$
$(p/(N_x \times N_y \times N_z))*G_1$

Tarang scaling

On Shaheen at KAUST



(a) SFF I/RBC
T^{-1}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{3}
10^{4}
10^{5}
p
(b) SFF I/RBC
T^{-1}
10^{1}
10^{-1}
10^{-3}
10^{1}
10^{3}
10^{5}
$(p/N^3)*768^3$

Average flop rating/core

(~8%)

Overlap Communication & Computation

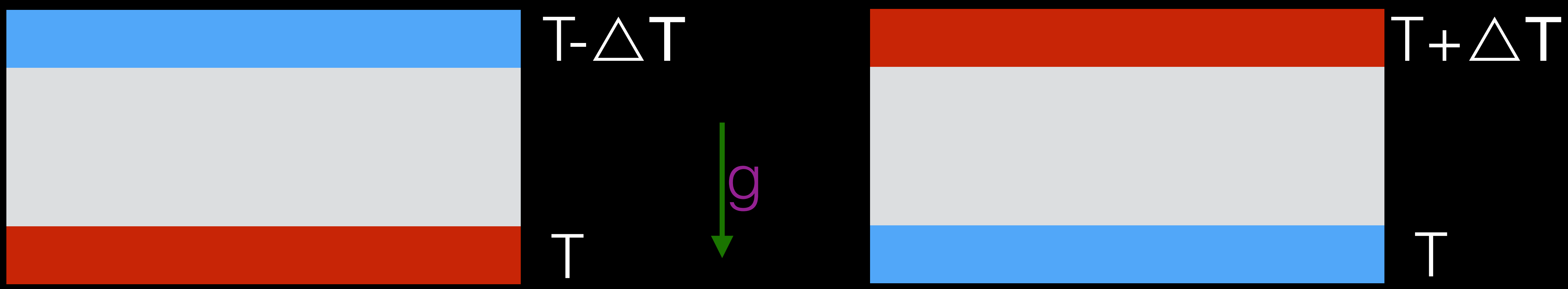
GPUs ??

Xeon Phi ??

Examples

Energy spectrum of stably-stratified flows and Rayleigh Benard convection

Kumar, Chatterjee, Verma, PRE 2014



RBC
Unstable

Stably Stratified flow
Stable

Stably stratified flows
Simulation results

Pr=1

Forcing the VELOCITY field
(Random)

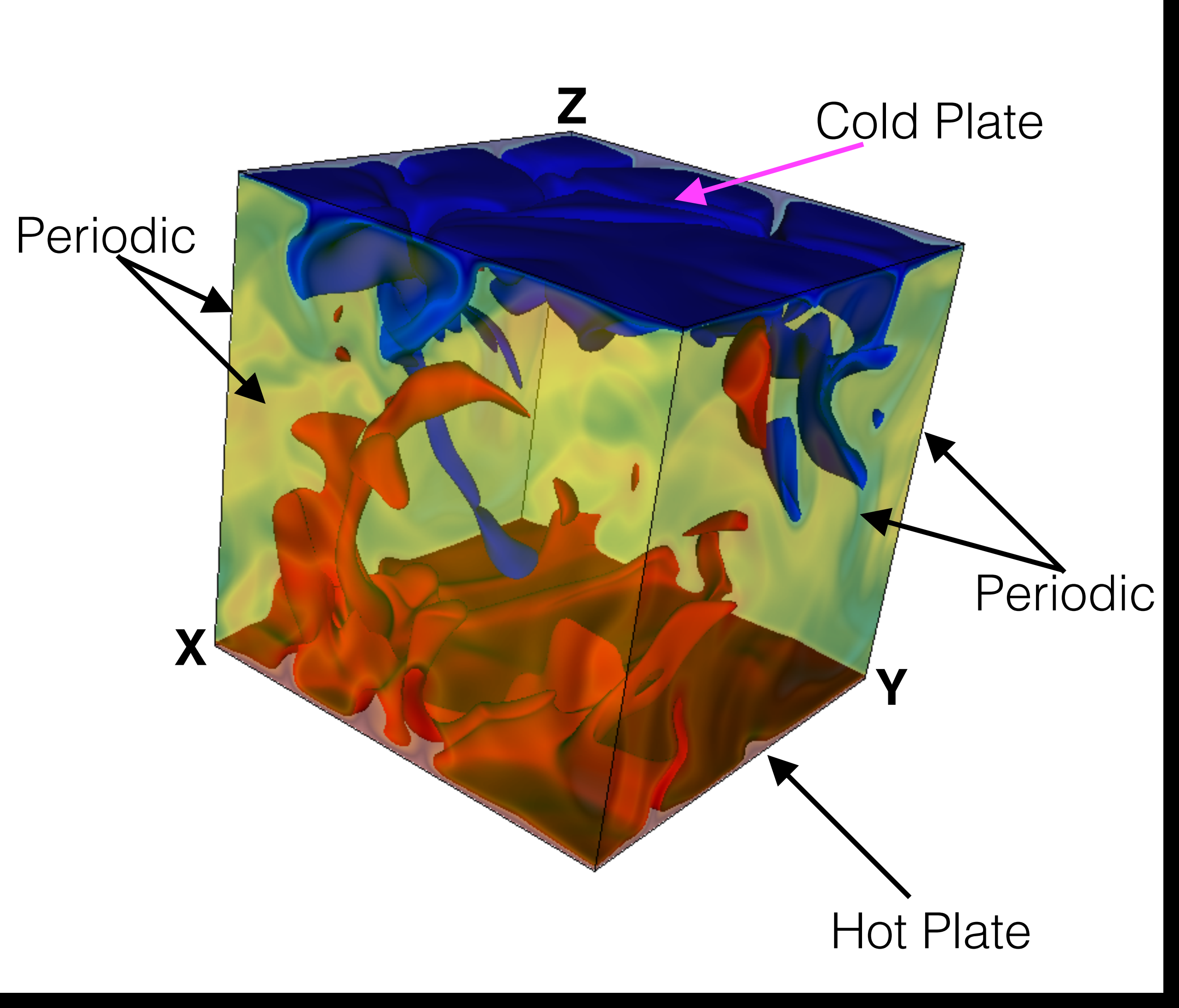
Periodic BC   (**u**,θ)

