

Numerical simulations of highly turbulent flows

PhD

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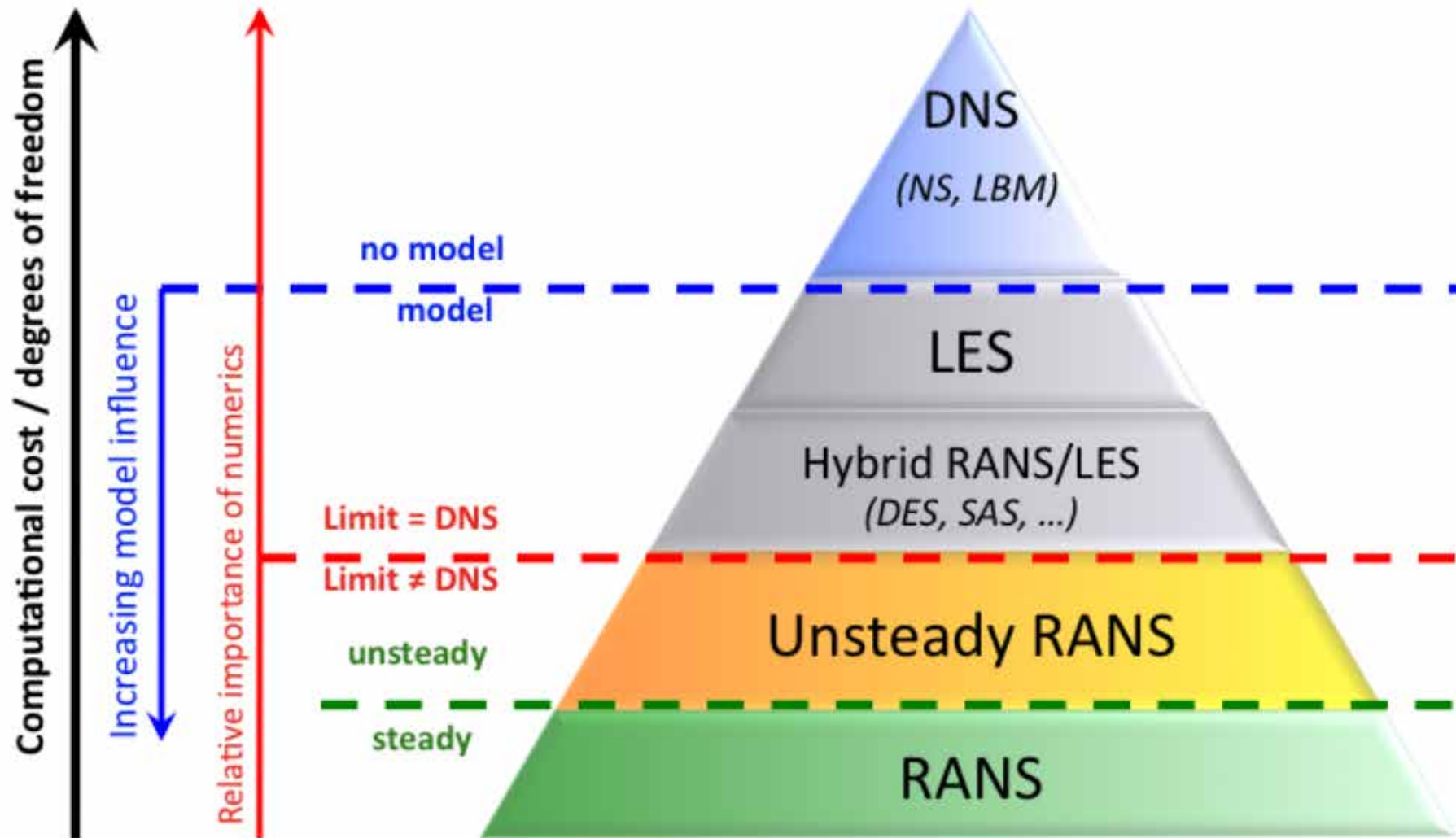
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Physics of Fluids

UNIVERSITY OF TWENTE.

Modeling approaches



Multiscale & Multiresolution approaches for turbulence

Sagaut, Deck & Terracol, Imperial College Press, 2006

Industrial framework

- Need to simulate complex flows
 - Multi-components problems (airplane, car)
 - Non-homogeneous flows
 - High Reynolds numbers
 - Multi phase or reacting flows
- Need a result in 1 hour to maximum 1 day
 - Research and development tool
 - Large number of parameters to investigate
- Limited computational resources
- The cost of the numerical simulations is important

- Need fast and robust methodologies
- Does not have the time to understand the physics.

Research framework

- Restricted to simple (or simplified) geometries
 - Isotropic turbulence (period boundary conditions)
 - Turbulent boundary layer flows
 - Rayleigh-Benard flow
 - Pipe, channel flow, etc.
- Not limited in time: can afford a one year simulation
- Access to largest computers (>10 Peta Flops)
- The cost is not so important
 - The cost is focused in some large simulations
 - The data are accessible to the research community
 - Cost needs to be related to the scientific outcome
- Numerical simulation is a tool to understand physics
- Need optimized algorithm and accurate results

Industrial and research practices

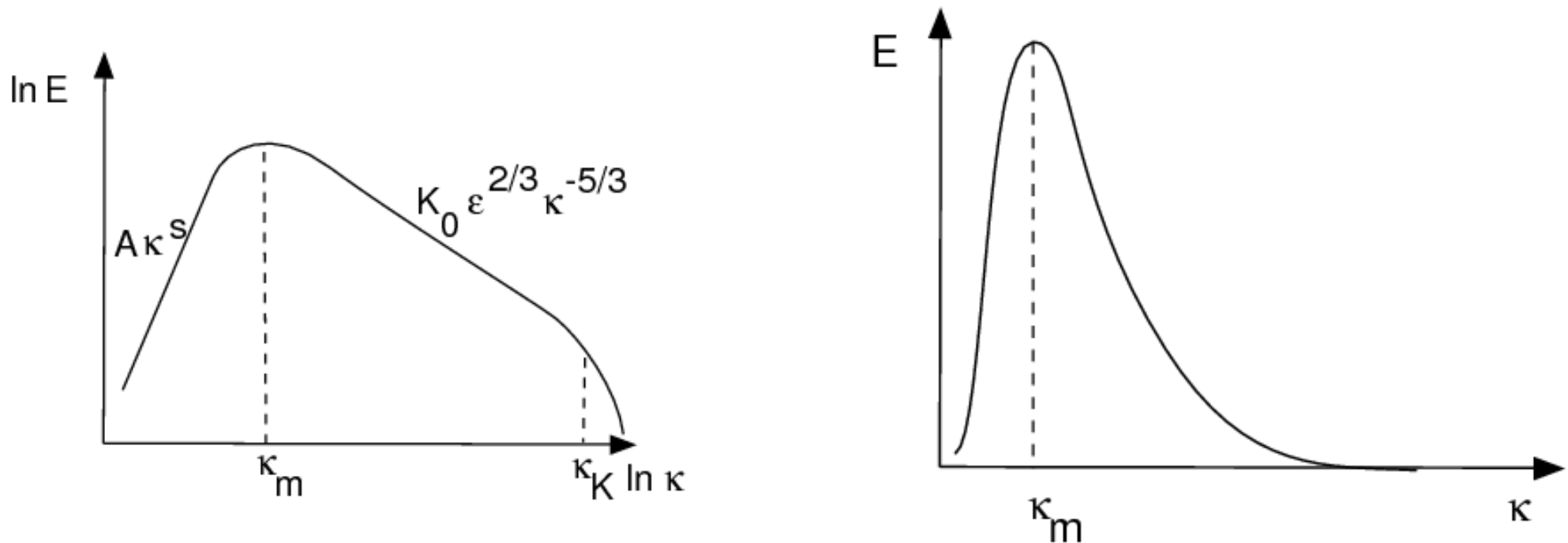
- Industrial practices
 - Most of simulations in steady states (RANS models)
 - Unsteady simulations restricted to specific parts of the flow (URANS, DES, LES)
 - Use of robust numerical techniques (usually not accurate)
- Research practice
 - Interest on unsteady flows (turbulence) to understand the physics
 - Increasing popularity and use of DNS and LES
 - Intensive research on turbulence models
 - Increasing number of LES models since 1980's
 - New development in RANS models (more than 100 models !)

How to select your model?

- What is the Reynolds number?
- Is the flow turbulent?
- Can I perform a DNS of this flow at reasonable cost?
- What is the maximum cost (money and time) I can afford?
- Is it important to do unsteady simulations (noise emission, ...) ?
- Do I need statistics at small scales (chemical reactions, ...)?

Then, you must do some **compromises** between the accuracy and the cost of your simulation.

Energy spectrum of turbulent flows

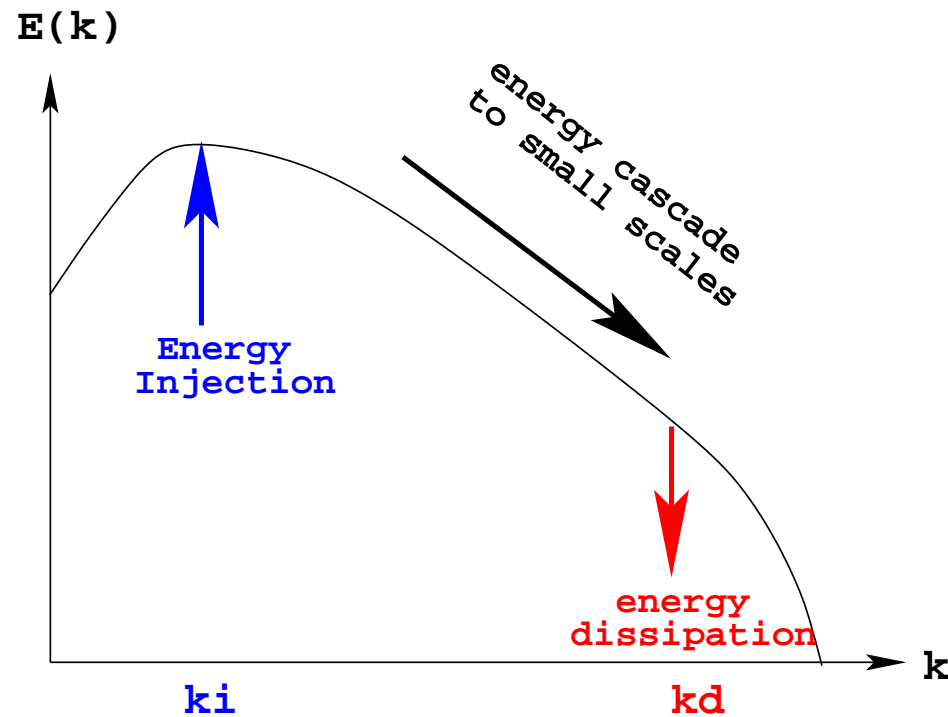


$$E(\kappa) = \begin{cases} A\kappa^s & \text{when } \kappa \leq \kappa_m \\ K_0 \epsilon^{2/3} \kappa^{-5/3} & \text{when } \kappa \geq \kappa_m \end{cases}$$

