ICMM

НАУЧНАЯ КОНФЕРЕНЦИЯ
Суперкомпьютерные дни в России

IIT Kanpur

Multi-node GPU-enabled pseudo-spectral solver «Tarang» for turbulence problems

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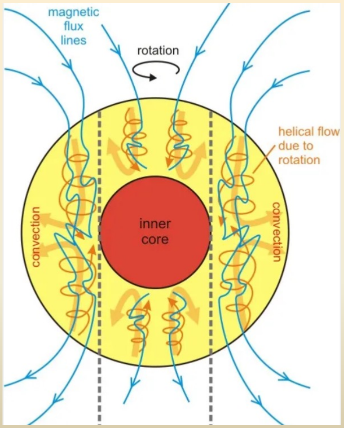
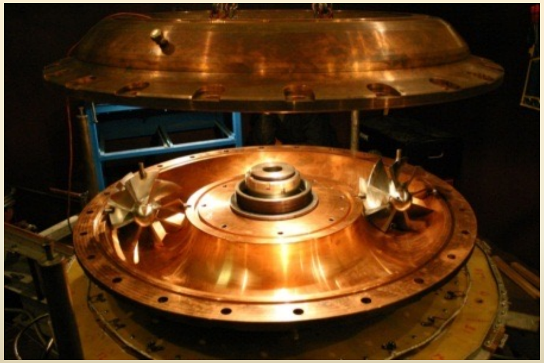
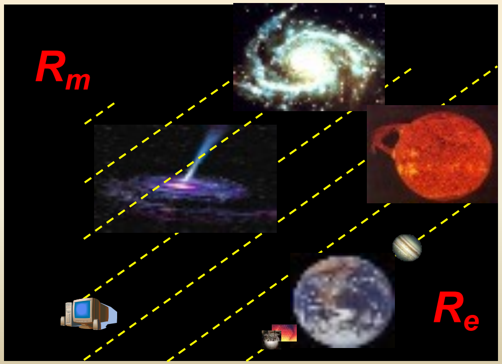
Magnetohydrodynamics of extreme parameters

MHD dynamo

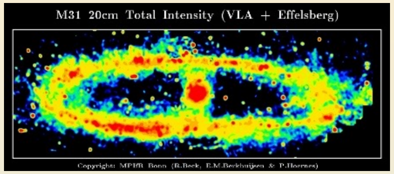




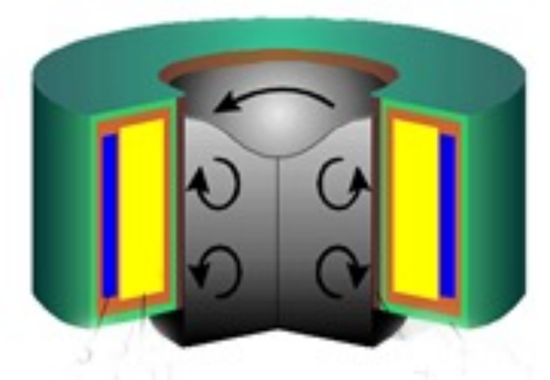
MHD turbulence



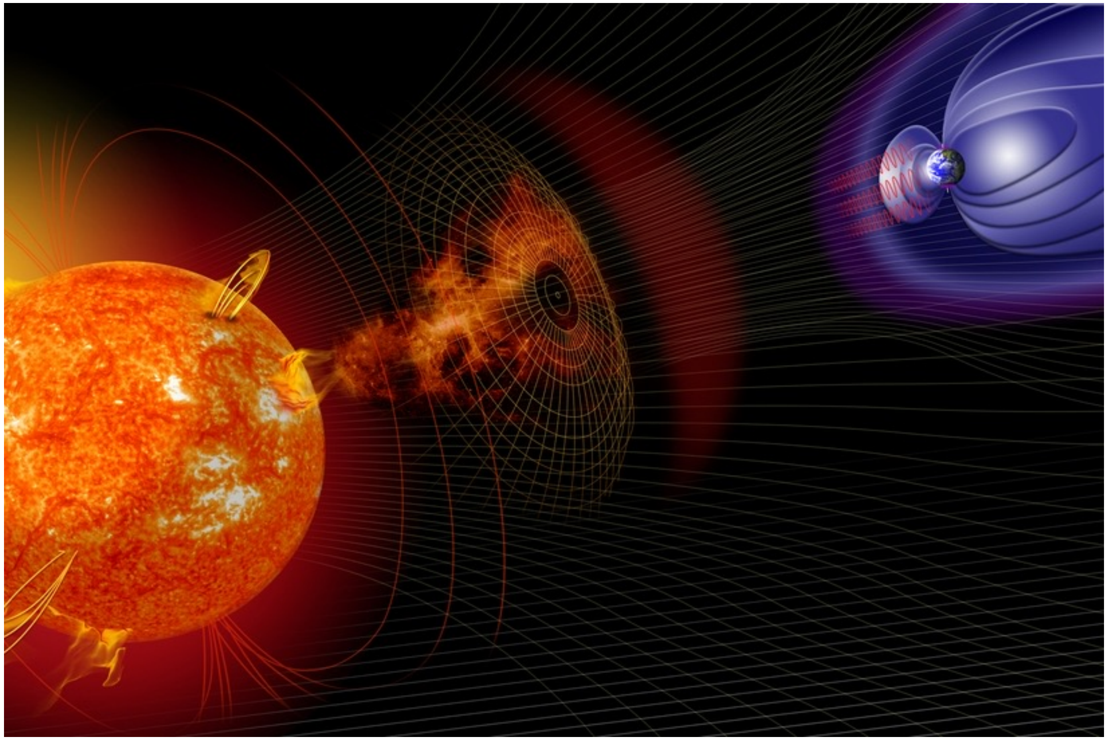
Cosmic magnetic fields



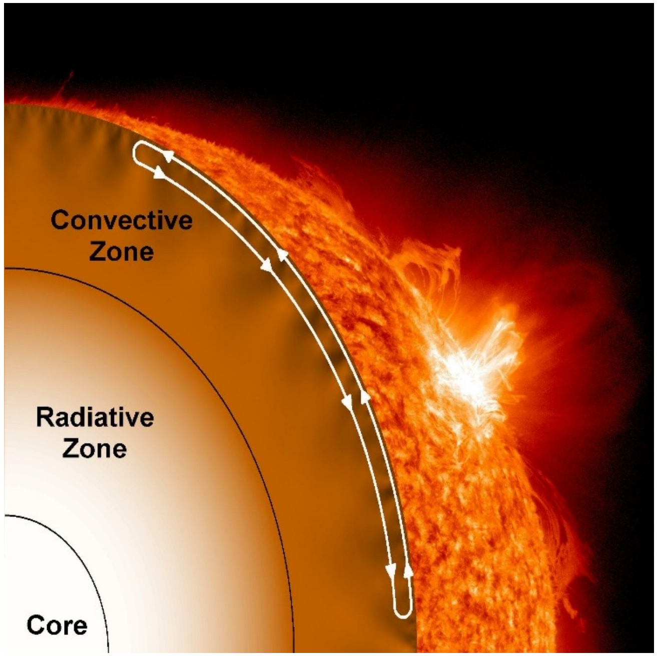
MHD technology



Space battle - “Solar-Dynamo" VS "Earth-Dynamo"



Построение модели солнечного и прогнозирование солнечной активности



Цель работы – верифицировать модели замыкания уравнений среднего поля для турбулентной конвекции с использованием данных прямого численного моделирования и эксперимента.