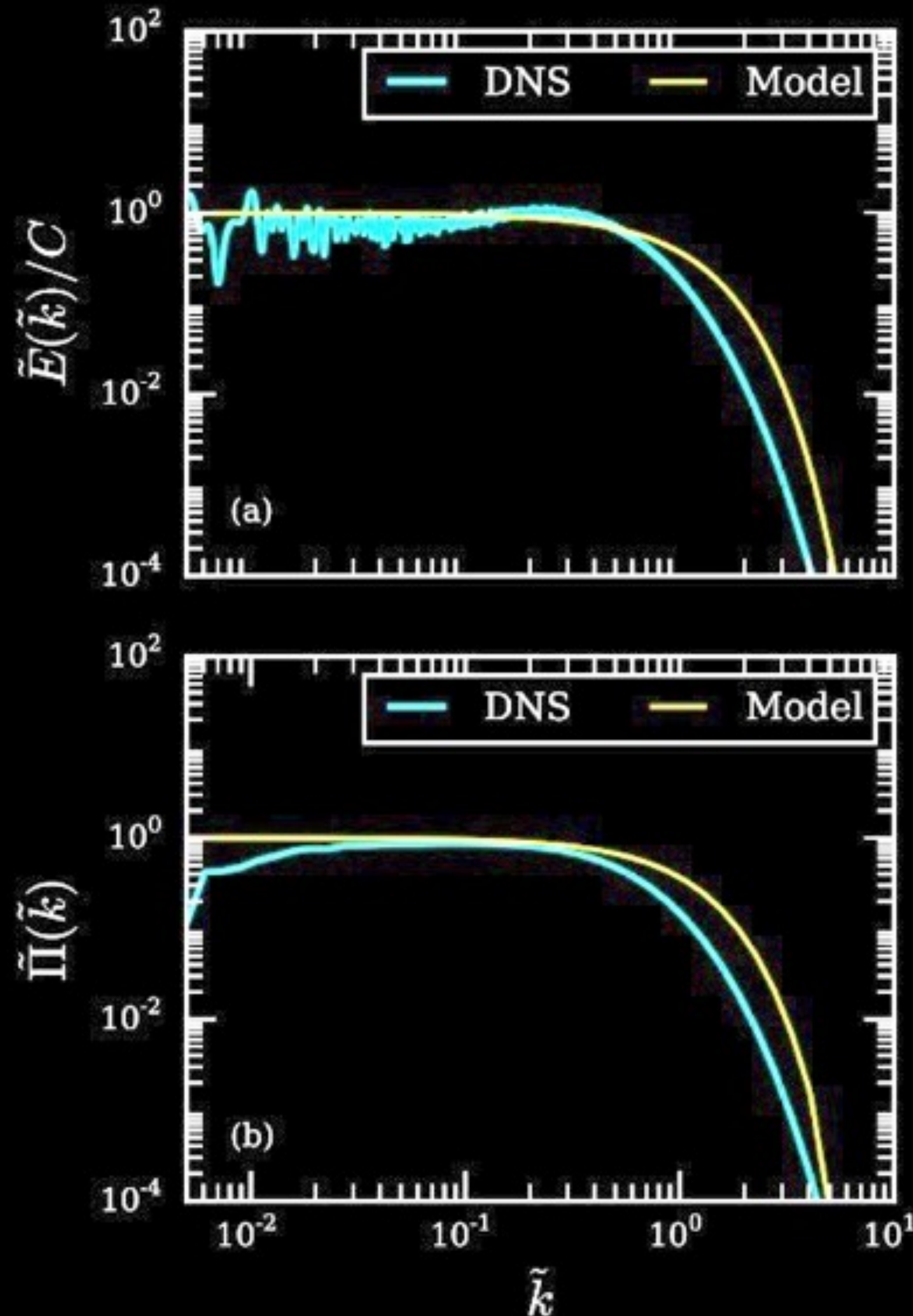
RBC
Simulation results

Pr=1

Free-slip BC
$$u_z = 0$$
$$\partial_z u_x = \partial_z u_y = 0$$

Conducting plates $\theta = 0$


Z
Cold Plate
Periodic
X
Periodic
Y
Hot Plate

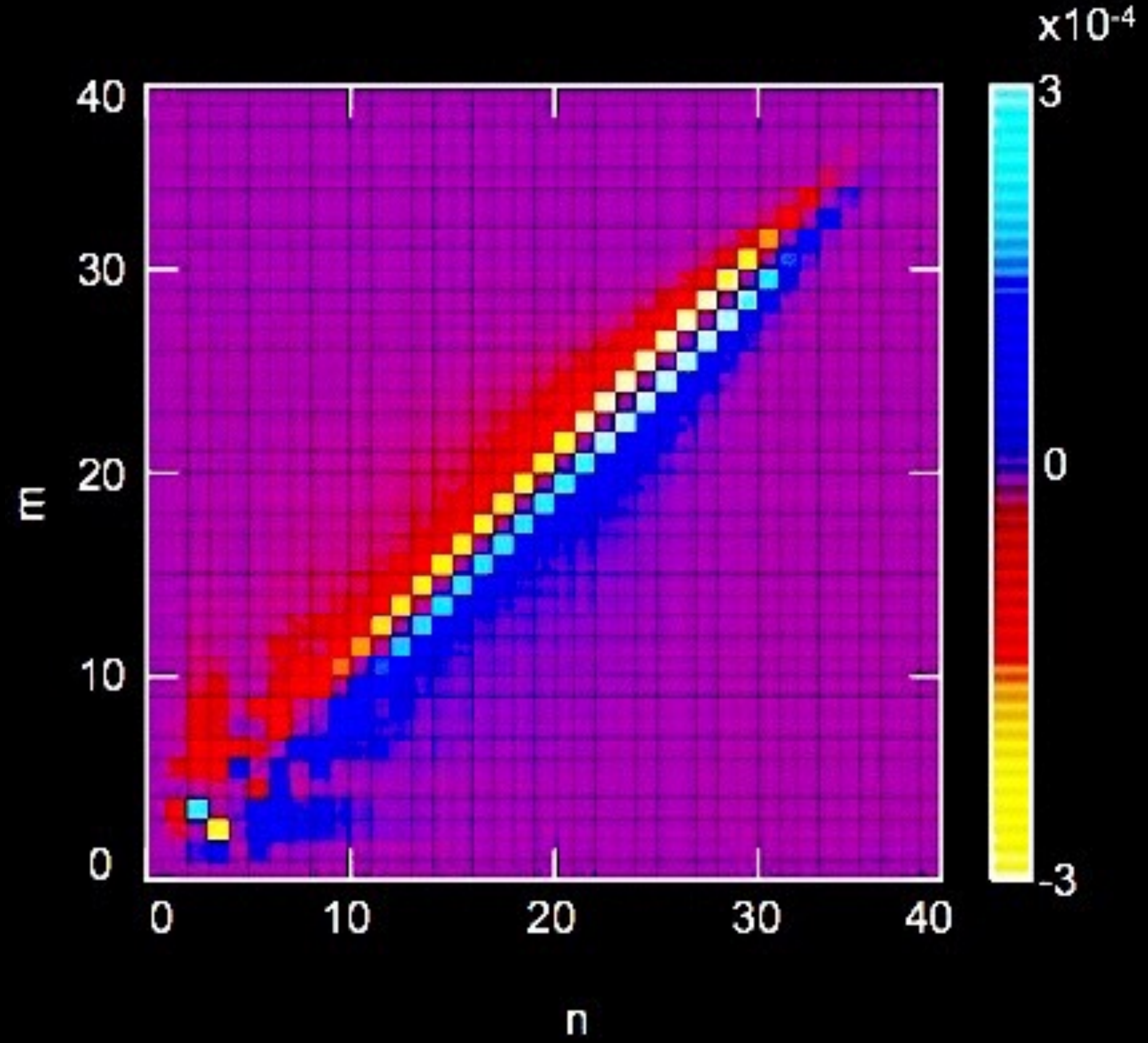