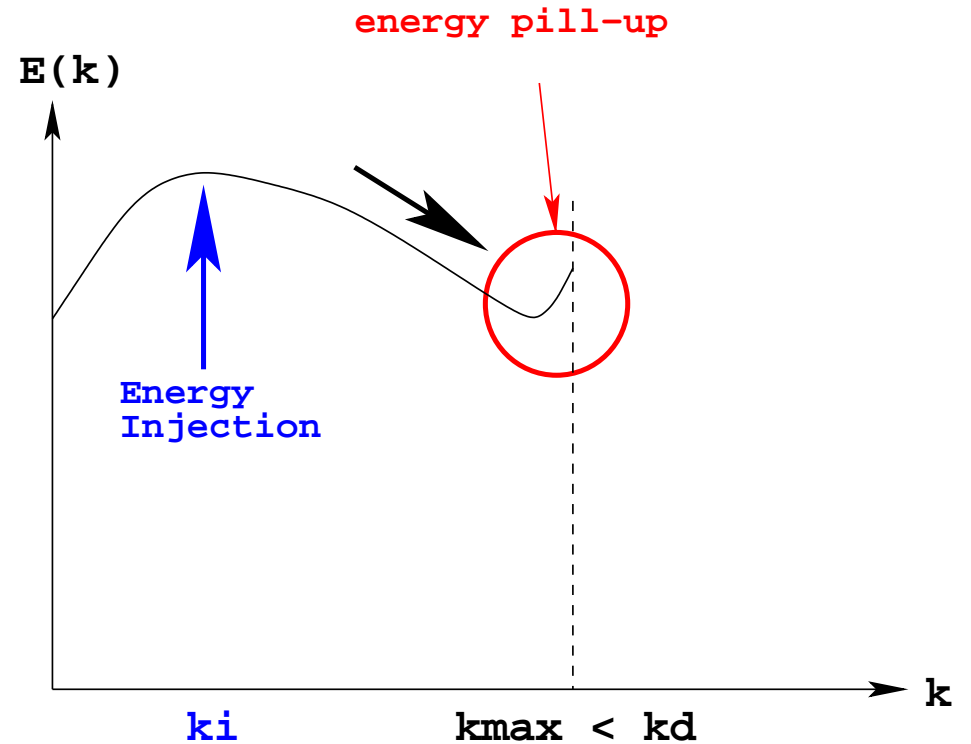
$\Rightarrow k_m$ is the inverse of the energy injection scale

Why do we need models

Direct Numerical Simulation (DNS)

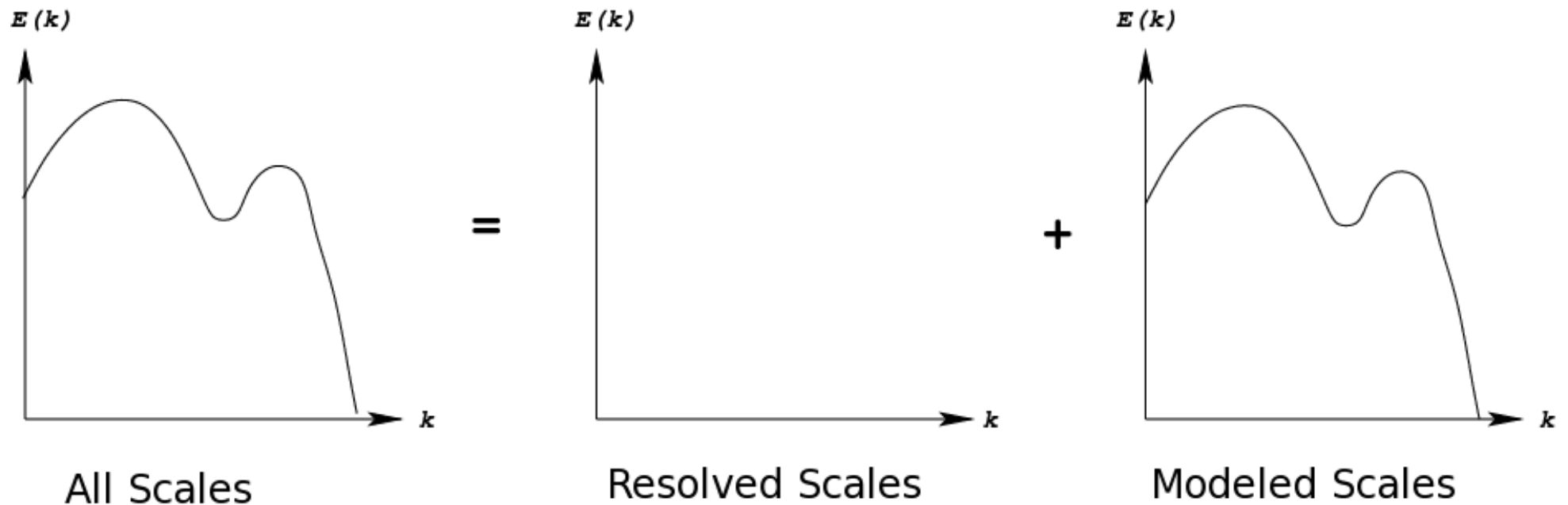


truncated simulation
(without model)



RANS modeling

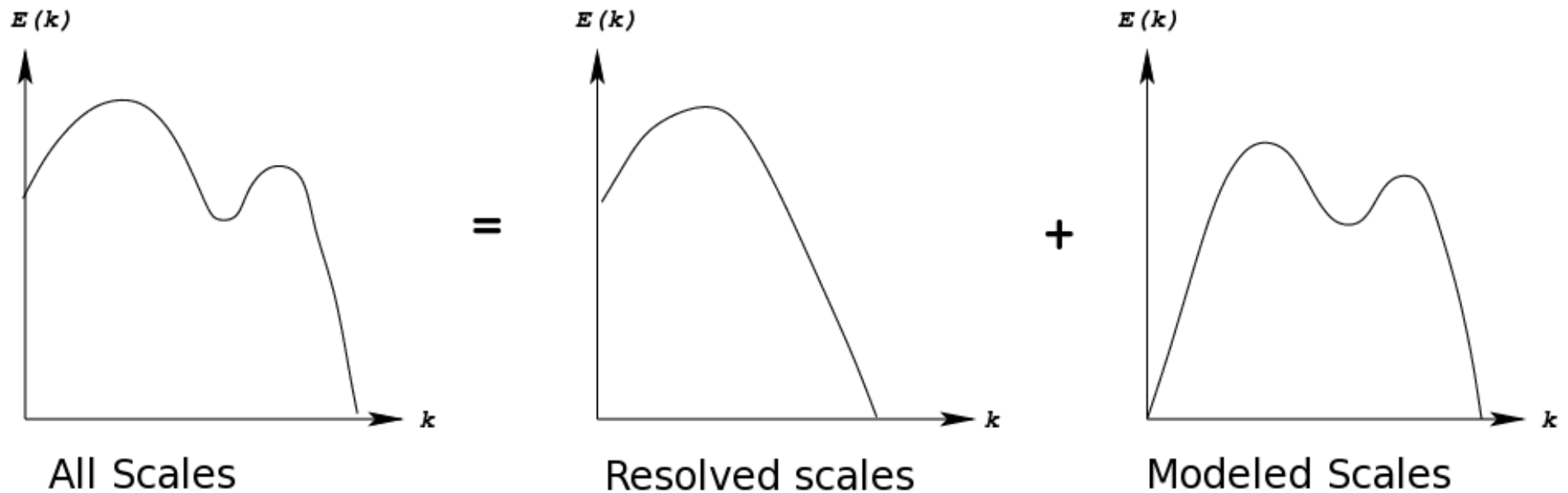
Reynold Averaged Navier Stokes (RANS)



- ⇒ Simulation of the statistical average
- ⇒ All physical scales are modeled

URANS modeling

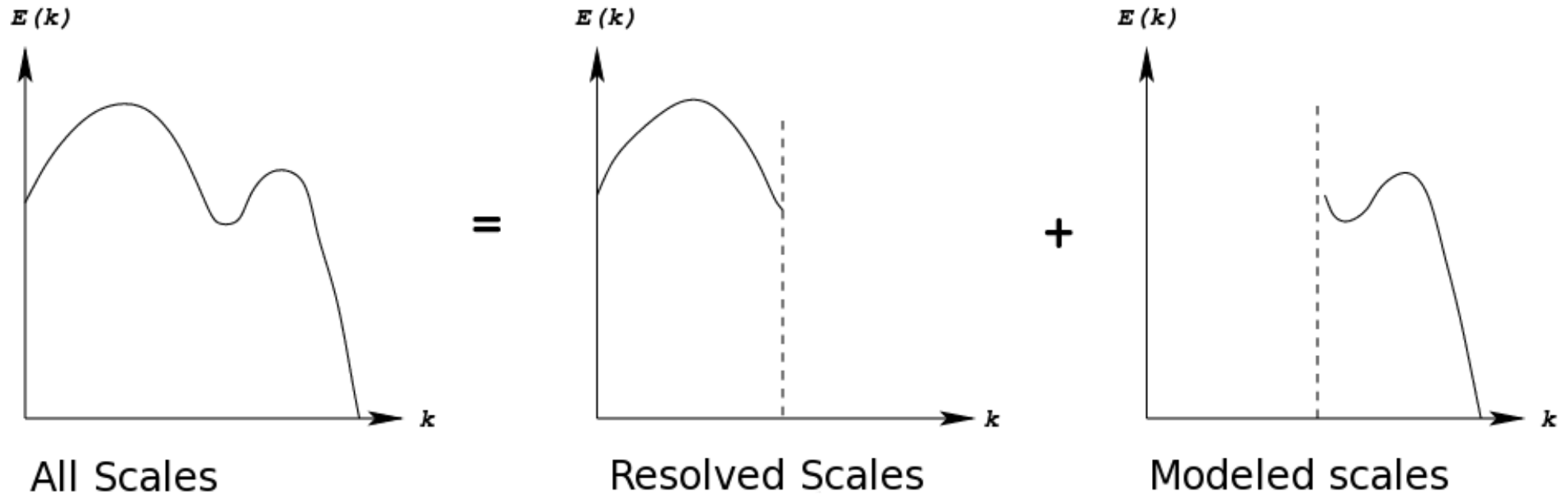
Unsteady Reynolds Averaged Navier Stokes (URANS)