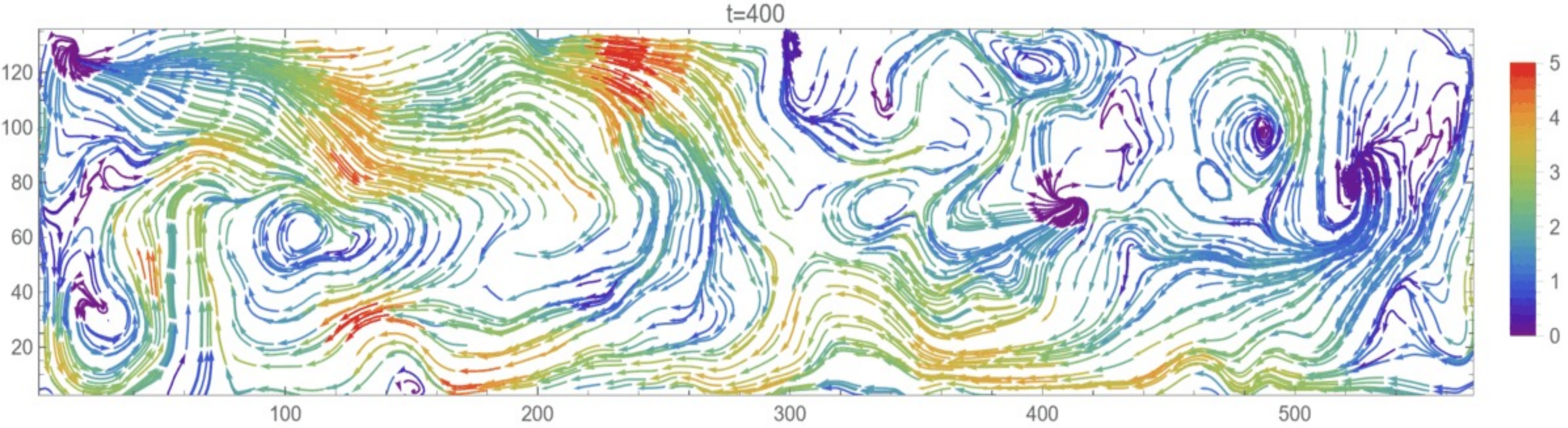
Проект РНФ ОИ-21-72-20067 - Анализ механизмов нерегулярного поведения цикла магнитной активности Солнца на основе численного и лабораторного моделирования анизотропной конвективной турбулентности и обработки наблюдений

Расчеты на суперкомпьютерах: «Ломоносов-2» НИВЦ МГУ, «Уран» ИММ УрО РАН

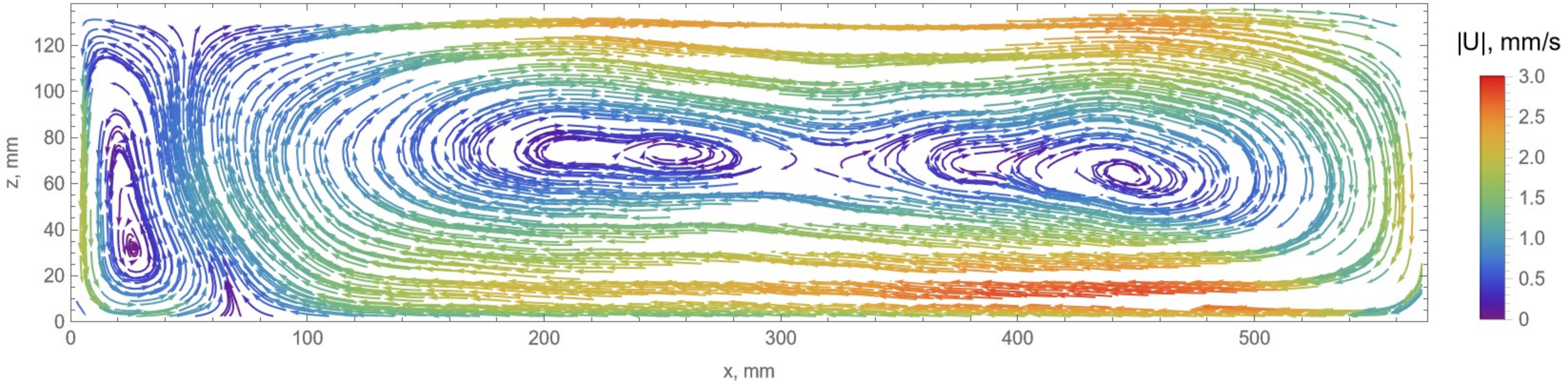
Turbulent convection in horizontally extended cell

Evolution in time

Velocity streamlines in vertical plain



After averaging



Governing equations of MHD

$$\partial_t \mathbf{U} + \mathbf{U}\cdot\boldsymbol{\nabla}\mathbf{U} = \rho^{-1}(-\boldsymbol{\nabla}P + \mathbf{j}\times\mathbf{B}) + \nu\Delta\mathbf{U},$$

$$\partial_t \mathbf{B} = \boldsymbol{\nabla}\times(\mathbf{U}\times\mathbf{B}) + \eta\Delta\mathbf{B},$$

$$\boldsymbol{\nabla}\cdot\mathbf{U} = 0,$$

$$\boldsymbol{\nabla}\cdot\mathbf{B} = 0.$$

Dimensionless form

$$\partial_t \mathbf{U} + \mathbf{U}\cdot\boldsymbol{\nabla}\mathbf{U} - \mathbf{B}\cdot\boldsymbol{\nabla}\mathbf{B} = -\boldsymbol{\nabla}(P + B^2/2) + \mathrm{Re}^{-1}\Delta\mathbf{U},$$

$$\partial_t \mathbf{B} + \mathbf{U}\cdot\boldsymbol{\nabla}\mathbf{B} - \mathbf{B}\cdot\boldsymbol{\nabla}\mathbf{U} = \mathrm{Rm}^{-1}\Delta\mathbf{B},$$