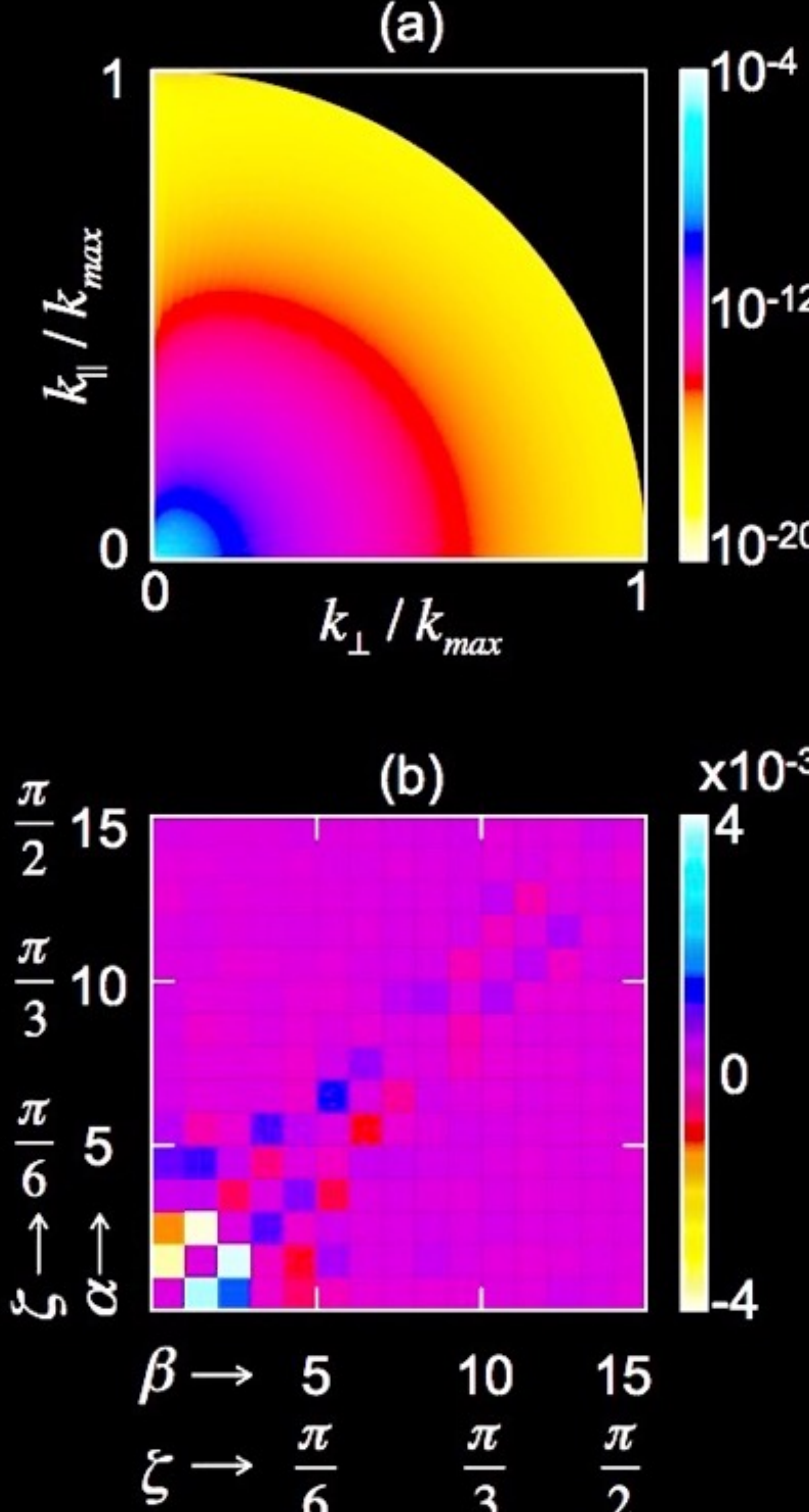
4096^3 simulations

Ra = 1.1×10^{11}

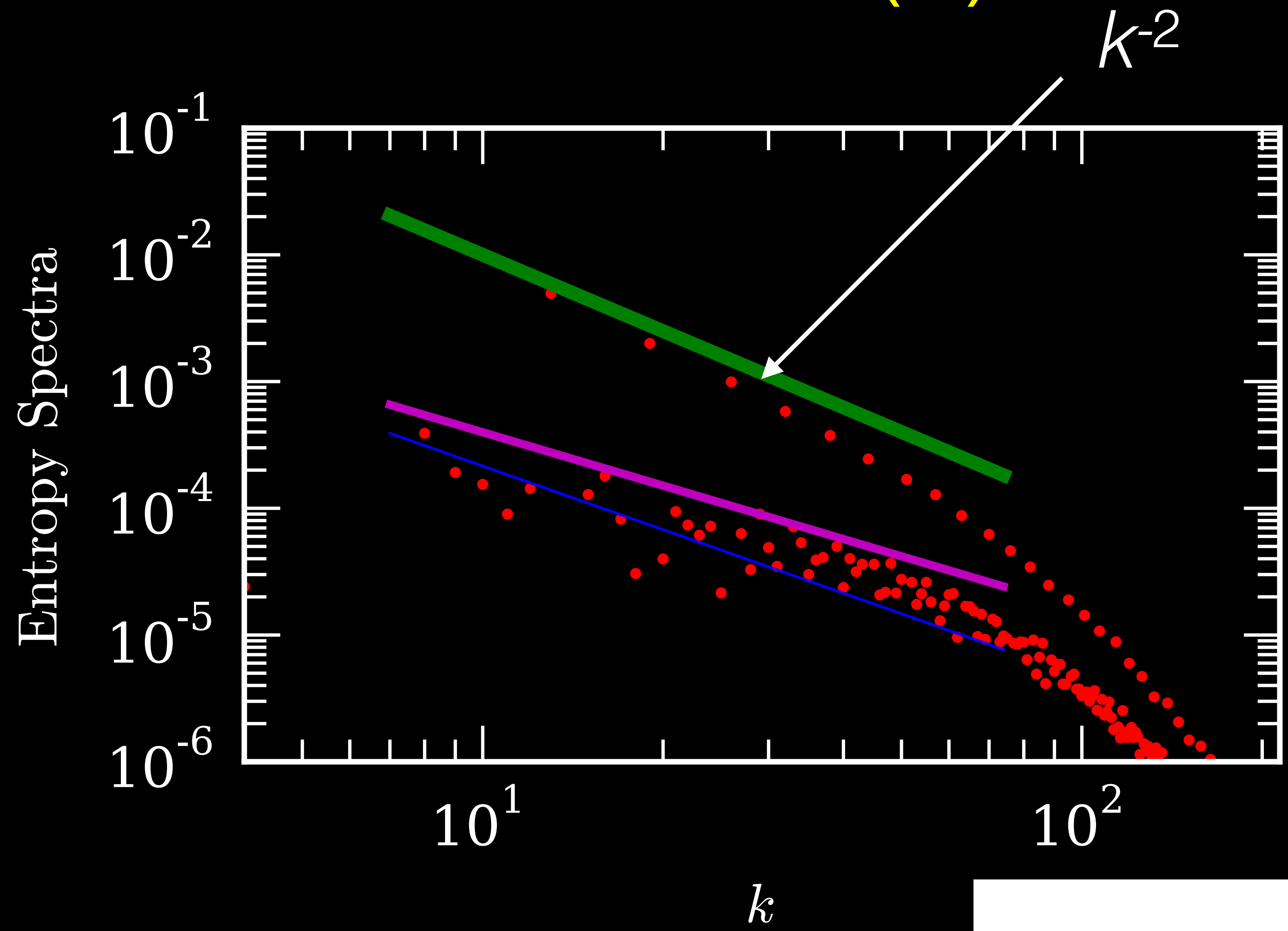
Pr = 1

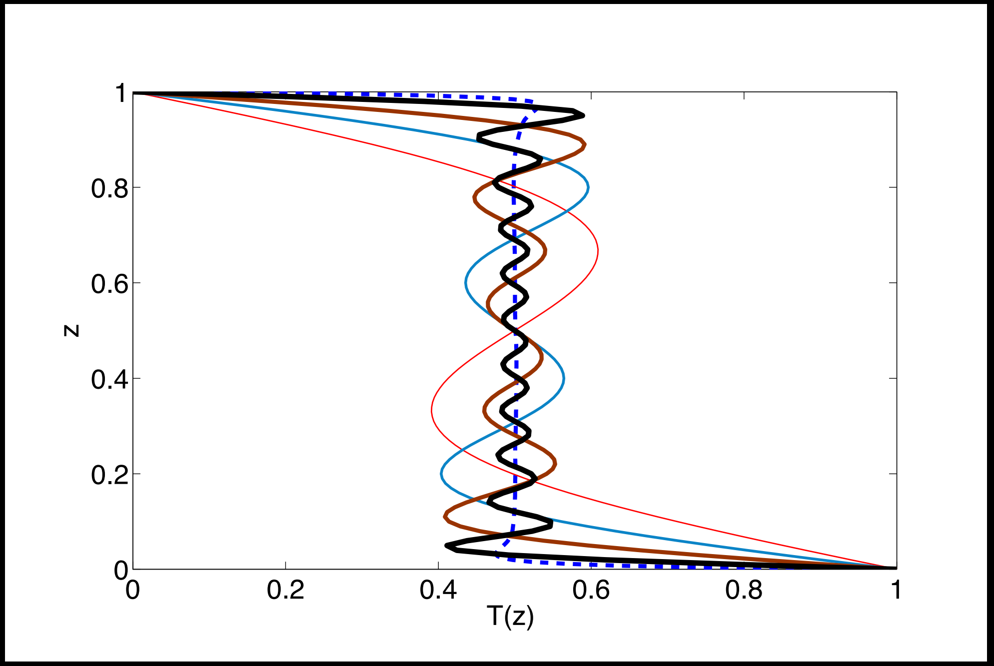
65536 cores of Shaheen II (KAUST)


x10^-4
3
0
-3
40
30
20
10
0
m
0
10
20
30
40
n


(a)
1
0
0
1
$k_{\parallel} / k_{max}$
$k_{\perp} / k_{max}$
10^{-4}
10^{-12}
10^{-20}
(b)
x10^-3
4
0
-4
15
10
5
$\frac{\pi}{2}$
$\frac{\pi}{3}$
$\frac{\pi}{6}$
$\zeta \rightarrow$
$\alpha \rightarrow$
$\beta \rightarrow$ 5 10 15
$\zeta \rightarrow$ $\frac{\pi}{6}$ $\frac{\pi}{3}$ $\frac{\pi}{2}$