- ⇒ Unsteady simulation of the largest scales
- ⇒ All physical scales are affected by the model

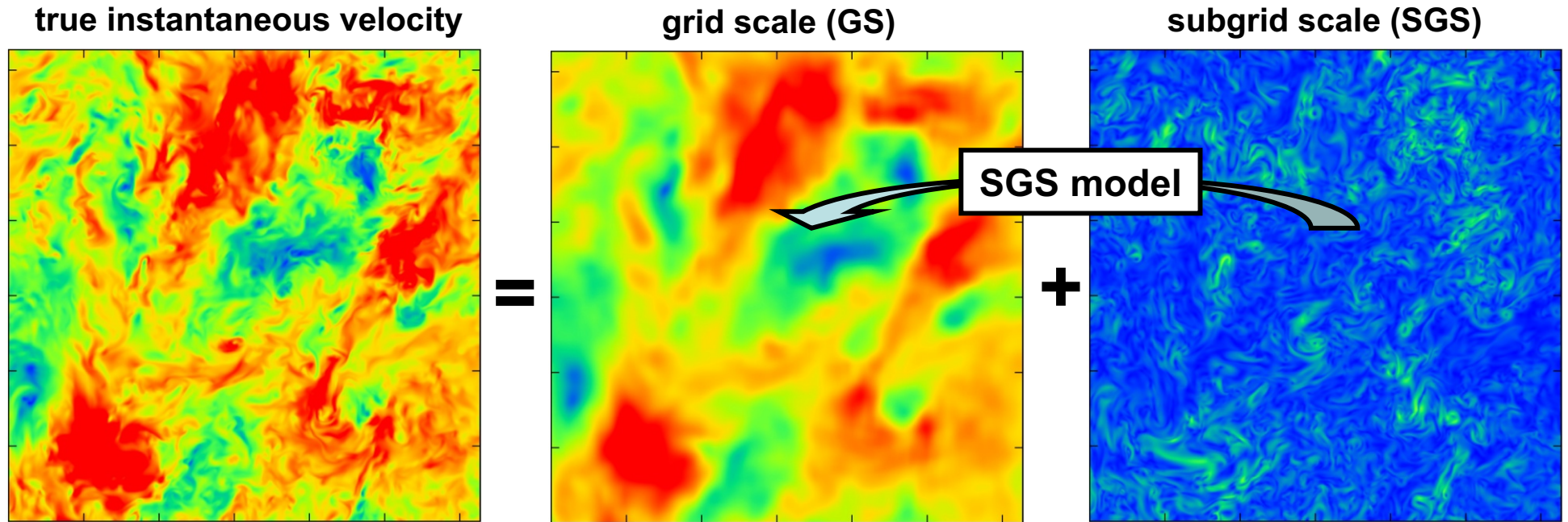
LES modeling

Large Eddy Simulation (LES)



- ⇒ Unsteady simulation of large scales
- ⇒ Modeling of sub-grid scales only

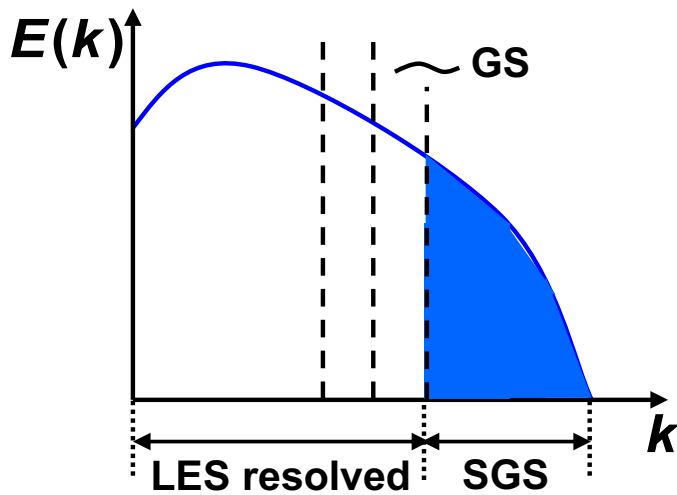
Large Eddy Simulations (LES)



$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial u_i}{\partial x_j} \right)$$

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial \tilde{u}_i}{\partial x_j} \right) + \frac{\partial \tau_{ij}^{SGS}}{\partial x_j}$$

$$\tau_{ij}^{SGS} = \widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j$$

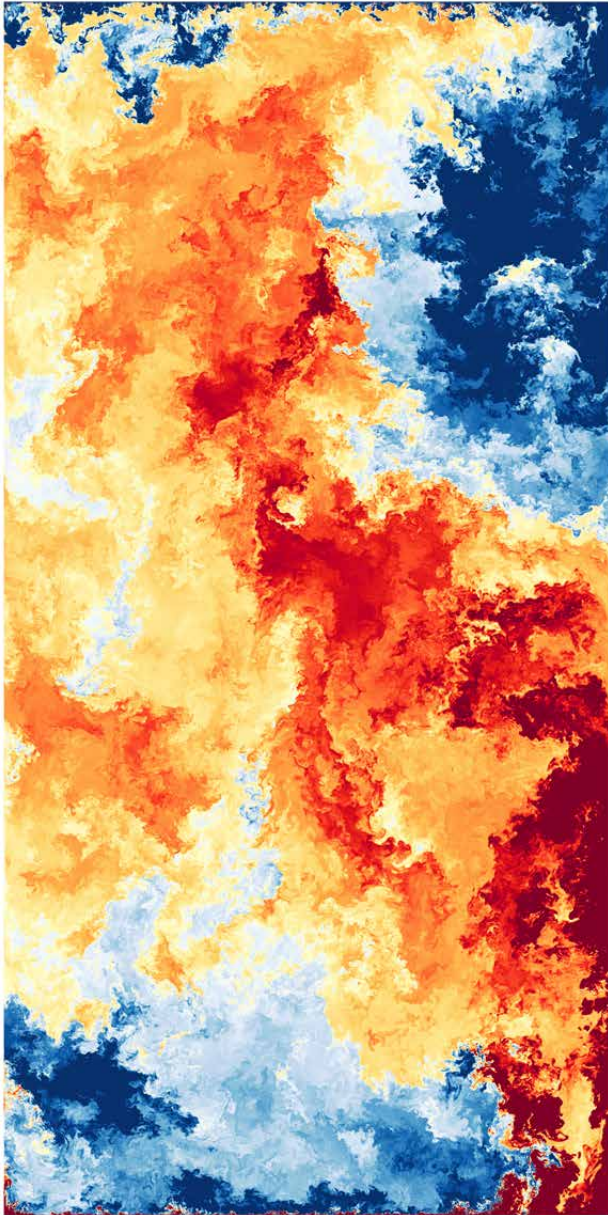


➤ Eddy viscosity type subgrid-scale model:

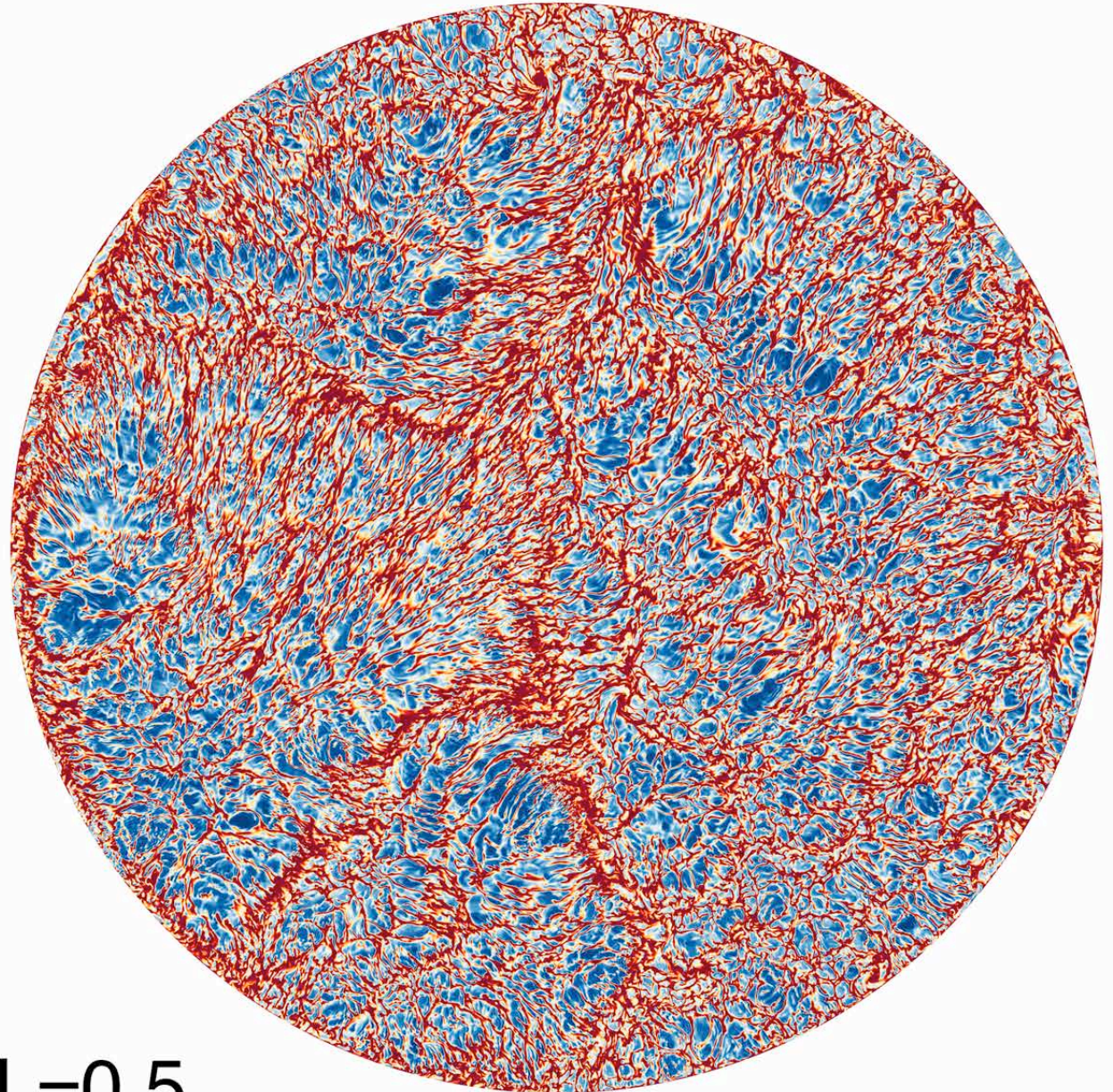
$$\tau_{ij}^{SGS} = -2\nu_t \tilde{S}_{ij} \quad \nu_t = c_s^2 \Delta^2 |\tilde{S}|$$