$\mathrm{Re} = LU/\nu$ - Reynolds number

$\mathrm{Rm} = LU/\eta$ - magnetic Reynolds number

$\mathrm{Pm} = \mathrm{Rm}/\mathrm{Re} = \nu/\eta$ - magnetic Prandtl number

Conservation laws

при $\nu = \eta = 0,\qquad \dot{E} \square \dot{H}_C \square \dot{H}_m \square 0$

$$\mathcal{H} = \int \boldsymbol{u} \cdot \boldsymbol{\omega} \, dV$$

- hydrodynamic helicity

$$H_m = \int_V \mathbf{A} \cdot \mathbf{B} dV$$

- magnetic helicity (**A** is the vector potential of the magnetic field)

$$H_c = \int_V \mathbf{u} \cdot \mathbf{B} dV$$

- Cross helicity

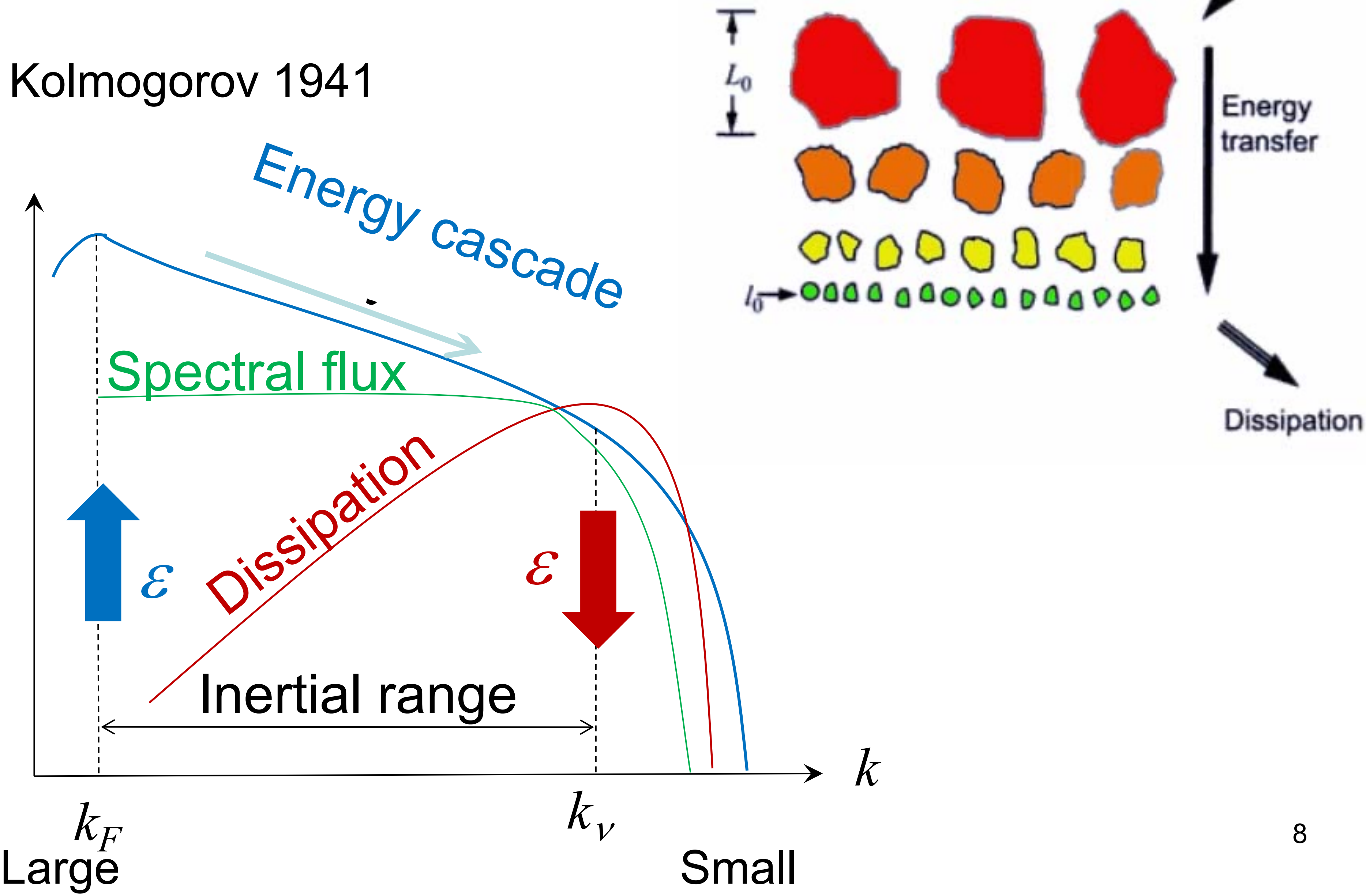
$$E = \int_V \rho \mathbf{u}^2/2 + \mathbf{B}^2/(2\mu) dV$$