$E_\theta(k)$

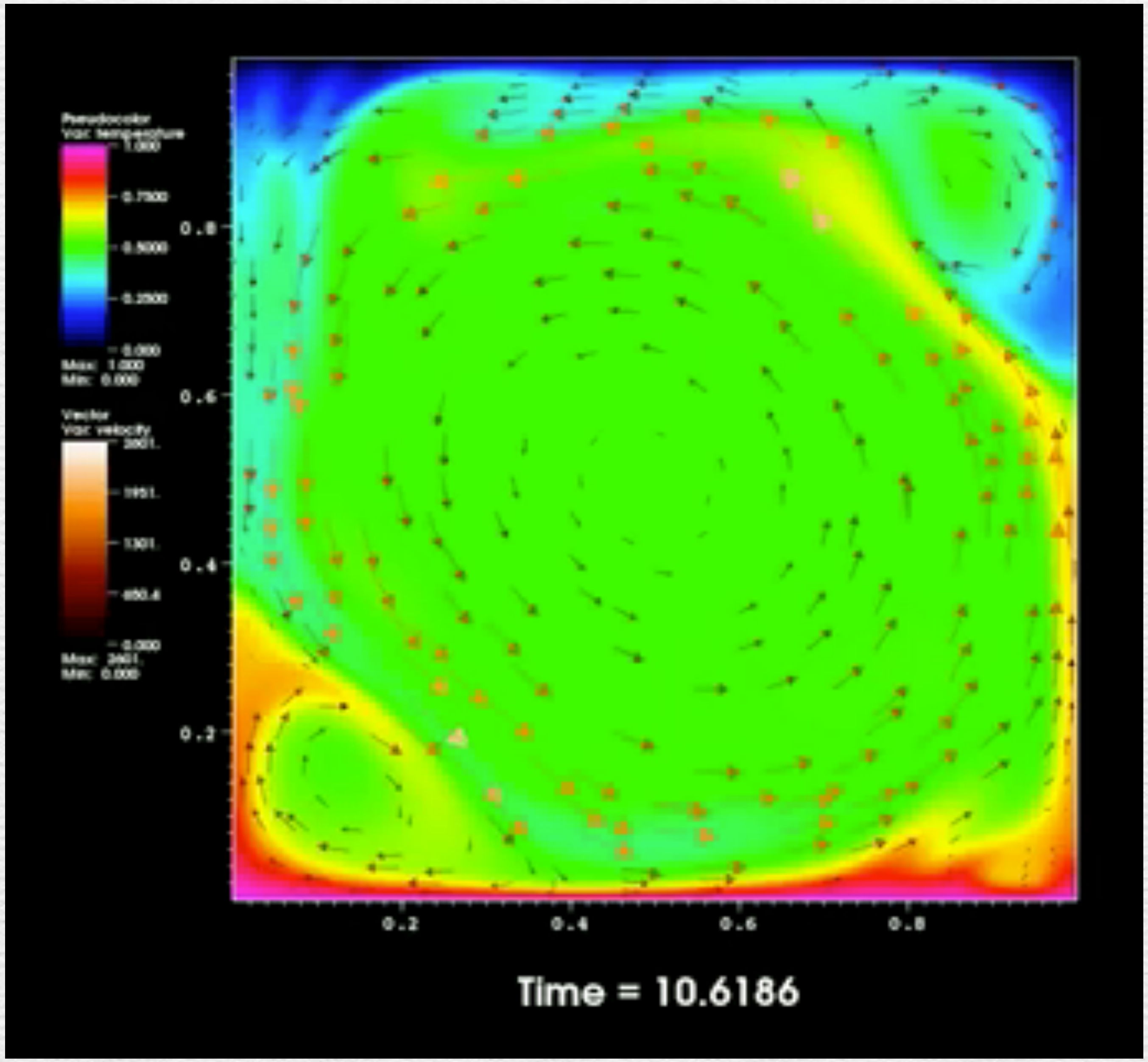




$\theta_K \approx -1/(2n\pi)$

Flow reversal

2D box:Chandra et al. 2010



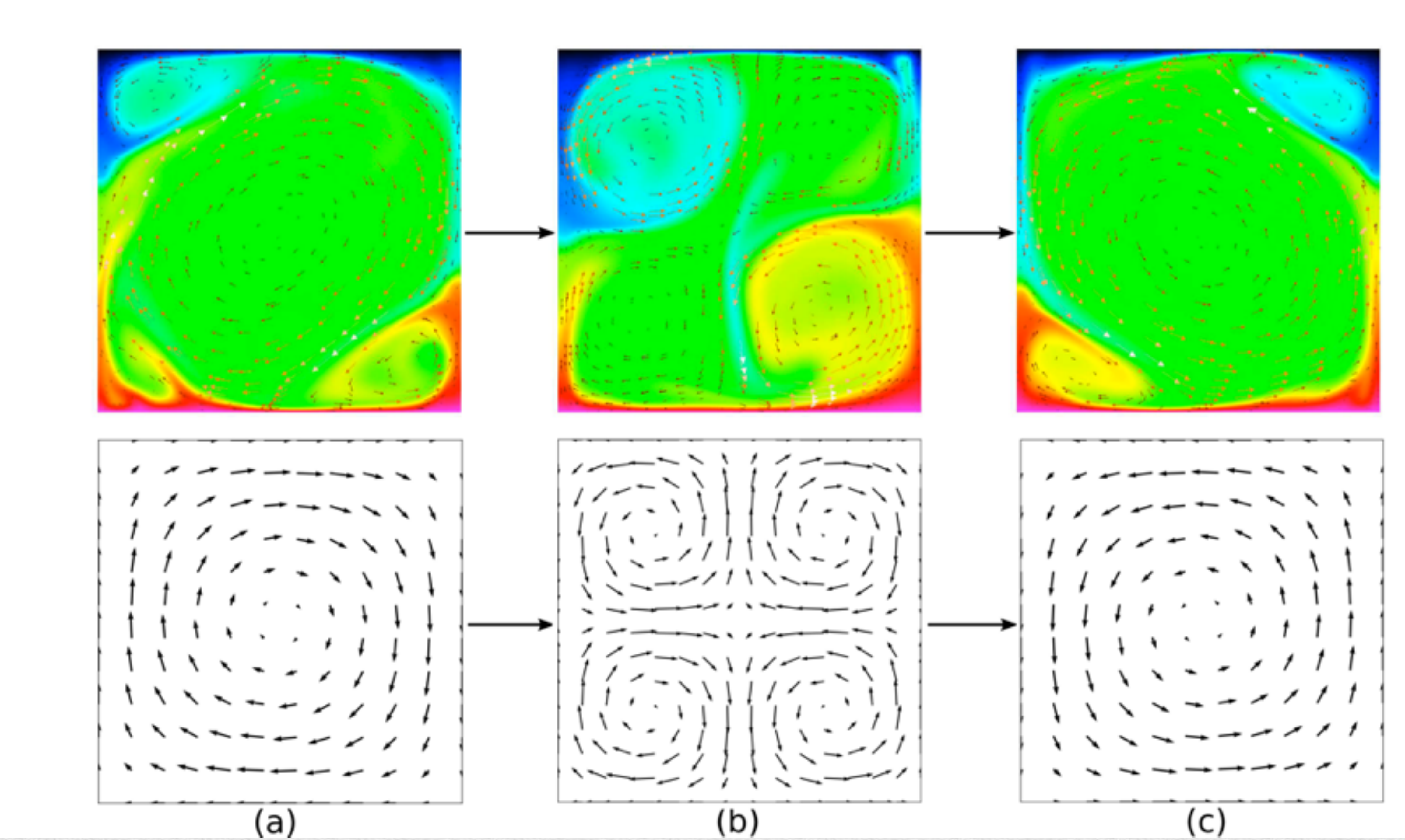
Similar to Sugiyama

28x28 elements
7thx7th order polynomials

Chandra & Verma, PRL 2013

(1,1)->(2,2)->(1,1)