Lagrangian-averaged scale-dependent dynamic model

Direct Numerical Simulations (DNS)



$D/L=0.5$



Navier-Stokes equations for incompressible flow

Conservation of momentum

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}$$

Conservation of mass

$$\frac{\partial u_i}{\partial x_i} = 0$$

4 equations for 4 unknowns (3 velocity components and pressure)

Closed system of equations for given initial and boundary conditions

Scaling of the smallest eddies

Dynamics of the smallest scales in turbulence are dominated by viscous dissipation \rightarrow parameters ν and ϵ

Smallest turbulence scales are the Kolmogorov scales

$$\eta = (\nu^3/\epsilon)^{1/4}$$

$$u_\eta = (\epsilon\nu)^{1/4}$$

$$\tau_\eta = (\nu/\epsilon)^{1/2}$$

Low Re consistent with dominance of viscous dissipations

$$Re = \frac{\eta u_\eta}{\nu} = 1$$

Ratio of Kolmogorov scales to macroscales

$$\eta/l_0 = Re_0^{-3/4}$$

$$u_\eta/u_0 = Re_0^{-1/4}$$

$$\tau_\eta/\tau_0 = Re_0^{-1/2}$$

Example

$$Re_0 = \frac{u_0 l_0}{\nu} = 10^5$$

$$\eta/l_0 \sim \frac{1}{6 \cdot 10^3}$$

Increase in range of scales with increasing Reynolds number

Required spatial resolution

$$N = \frac{L}{\eta}$$

$$\eta = \frac{\nu^{3/4}}{\epsilon^{1/4}}$$

$$\epsilon = \frac{U^3}{L}$$

$$\eta = \frac{\nu^{3/4} L^{1/4}}{U^{3/4}}$$

Required spatial resolution

$$N = \frac{L}{\eta}$$

$$\eta = \frac{\nu^{3/4}}{\epsilon^{1/4}}$$

$$\epsilon = \frac{U^3}{L}$$

$$\frac{L}{\eta} \sim L \frac{U^{3/4}}{\nu^{3/4} L^{1/4}}$$

$$\eta = \frac{\nu^{3/4} L^{1/4}}{U^{3/4}}$$

Required spatial resolution

$$N = \frac{L}{\eta} \quad \eta = \frac{\nu^{3/4}}{\epsilon^{1/4}} \quad \epsilon = \frac{U^3}{L}$$

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Required spatial resolution

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$$\frac{L}{\eta} \sim \frac{L^{3/4} U^{3/4}}{\nu^{3/4}}$$

$$\frac{L}{\eta} \sim Re_L^{3/4}$$

$$Re_L^{1/2} \sim Re_\lambda$$

Required spatial resolution

$$N = \frac{L}{\eta} \quad \eta = \frac{\nu^{3/4}}{\epsilon^{1/4}} \quad \epsilon = \frac{U^3}{L}$$

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$$\frac{L}{\eta} \sim \frac{L^{3/4} U^{3/4}}{\nu^{3/4}}$$