- Total energy

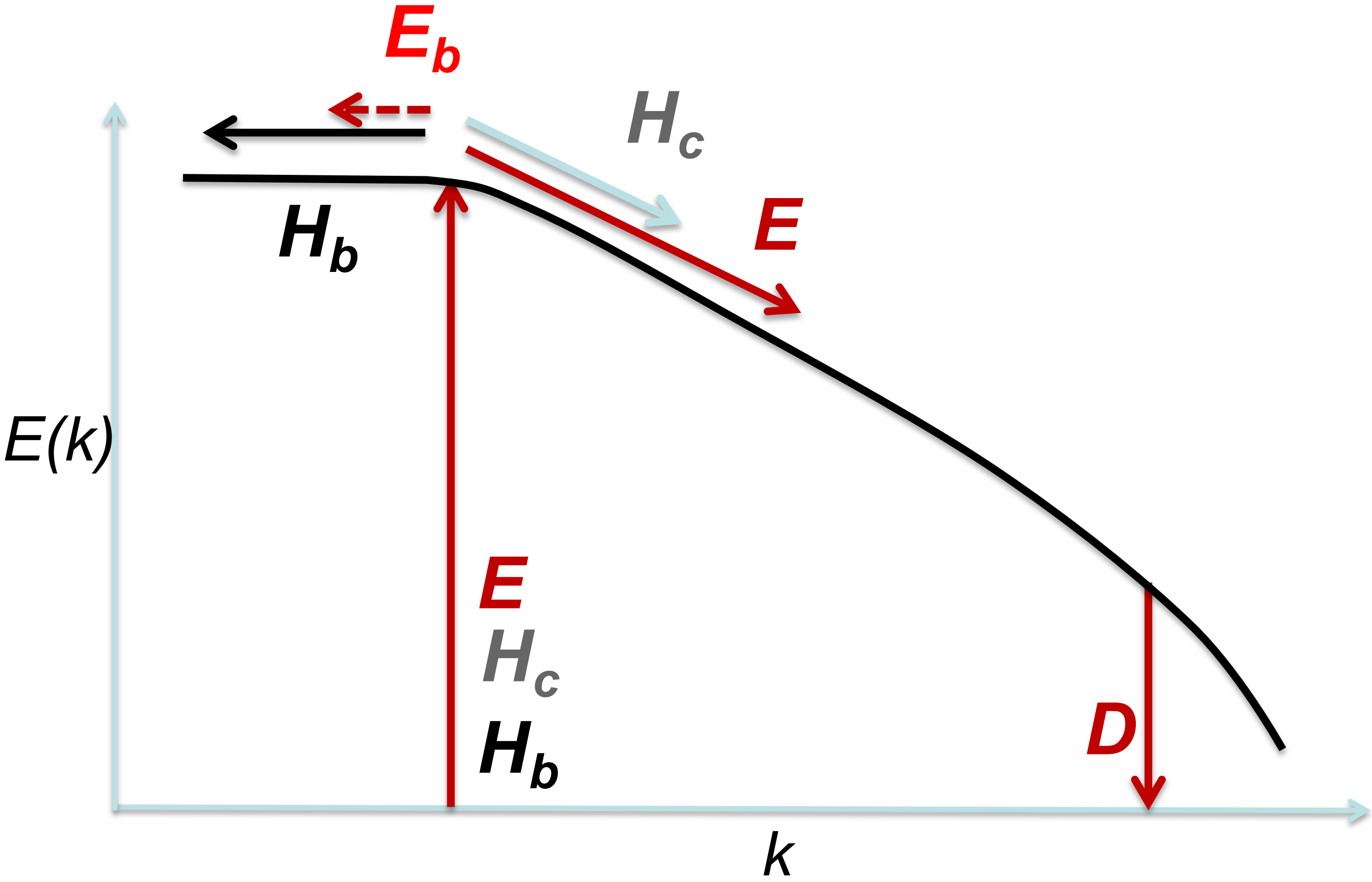
Concepts of turbulence

Richardson 1926

Kolmogorov 1941

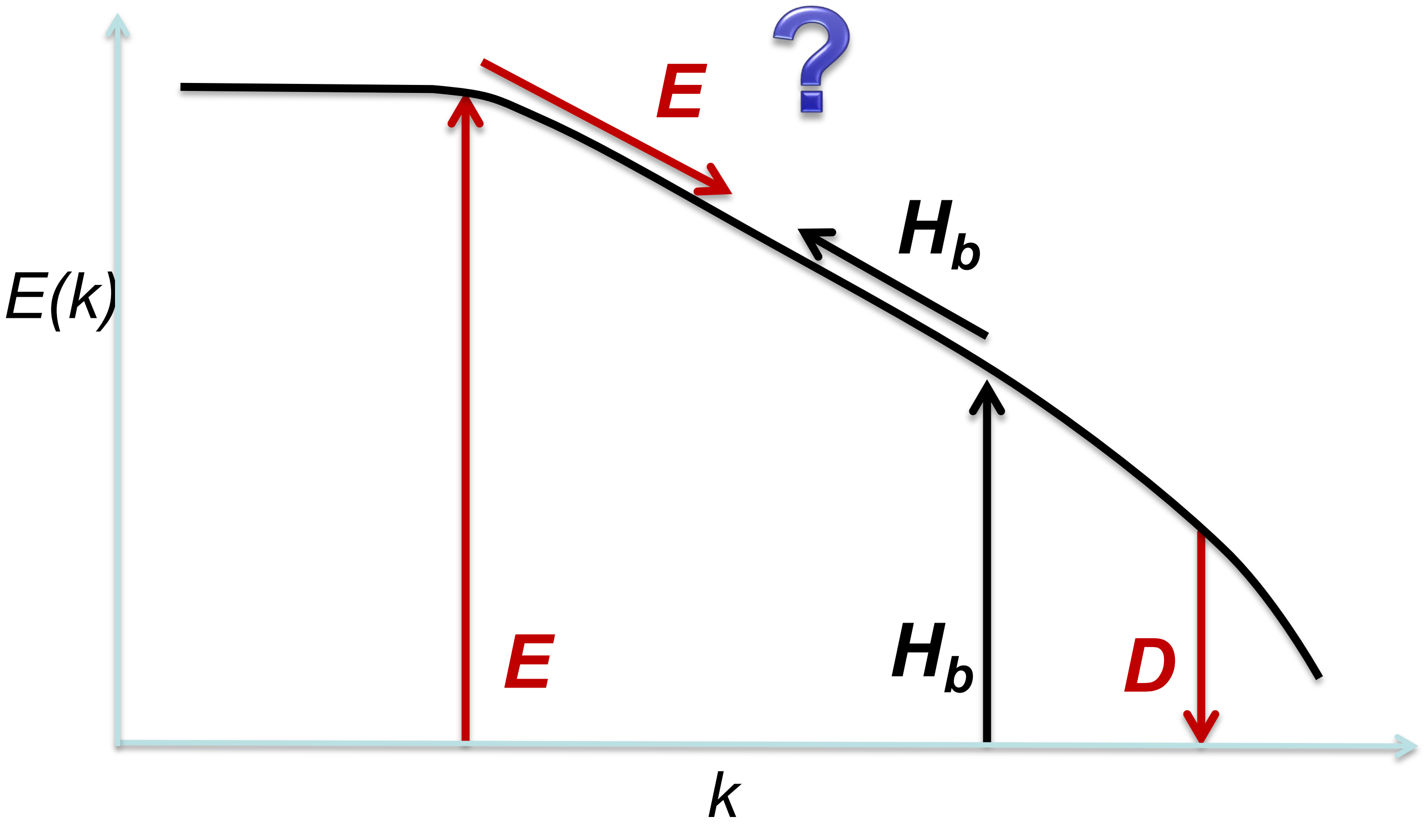


Joint injection of energy, helicities



Stepanov R., Frick P., Mizeva I. // Magnetohydrodynamics, 2013. V.49. N.1-2. P.15-21.

Separate injections of energy and magnetic helicity

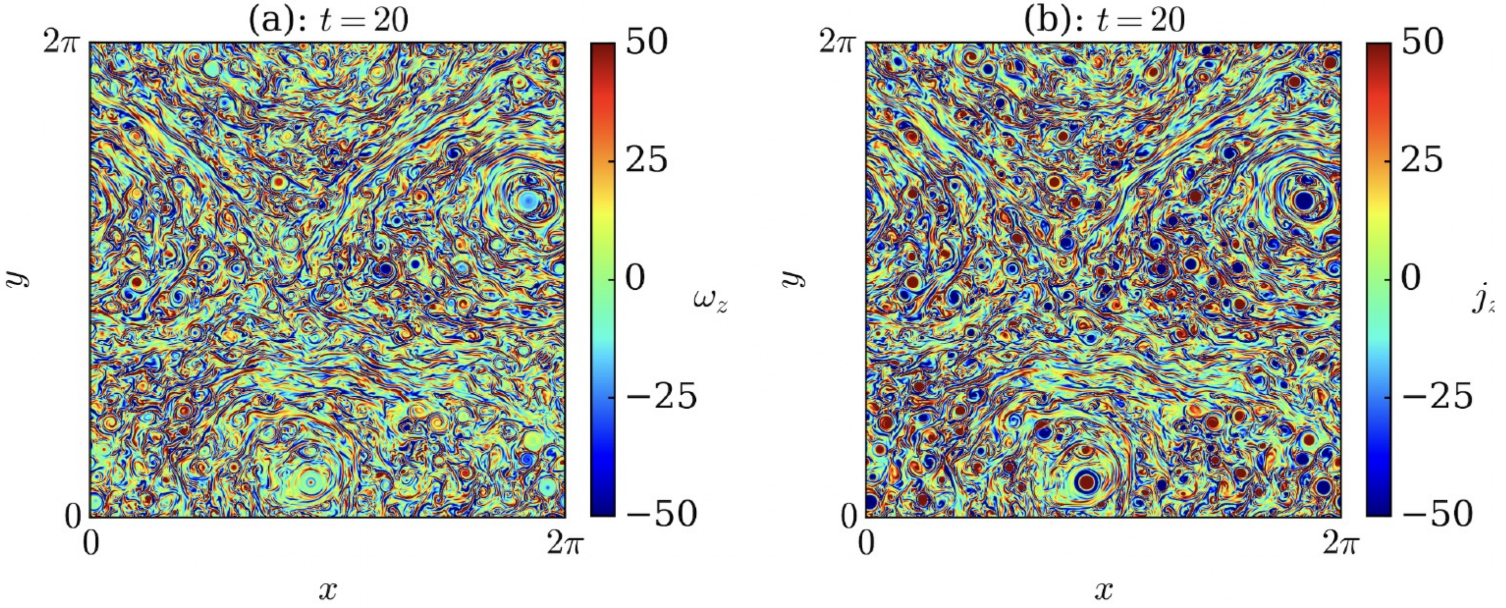


«Magnetic bottleneck effect»