Fourier modes in action



Instability analysis

Prandtl No Pr =0

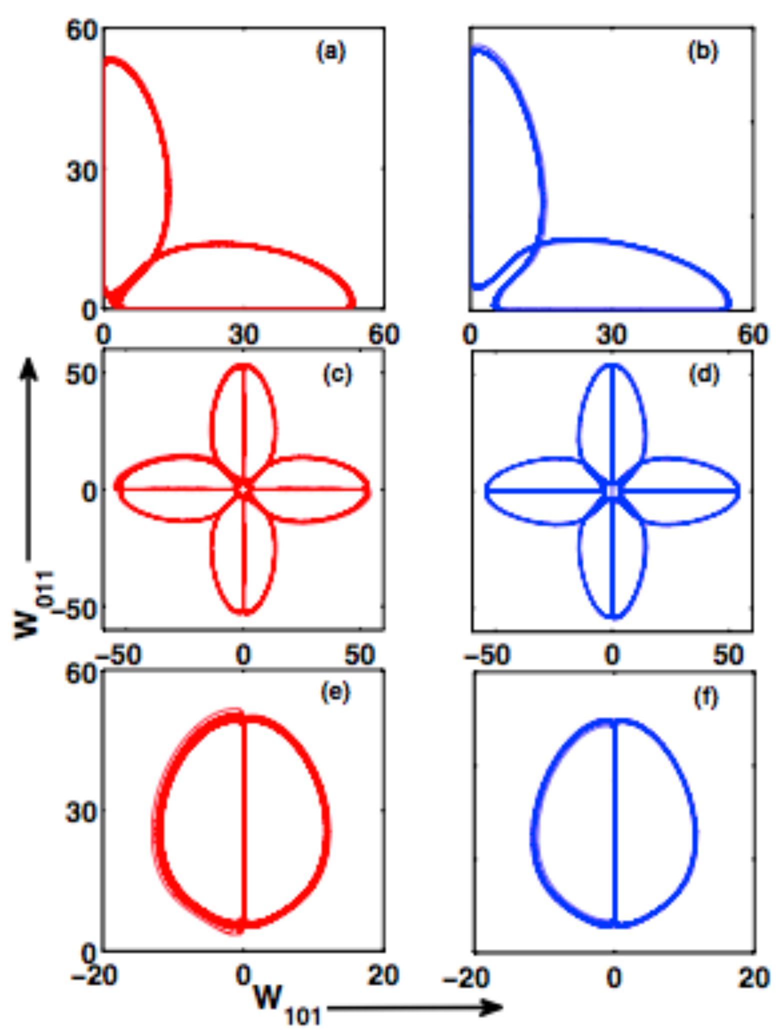
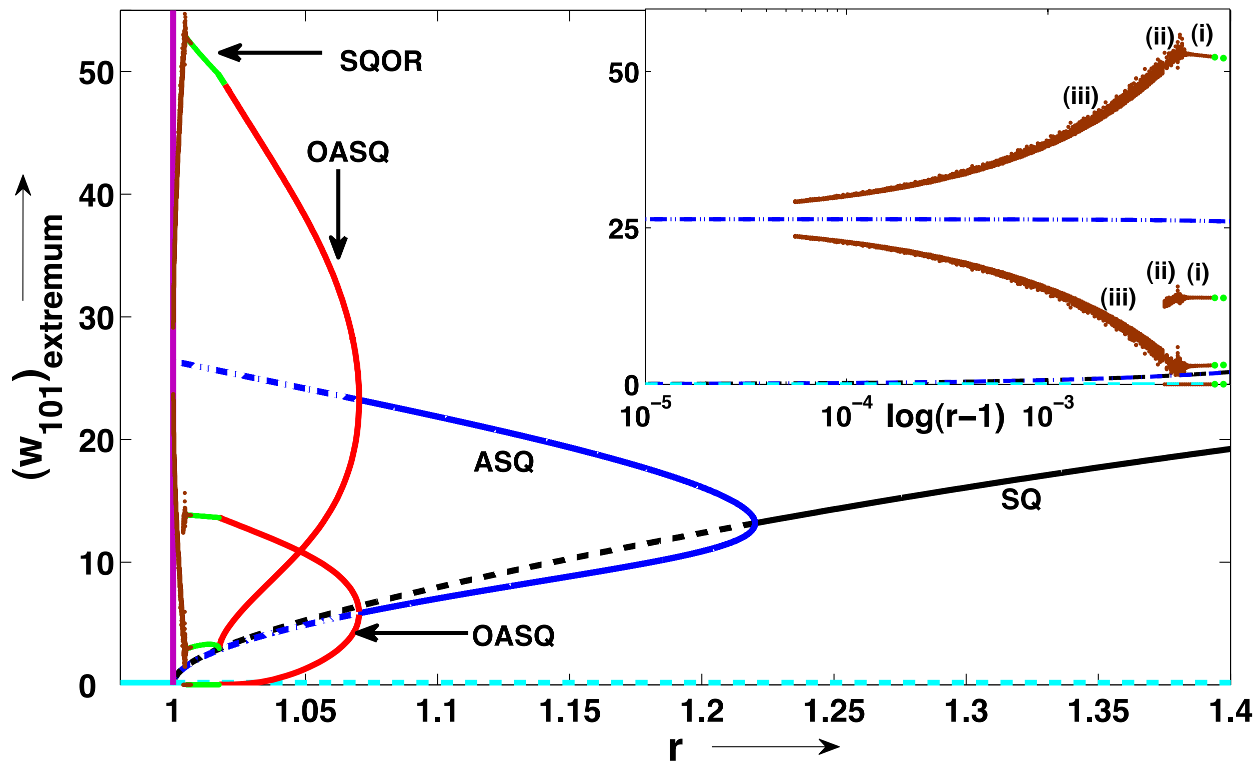
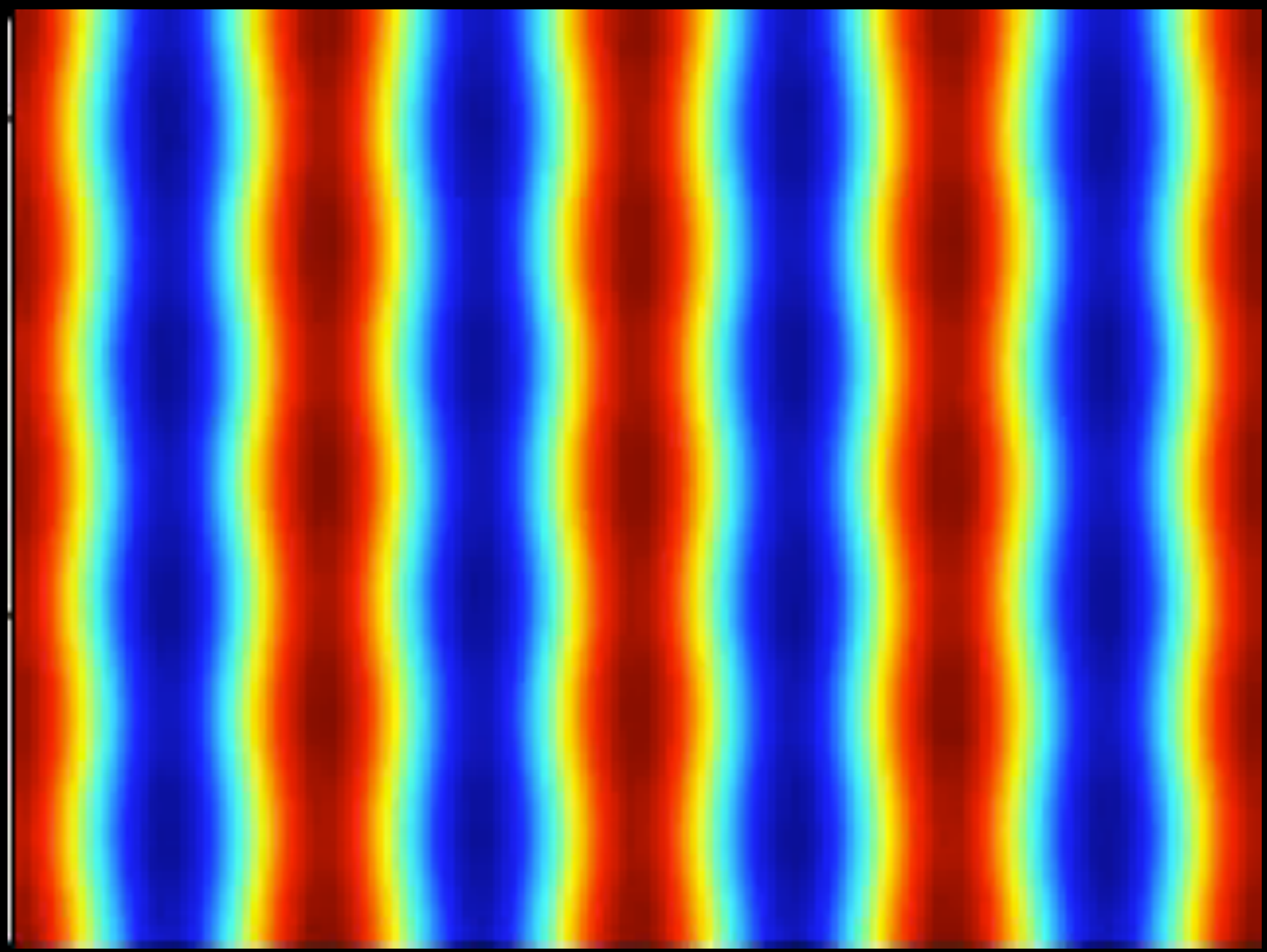