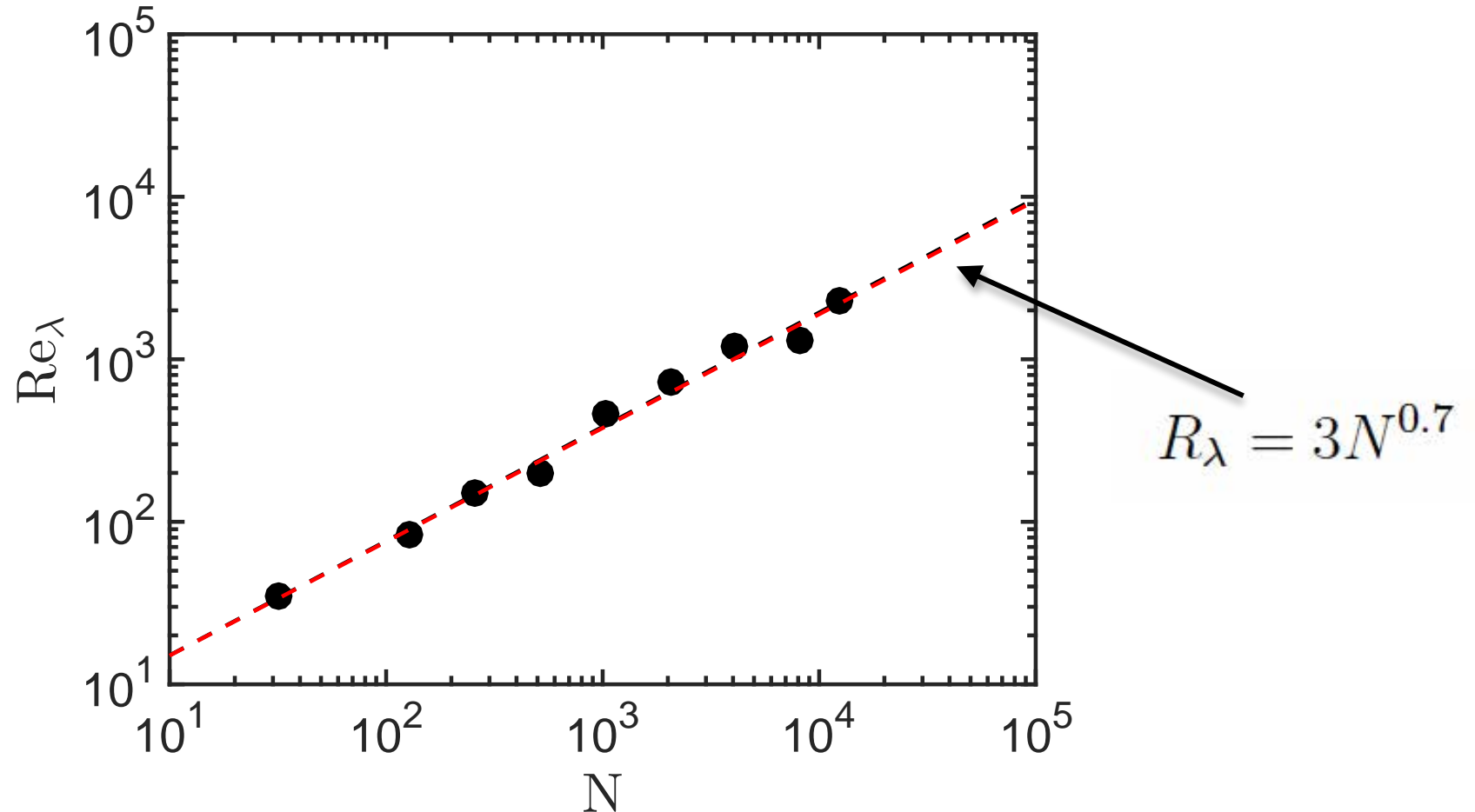
$$\frac{L}{\eta} \sim Re_L^{3/4}$$

$$\frac{L}{\eta} \sim Re_\lambda^{3/2}$$

$$Re_L^{1/2} \sim Re_\lambda$$

$$Re_\lambda \sim N^{2/3}$$

Taylor-based Reynolds number



Data points

$$R_\lambda = 2.3N^{3/4}$$

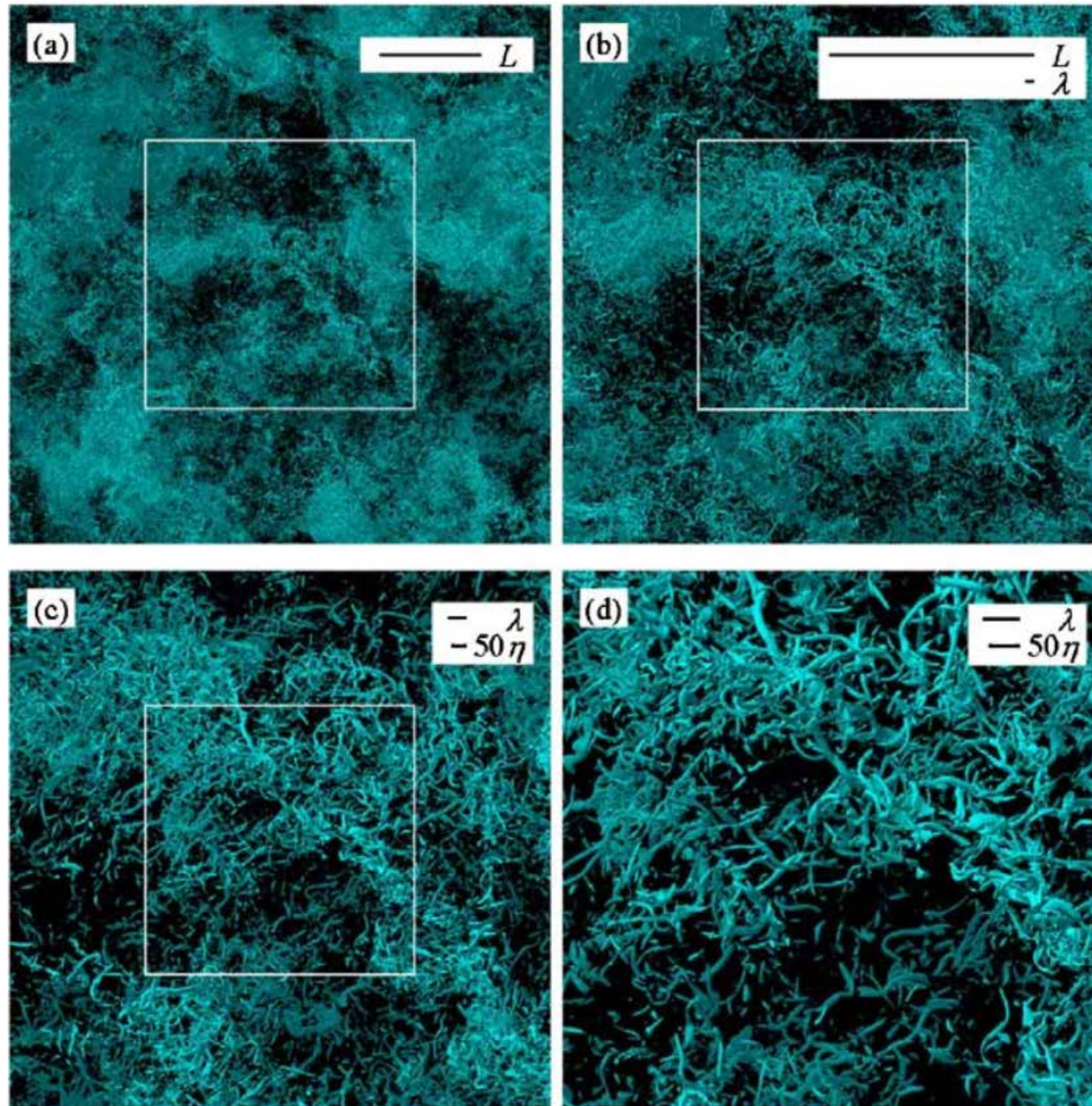
Dimensional analysis

$$R_\lambda \sim N^{2/3}$$

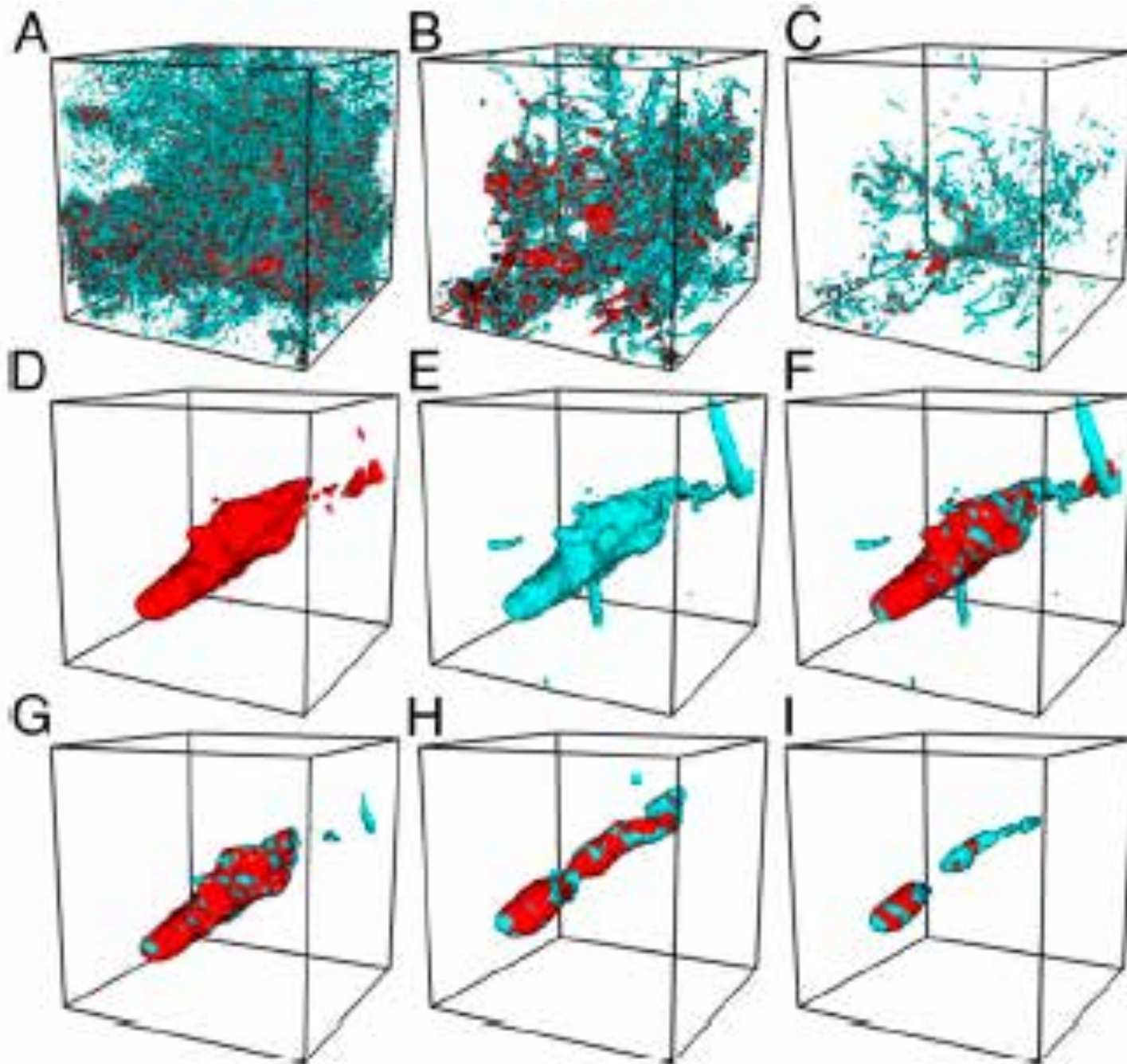
Recent results might be marginally resolved.

A. Celani, Journal of Turbulence, The frontiers of computing in turbulence: challenges and perspectives 8, 2007

Kaneda et al. 2003 DNS 4096³



Yeung et al. 2015 DNS 8192³



**Ishihara, Morishita, Yokokawa, Uno,
Kaneda 2016 DNS 12288³**

How much CPU time is required?

$$N = \frac{L}{\eta} \quad \frac{L}{\eta} \sim Re_\lambda^{3/2}$$

Calculate the total number of modes

$$N^3 = \left(\frac{L}{\eta}\right)^3 \sim Re_L^{9/4} \sim Re_\lambda^{9/2}$$

How much CPU time is required?

$$N = \frac{L}{\eta} \quad \frac{L}{\eta} \sim Re_{\lambda}^{3/2}$$

Calculate the total number of modes

$$N^3 = \left(\frac{L}{\eta}\right)^3 \sim Re_L^{9/4} \sim Re_{\lambda}^{9/2}$$

Time advancement also depends on Re_L

$T =$ Large eddy turnover time $\sim \frac{U^2}{\epsilon}$

$$\tau_{\eta} = \left(\frac{\nu}{\epsilon}\right)^{1/2}$$

How much CPU time is required?

$$M = \frac{T}{\tau_\eta} = \frac{U^2 \epsilon^{1/2}}{\epsilon \nu^{1/2}}$$

How much CPU time is required?

$$M = \frac{T}{\tau_\eta} = \frac{U^2 \epsilon^{1/2}}{\epsilon \nu^{1/2}}$$
$$M = \frac{U^2}{\nu^{1/2} \epsilon^{1/2}}$$

How much CPU time is required?

$$M = \frac{T}{\tau_\eta} = \frac{U^2 \epsilon^{1/2}}{\epsilon \nu^{1/2}}$$

$$M = \frac{U^2}{\nu^{1/2} \epsilon^{1/2}}$$

$$M = \frac{U^2 L^{1/2}}{\nu^{1/2} U^{3/2}}$$

Remember $\epsilon = \frac{U^3}{L}$

How much CPU time is required?

$$\begin{aligned}M &= \frac{T}{\tau_\eta} = \frac{U^2 \epsilon^{1/2}}{\epsilon \nu^{1/2}} \\M &= \frac{U^2}{\nu^{1/2} \epsilon^{1/2}} \\M &= \frac{U^2 L^{1/2}}{\nu^{1/2} U^{3/2}} \\M &= \frac{U^{1/2} L^{1/2}}{\nu^{1/2}}\end{aligned}$$

How much CPU time is required?

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How much CPU time is required?

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$$M = \frac{U^2}{\nu^{1/2} \epsilon^{1/2}}$$

$$M = \frac{U^2 L^{1/2}}{\nu^{1/2} U^{3/2}}$$

$$M = \frac{U^{1/2} L^{1/2}}{\nu^{1/2}}$$

$$M = Re_L^{1/2} = Re_\lambda$$

$$\text{CPU-time} \sim N^3 M \sim Re_L^{11/2} \sim Re_\lambda^{11/4}$$

Remember $N^3 = \left(\frac{L}{\eta}\right)^3 \sim Re_L^{9/4} \sim Re_\lambda^{9/2}$