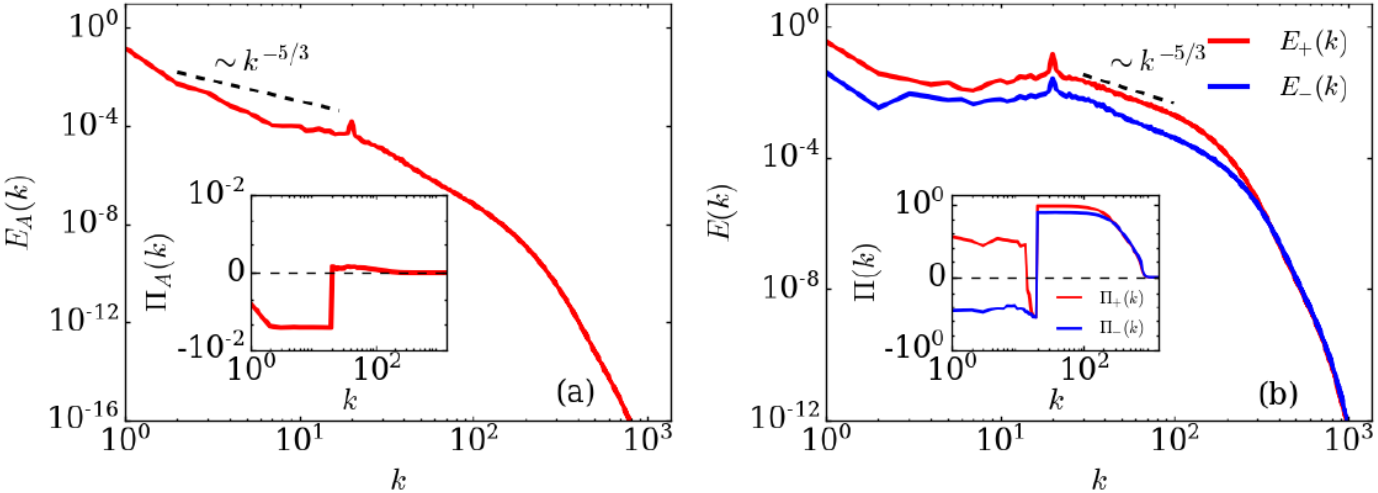
R. Stepanov, P. Frick, and I. Mizeva **Joint inverse cascade of magnetic energy and magnetic helicity in MHD turbulence // Astrophysical Journal Letters, 798:L35, 2015.**

Solving 2D MHD turbulence using TARANG (grid 4096^2)

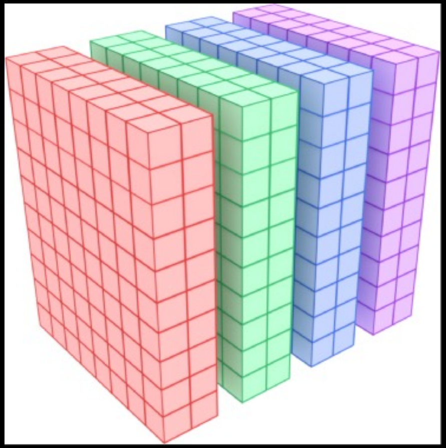
Real space distributions of vorticity and current density



Spectra and spectral fluxes



«Tarang» - psudo-spectral solver



C++ (Tarang[1,2]) [CPU]

C++ (Cuda) [GPU]

Python (CuPy) [GPU]

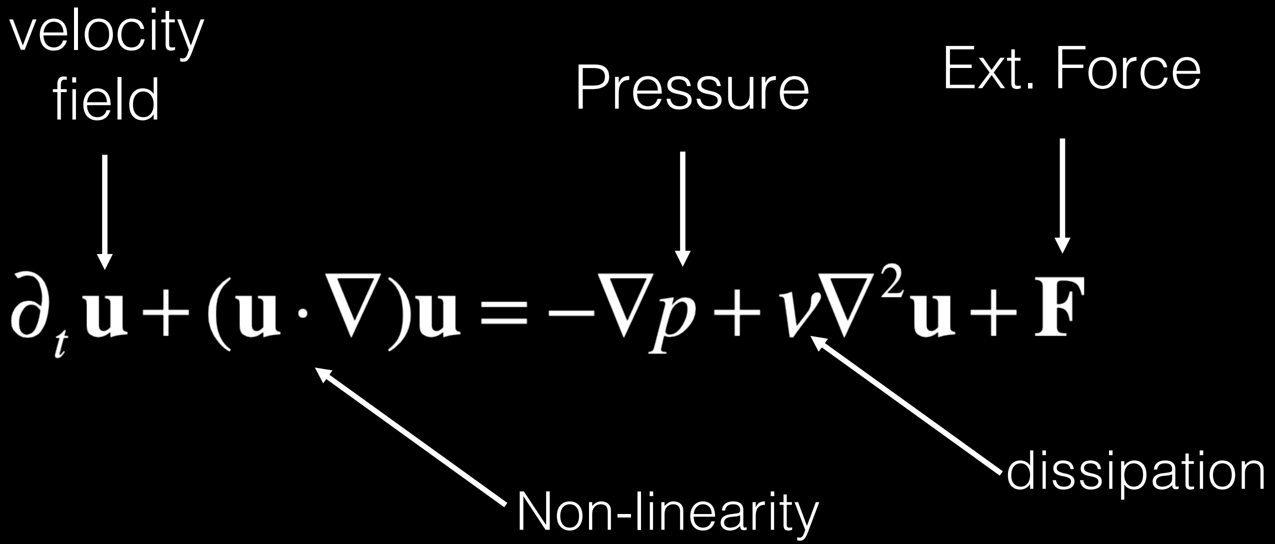
- Object-oriented design
- General PDE solver → Fluid, MHD, Convection etc.

http://turbulencehub.org

[1] Verma et al., Pramana-J. Phys., **81**, 617 (2013)

[2] Chatterjee et al., J. Parallel Distrib. Comput., 113, 77 (2018)