Fig. 5: (Colour on-line) The three different chaotic solutions observed near $r = 1$: Ch1 at $r = 1.0041$ for the model (a) and at $r = 1.0045$ in DNS (b); Ch2 at $r = 1.0038$ for the model (c) and at $r = 1.0030$ in DNS (d); Ch3 at $r = 1.0030$ for the model (e) and at $r = 1.0023$ in DNS (f). These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



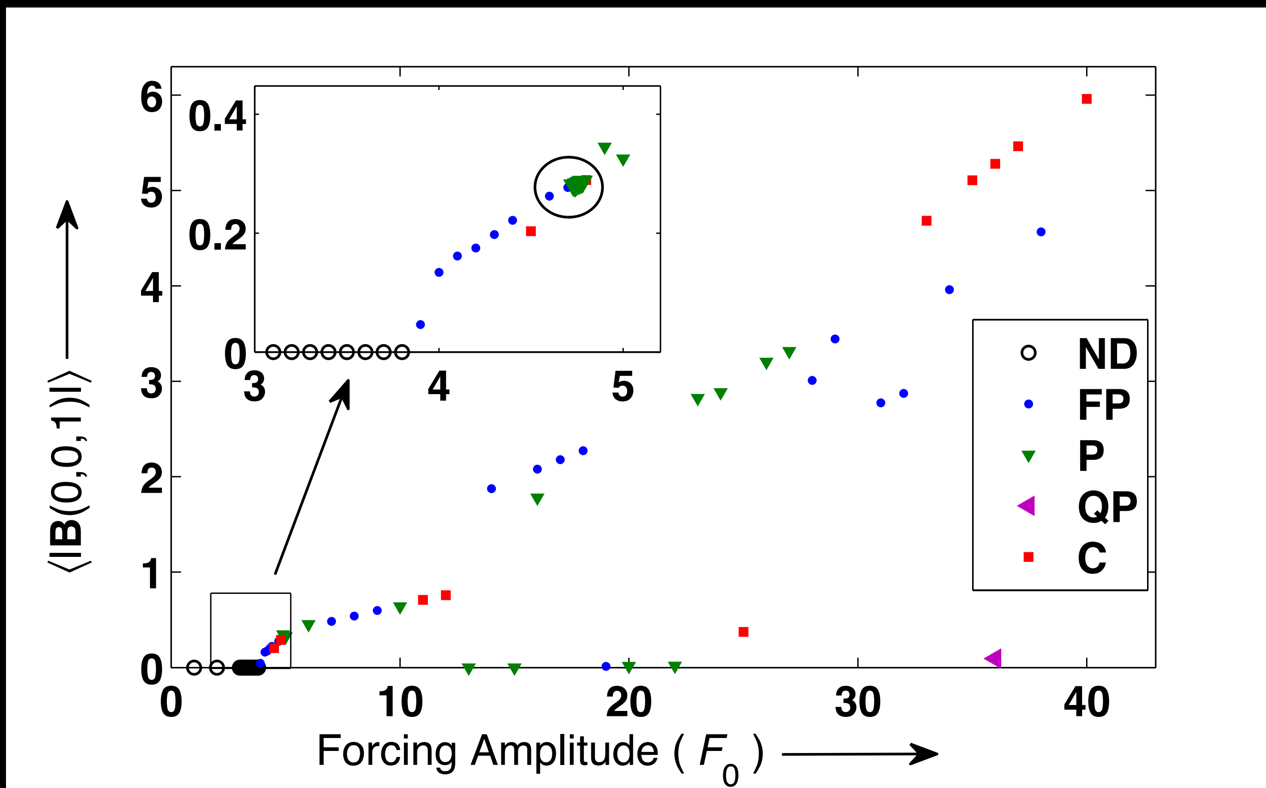
Pal et al., EPL 2009;
Mishra et al., EPL 2010