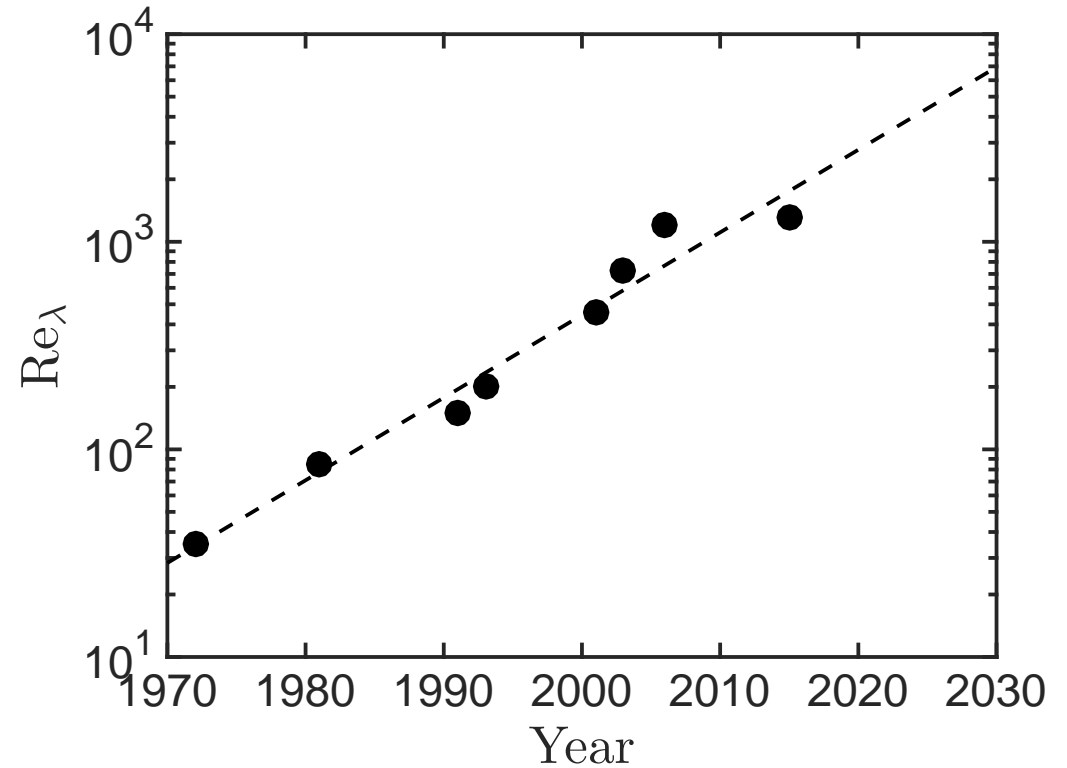
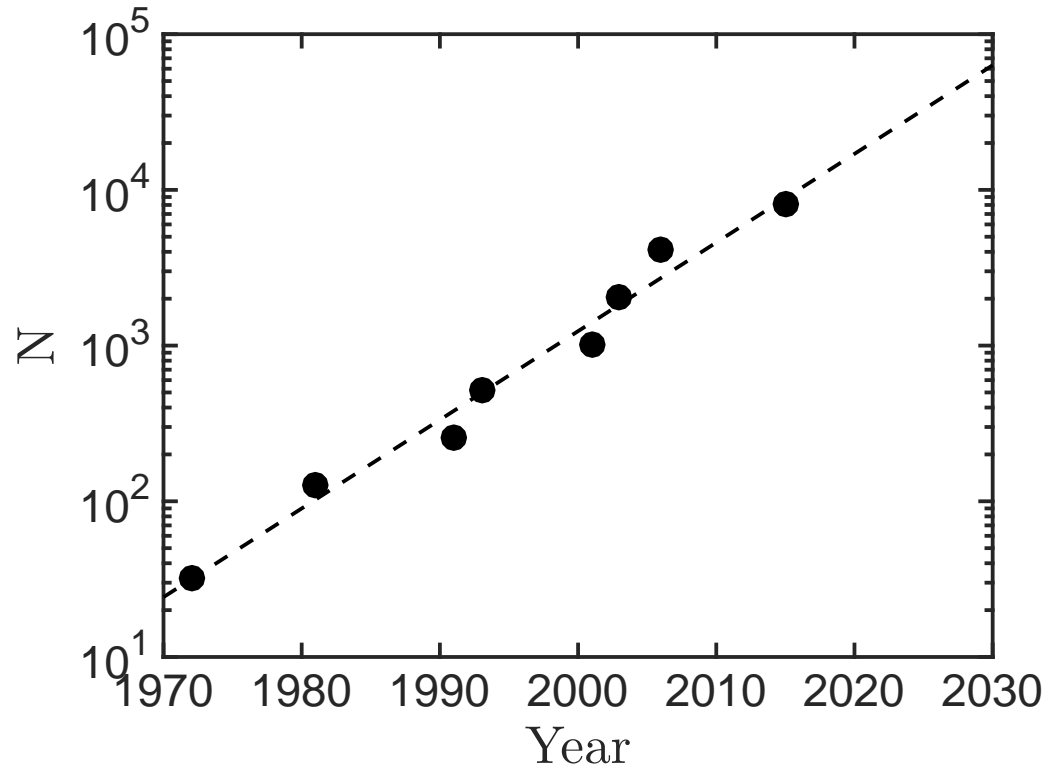
Development supercomputers



Top supercomputers

Rank	Site	System	Cores	(TFlop/s)	(TFlop/s)	(kW)
1	National Supercomputing Center in Wuxi China	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	Titan - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890
5	DOE/SC/LBNL/NERSC United States	Cori - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect Cray Inc.	622,336	14,014.7	27,880.7	3,939

Taylor-based Reynolds number



Resolution doubles every 5.5 years
Taylor Reynolds doubles every 8 years

Numerical methods

- Second order central finite difference
 - Energy conserving
 - Better for sharp shocks
 - Easier, more complex physics can be incorporated
 - Efficient, suitable for massively parallel machines.
- Pseudo spectral
 - Higher accuracy for given number degrees of freedom
 - Requires periodic boundary conditions

AFiD: An universal Navier-Stokes solver for wall-bounded flow

R. Verzicco & P. Orlandi, A finite-difference scheme for three-dimensional incompressible flow in cylindrical coordinates, *J. Comput. Phys.* 123, 402–413 (1996)

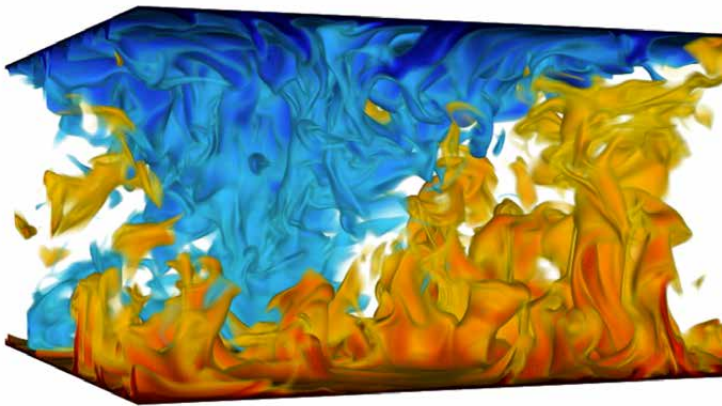
E. P. van der Poel, R. Ostilla-Monico, J. Donners, & R. Verzicco, A pencil distributed finite difference code for strongly turbulent wall-bounded flows, *Computers and Fluids* 166, 10-16 (2015).

R. Ostilla-Monico, Y. Yang, E. P. van der Poel, D. Lohse, R. Verzicco, A multiple-resolution strategy for Direct Numerical Simulation of scalar turbulence, *J. Computational Physics* 301, 308-321 (2015).

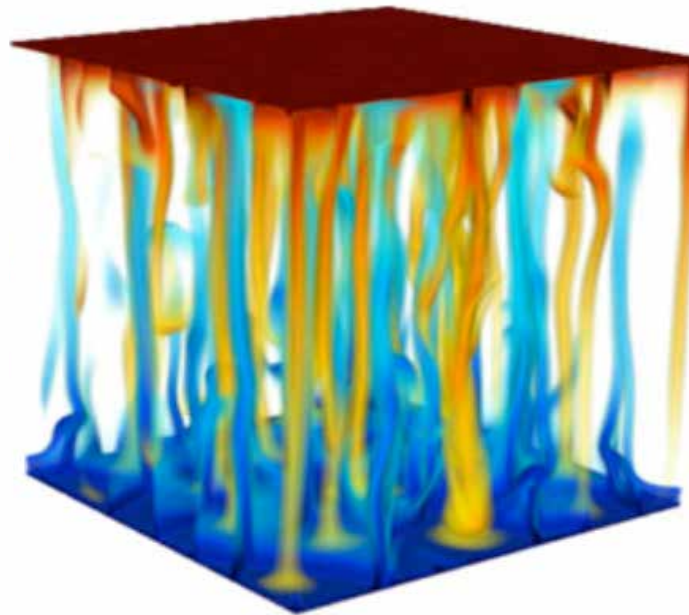
X. Zhu, E. Phillips, V. Spandan, J. Donners, G. Ruetsch, J. Romero, R. Ostilla-Mónico, Y. Yang, D. Lohse, R. Verzicco, M. Fatica, R.J.A.M. Stevens, AFiD-GPU: a versatile Navier-Stokes Solver for Wall-Bounded Turbulent Flows on GPU Clusters, Submitted to *Computer Physics Communications* (2017).

AFiD code for wall bounded turbulence

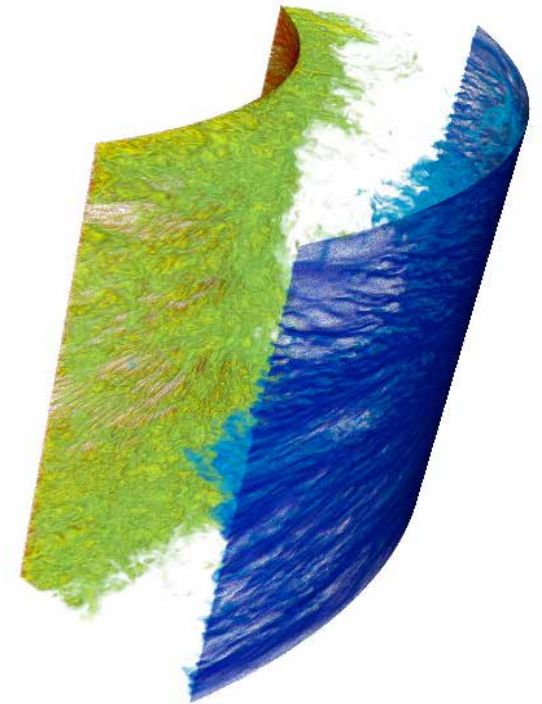
- Direct numerical simulation of Navier-Stokes equations, no turbulence modeling
- Spatial discretization: 2nd order finite differences
- Temporal discretization: mixed explicit & implicit treatment of some terms
- Pressure correction method: must solve Poisson equation exactly (**most expensive!**)