Incompressible Eqns



velocity field

Pressure

Ext. Force

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

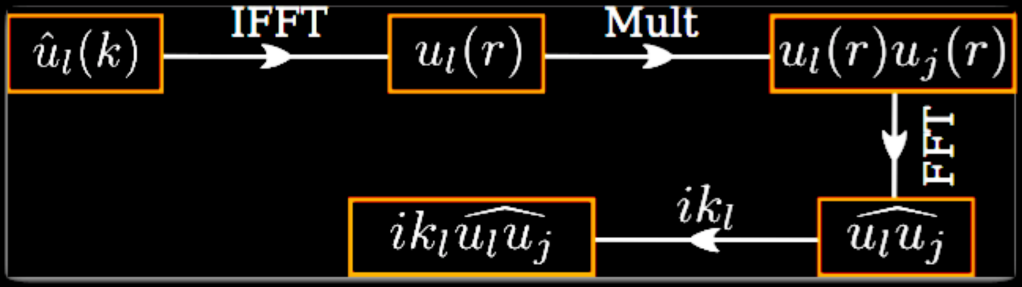
Non-linearity

dissipation

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

Incompressibility

Nonlinear term computation:



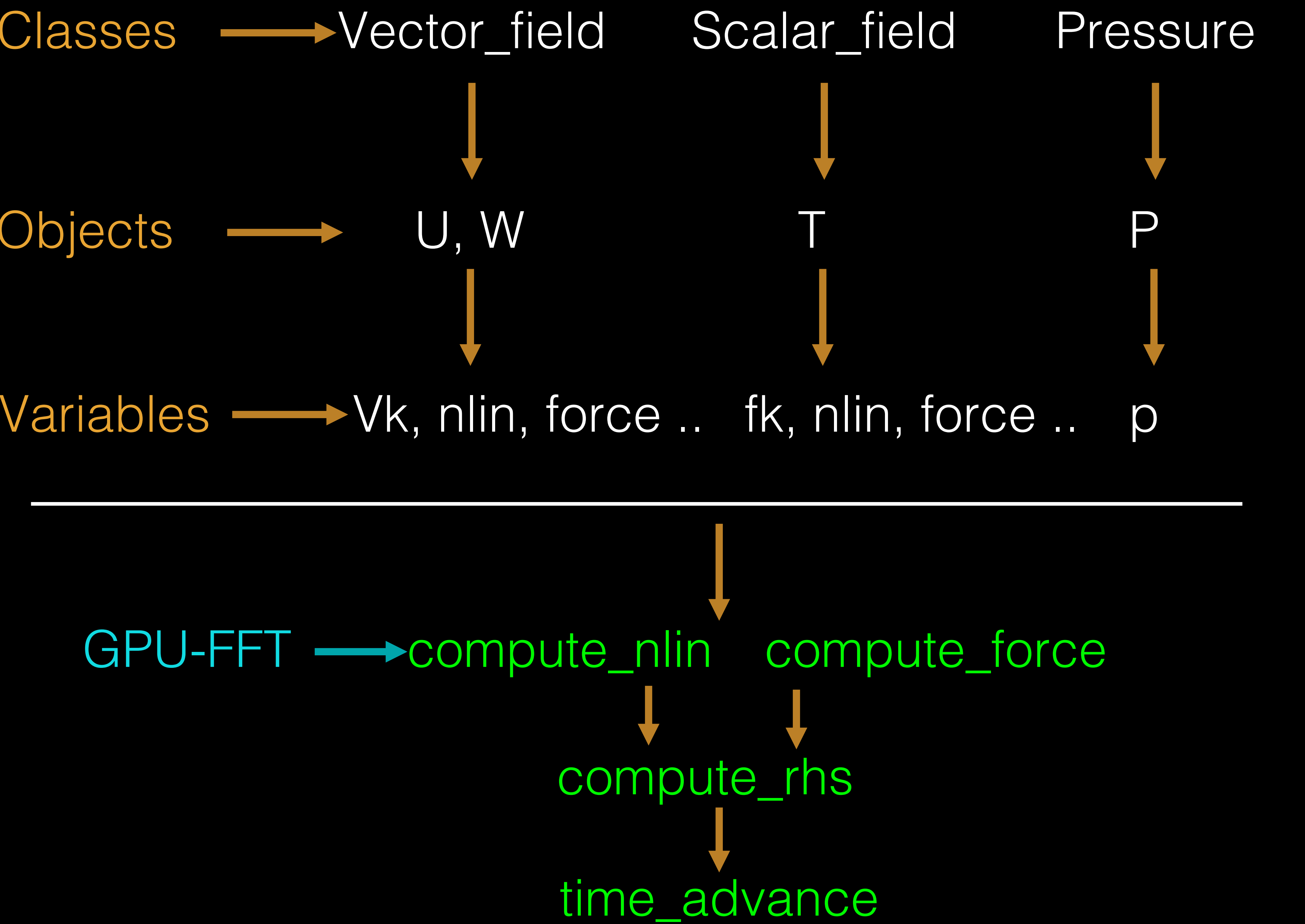
(pseudo-spectral)

Fourier transforms take around 80 % of total time.

↓

ported to GPU → GPU-FFT

Scalable Multi-node Fast Fourier Transform on GPUs
Manthan Verma et al., arXiv:2202.12756 (2022)