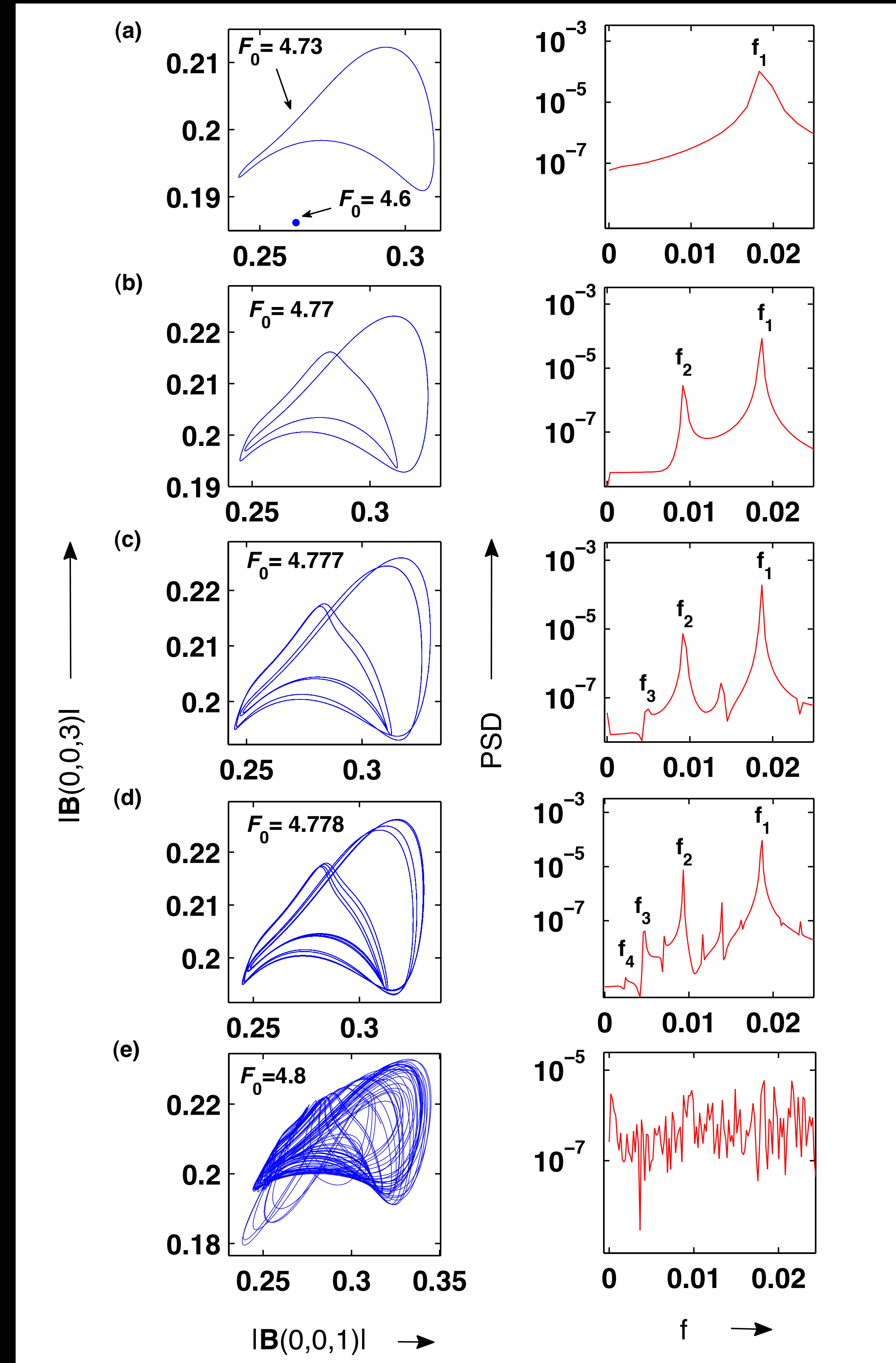
Dynamo simulation

Yadav et al., EPL 2010; PRE, 2012

64^3 128^3



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



(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
f_1
f_2
f_3
f_4
|B(0,0,3)|
PSD
|B(0,0,1)|
f

To Petascale & then Exascale

Finite difference code

General code: Easy porting to GPU, MiC, FPGA

Collaborators:
Gaurav Gautam
Tarang team (IITK)
Fahad Anwer (AMU)
Ravi Samtaney (KAUST)

Acknowledgements

Students:

Anando Chatterjee

Abhishek Kumar

Roshan Samuel

Sandeep Reddy

Mani Chandra

Sumit Kumar & Vijay

Faculty:

Ravi Samtaney

Fahad Anwer

Ported to:

PARAM, CDAC

Shaheen, KAUST

HPC system IITK

Funding

Dept of Science and Tech., India

Dept of Atomic Energy, India

KAUST (computer time)

Invite collaborations

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