Thermal convection

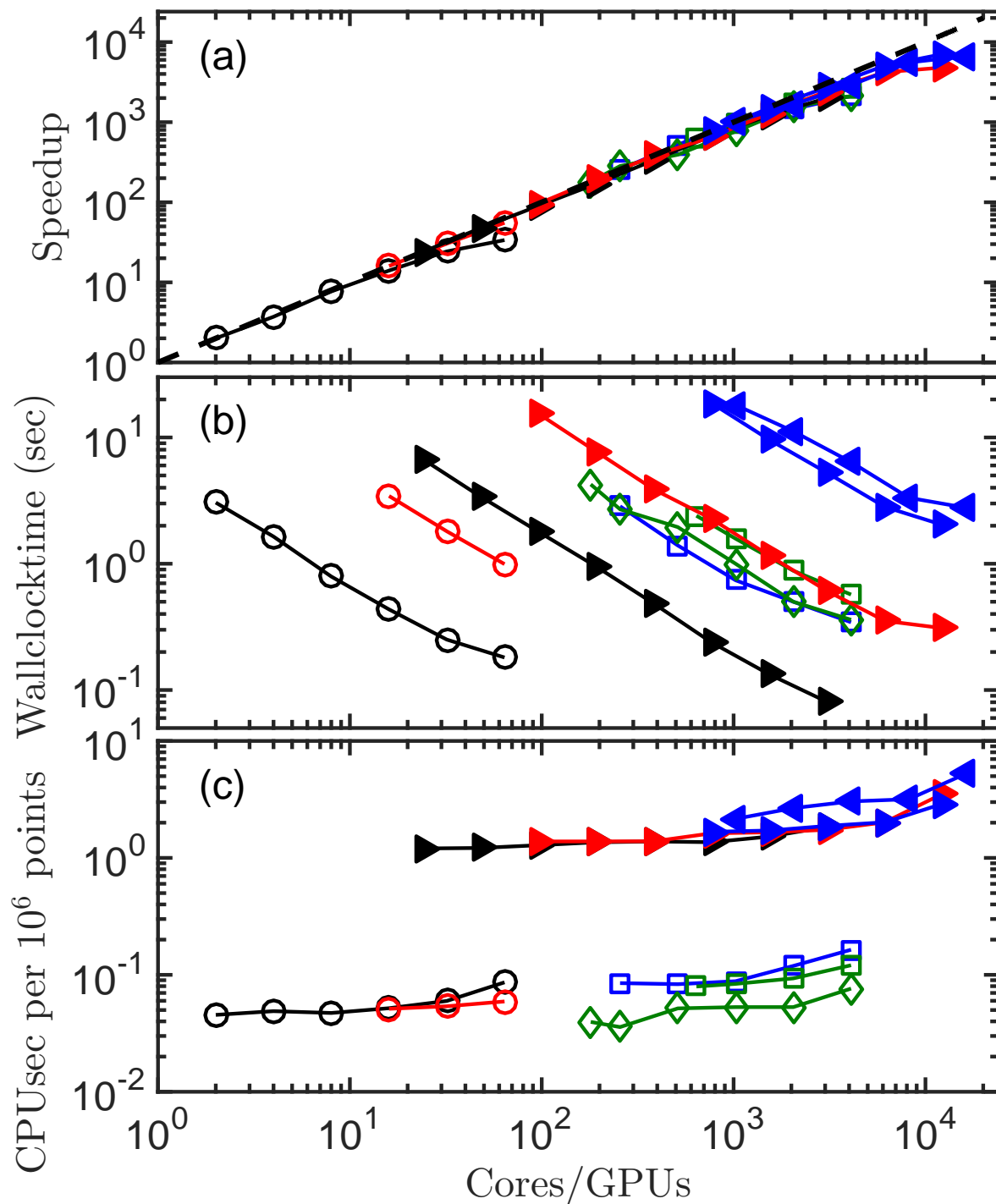


Double diffusive convection



Taylor-Couette flow

Scaling of AFiD code



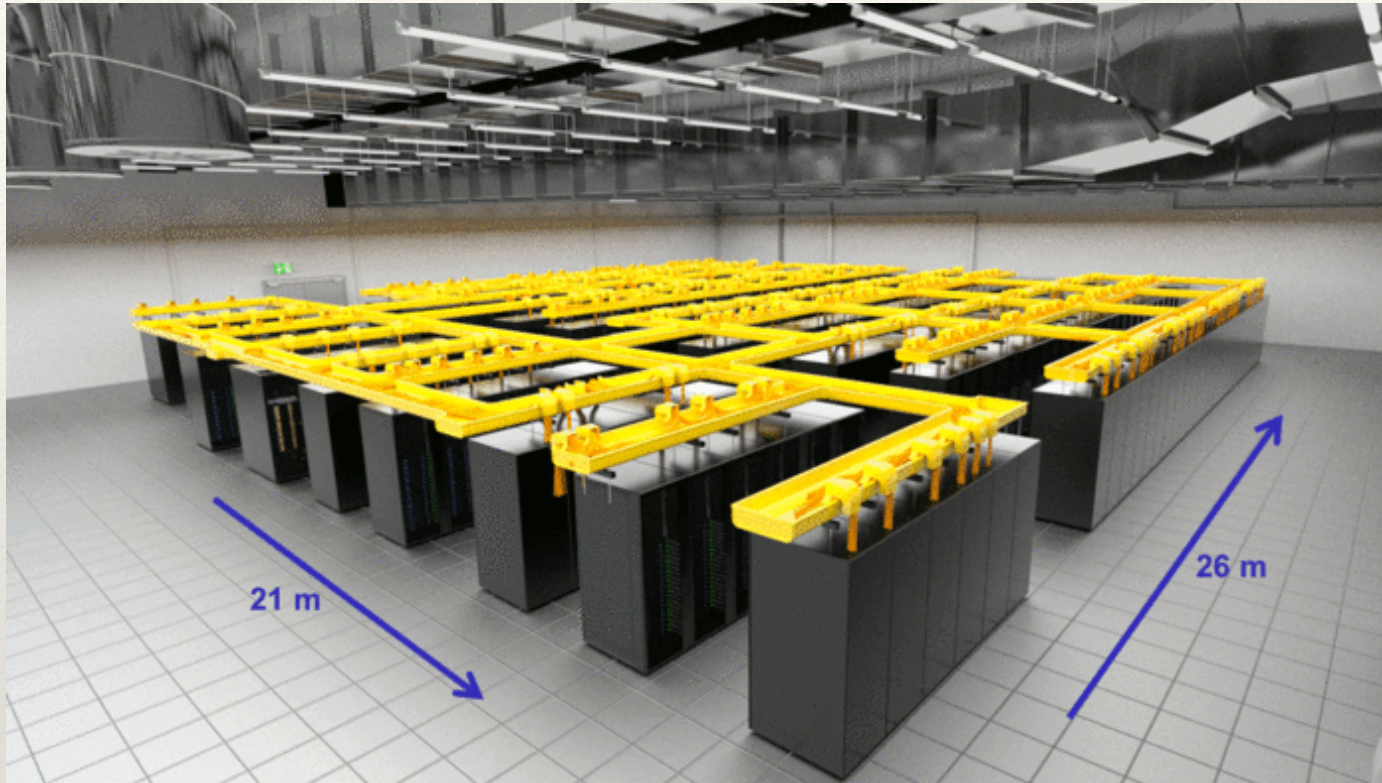
CPU

- 512³ (Haswell)
- 1024³ (Haswell)
- 2048³ (Haswell)
- 2048³ (Sandy Bridge)

GPU

- 512³ (K40m)
- 1024³ (K40m)
- 2048³ (K20X)
- 2048 × 3072² (K20X)
- 2048 × 3072² (P100)

Simulations performed on state of the art supercomputers



SuperMuc (Germany)

Marconi (Italy)

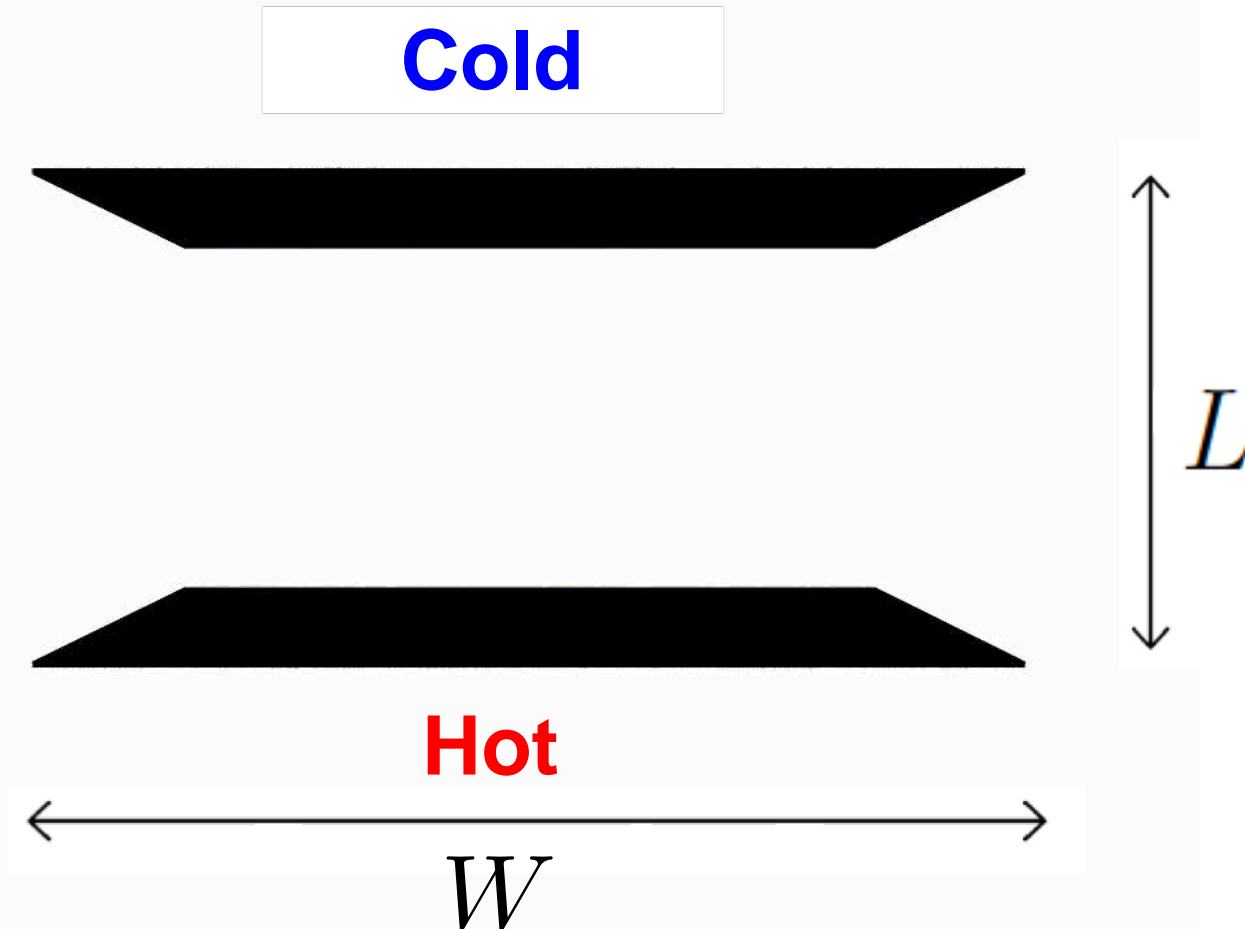
Piz Daint (Switzerland)