Classes → Vector_field Scalar_field Pressure

Objects → U, W T P

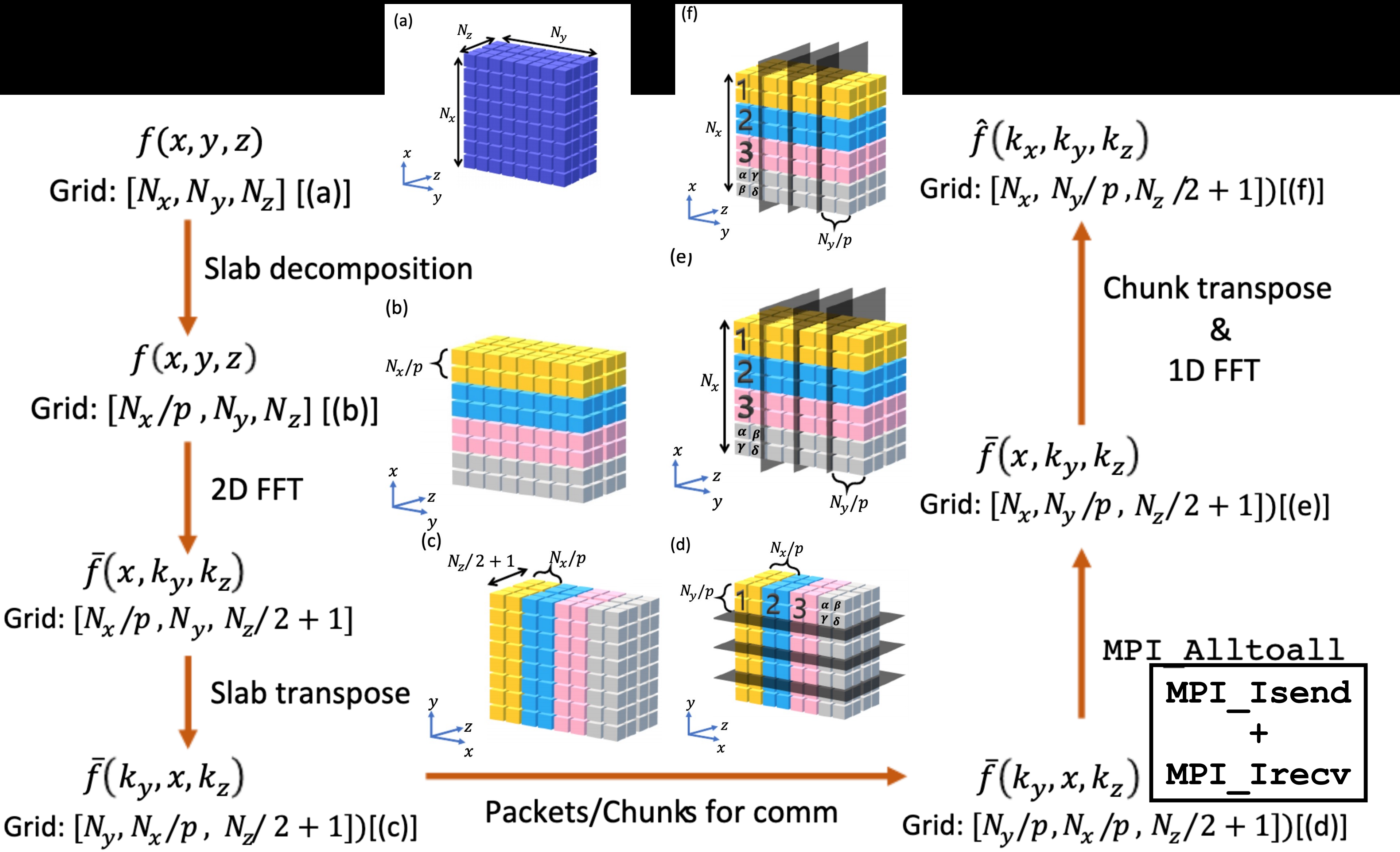
Variables → Vk, nlin, force .. fk, nlin, force .. p

GPU-FFT → compute_nlin compute_force

compute_rhs

time_advance

SLAB decomposition



$f(x,y,z)$

Grid: $[N_x, N_y, N_z]$ [(a)]

Slab decomposition

$f(x,y,z)$

Grid: $[N_x/p, N_y, N_z]$ [(b)]

2D FFT

$\bar{f}(x,k_y,k_z)$

Grid: $[N_x/p, N_y, N_z/2+1]$

Slab transpose

$\bar{f}(k_y,x,k_z)$

Grid: $[N_y, N_x/p, N_z/2+1])$[(c)]

Packets/Chunks for comm

$\bar{f}(k_y,x,k_z)$

Grid: $[N_y/p, N_x/p, N_z/2+1])$[(d)]

`MPI_Alltoall`

`MPI_Isend`
+
`MPI_Irecv`

$\bar{f}(x,k_y,k_z)$

Grid: $[N_x, N_y/p, N_z/2+1])$[(e)]

Chunk transpose
&
1D FFT

$\hat{f}(k_x,k_y,k_z)$

Grid: $[N_x, N_y/p, N_z/2+1])$[(f)]

Codes	Grid sizes	Time
FFTK (Shaheen II)	$1536^3, 3072^3$	42 ms, 179 ms
GPU-FFT (128 GPU)	2048^3	74 ms

- For a pair of double-precision forward and backward transforms.
- FFTK runs using12288 processors on Cray XC 40 (*Shaheen II*).
- GPU-FFT runs on 128 A100 GPUs on *Selene*.

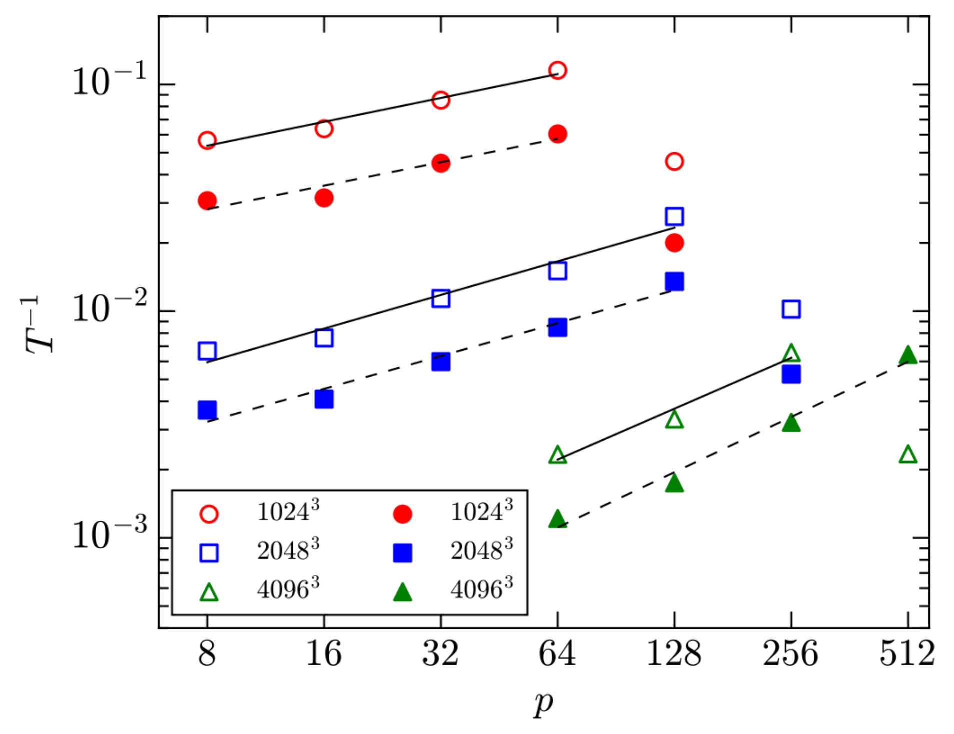
Selene supercomputer:

- 540 DGX boxes x 8 A100 GPU cards/box,
- NVSwitch and NVLink

Shaheen II, Cray XC40

- 196608 cores

Strong scaling



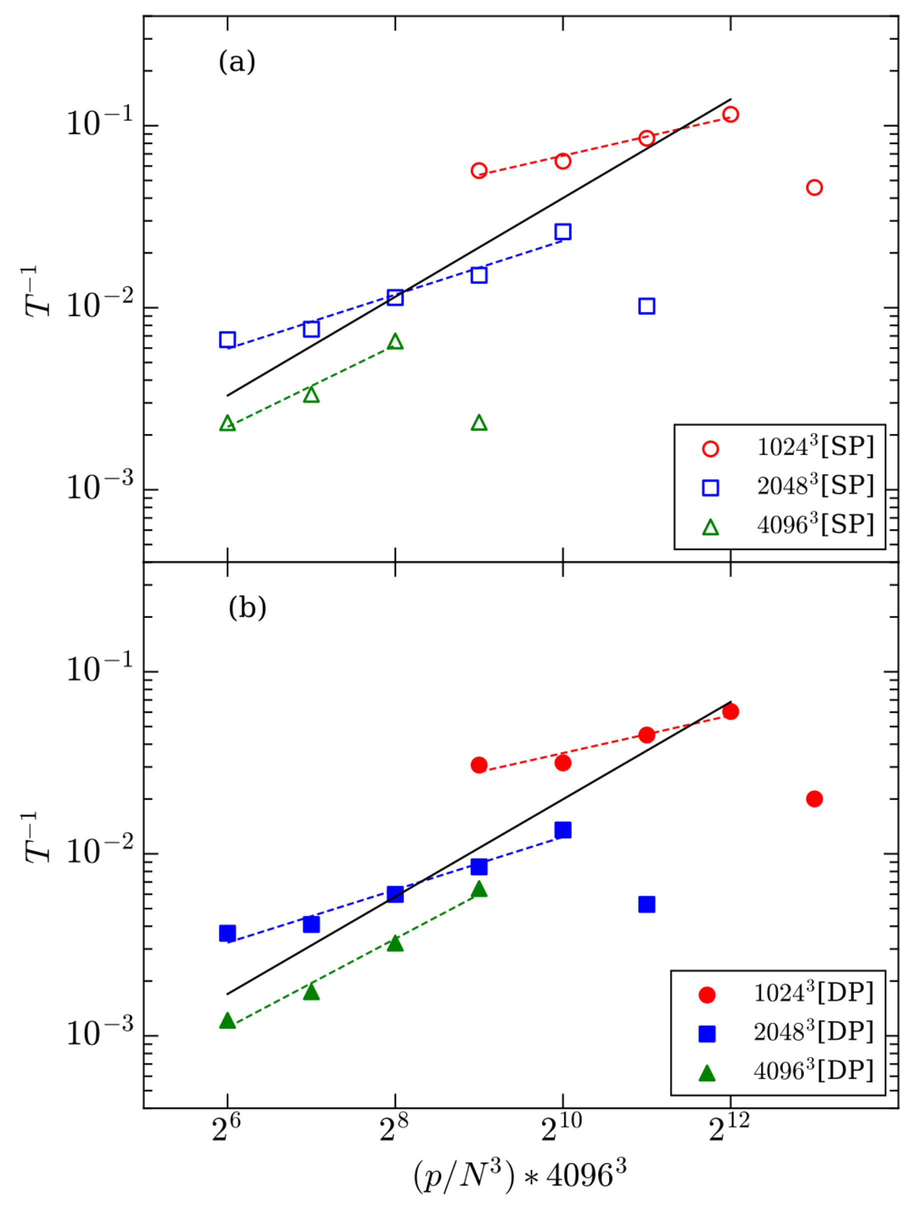
$$T^{-1} = Cp^{\gamma}$$

p = no. of GPUs,

T = total time in ms for a pair of transforms

Grid size	γ	
	SP	DP
1024^3	0.35 ± 0.05	0.34 ± 0.07
2048^3	0.49 ± 0.06	0.48 ± 0.05
4096^3	0.75 ± 0.13	0.71 ± 0.11

Weak scaling



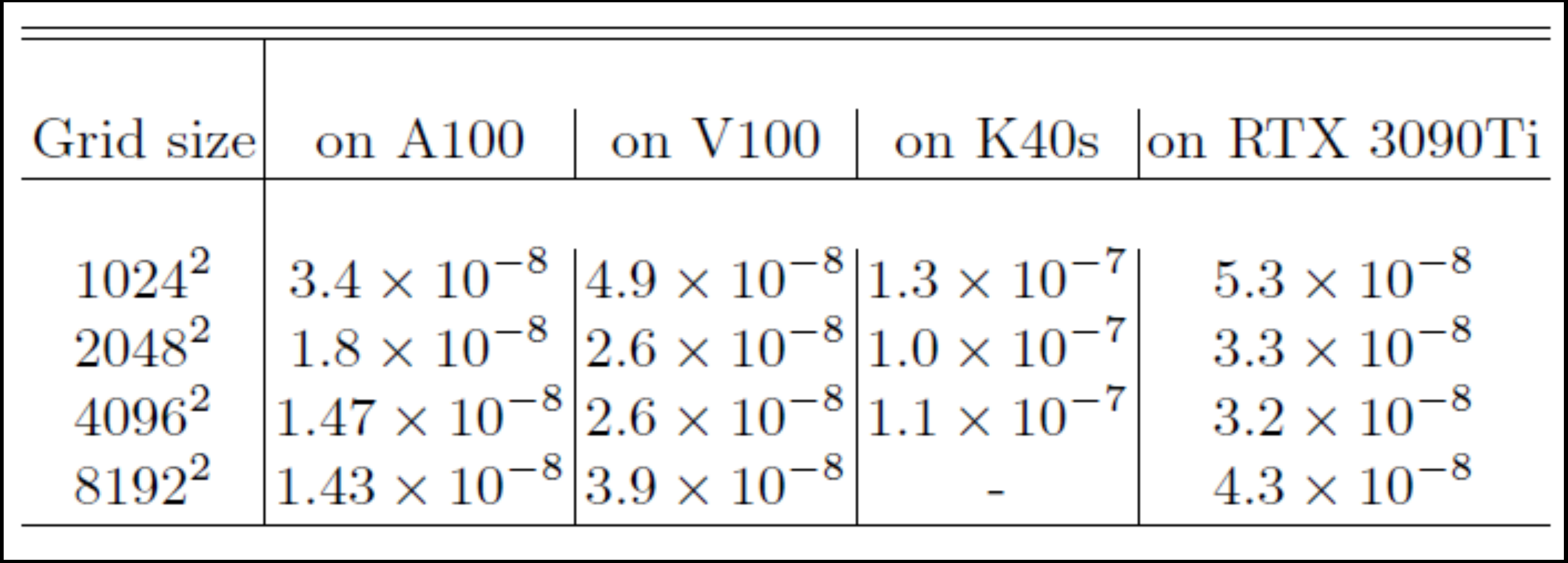
$$T^{-1} \sim p^{0.9}$$

timings

Grid size	CPU [Single Core]	Cuda-solver	Cupy-solver
512^3	~ 3 days	~ 5 mins	~15 mins
		1300 X	500 X

- 1000 time steps of hydro solver on single core CPU (Rome Processor) and a single A100 GPU.

Scaling of TARANG on single GPU: the timings (in secs) per step per grid point



Grid size	on A100	on V100	on K40s	on RTX 3090Ti
1024^2	3.4×10^{-8}	4.9×10^{-8}	1.3×10^{-7}	5.3×10^{-8}
2048^2	1.8×10^{-8}	2.6×10^{-8}	1.0×10^{-7}	3.3×10^{-8}
4096^2	1.47×10^{-8}	2.6×10^{-8}	1.1×10^{-7}	3.2×10^{-8}
8192^2	1.43×10^{-8}	3.9×10^{-8}	-	4.3×10^{-8}

Availability NVLink and NVSwitch are crucially important for multi-GPUs

Conclusions

- GPUs are key accelerators.
- They accelerate spectral solver many folds (~1000).
- Welcome to use open-source code «TARANG»

http://turbulencehub.org