Cartesius (Netherlands)

Archer (Great Britain)

**3 out of 5 fastest
supercomputers in
Europe**

Rayleigh-Bénard convection



Control parameters

Aspect ratio

$$\Gamma = \frac{W}{L}$$

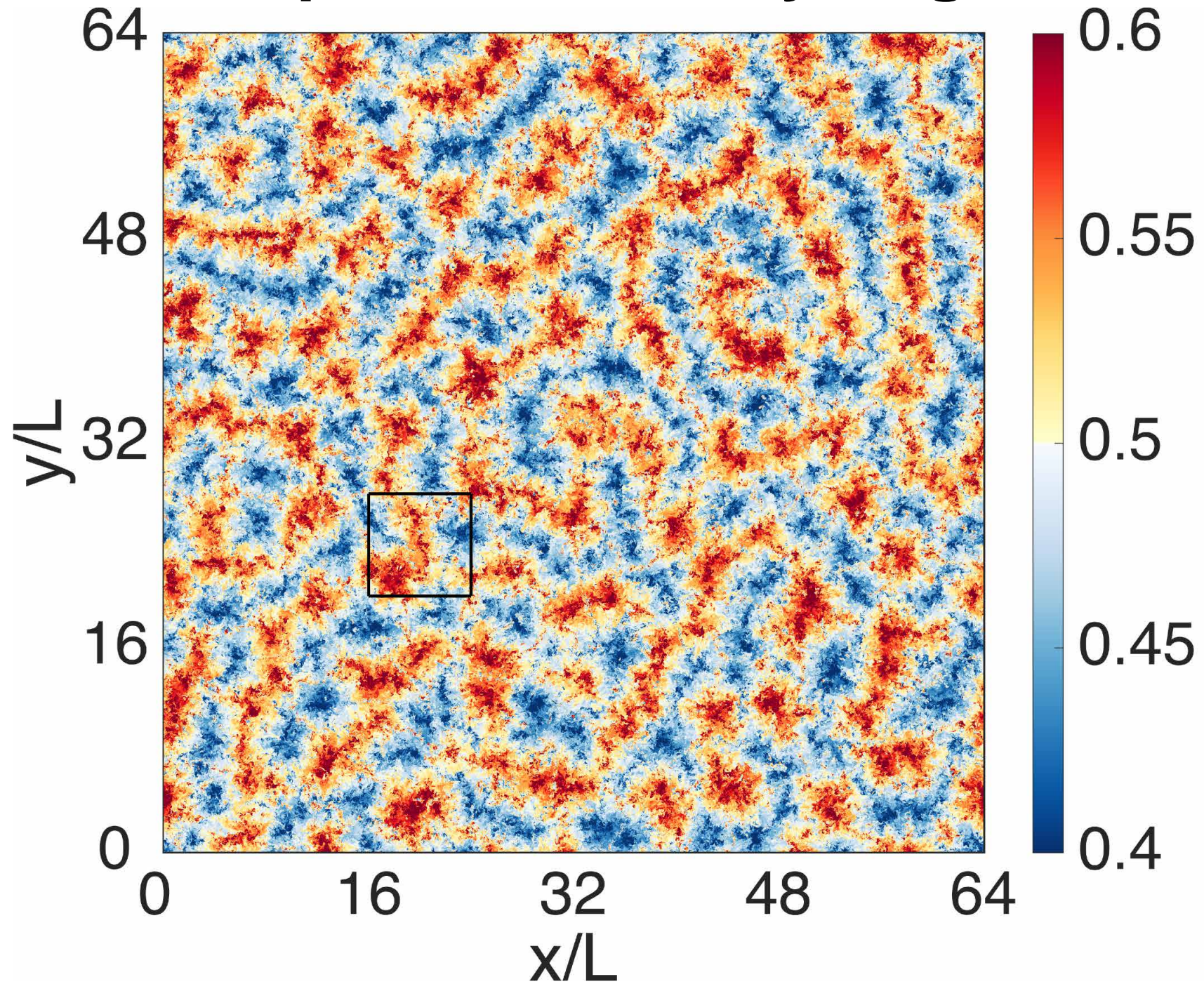
Rayleigh number

$$Ra = \frac{\beta g L^3 \Delta}{\nu \kappa}$$

Prandtl number

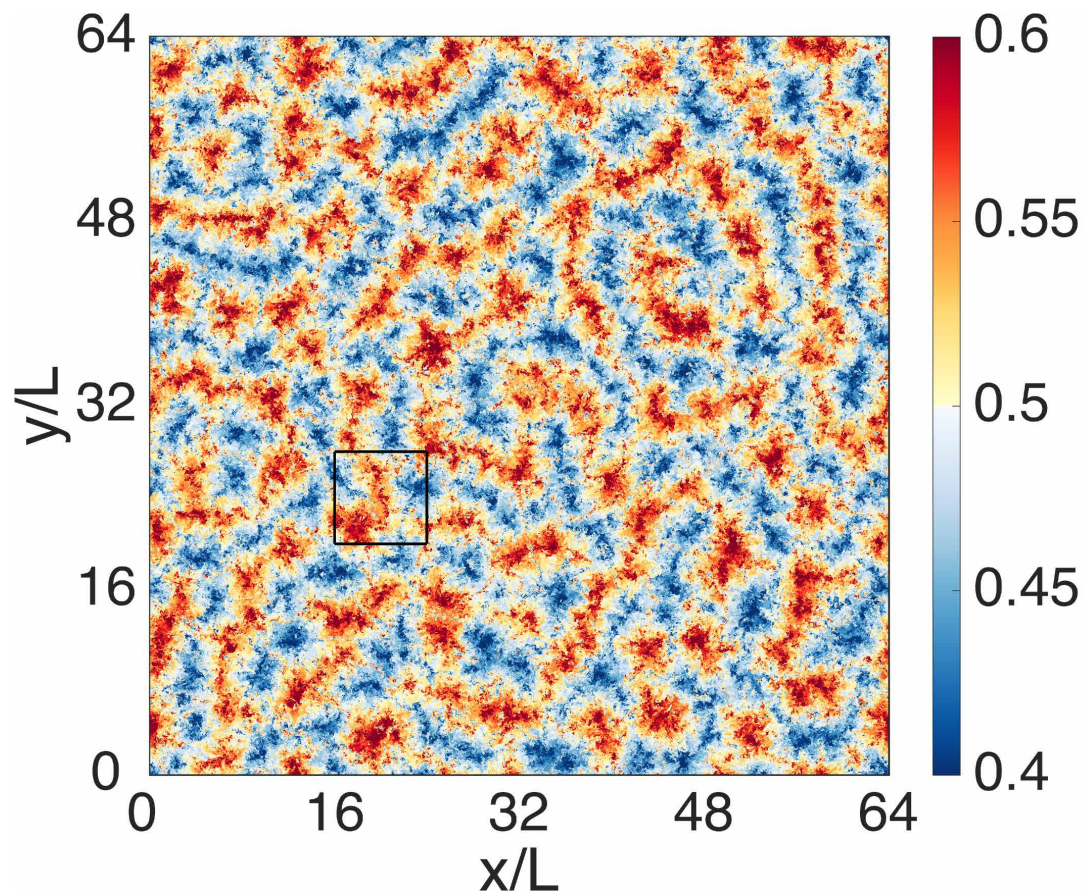
$$Pr = \frac{\nu}{\kappa}$$

Convection patterns in very large domains

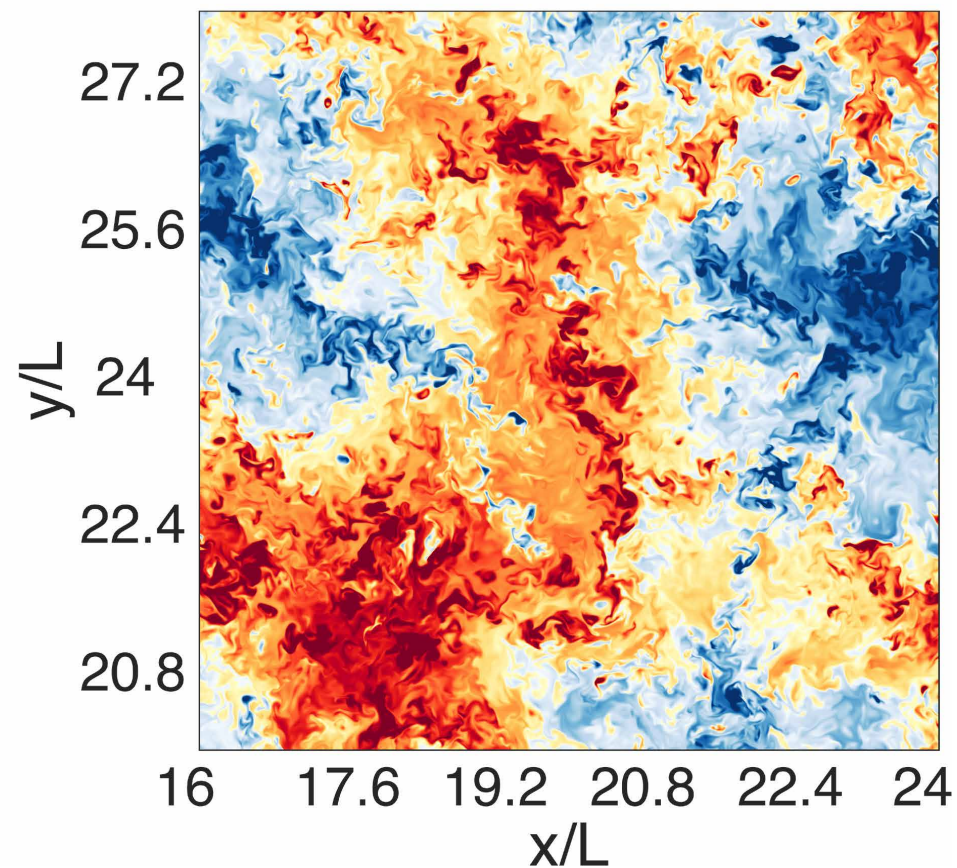


Convection patterns in very large domains

Full domain

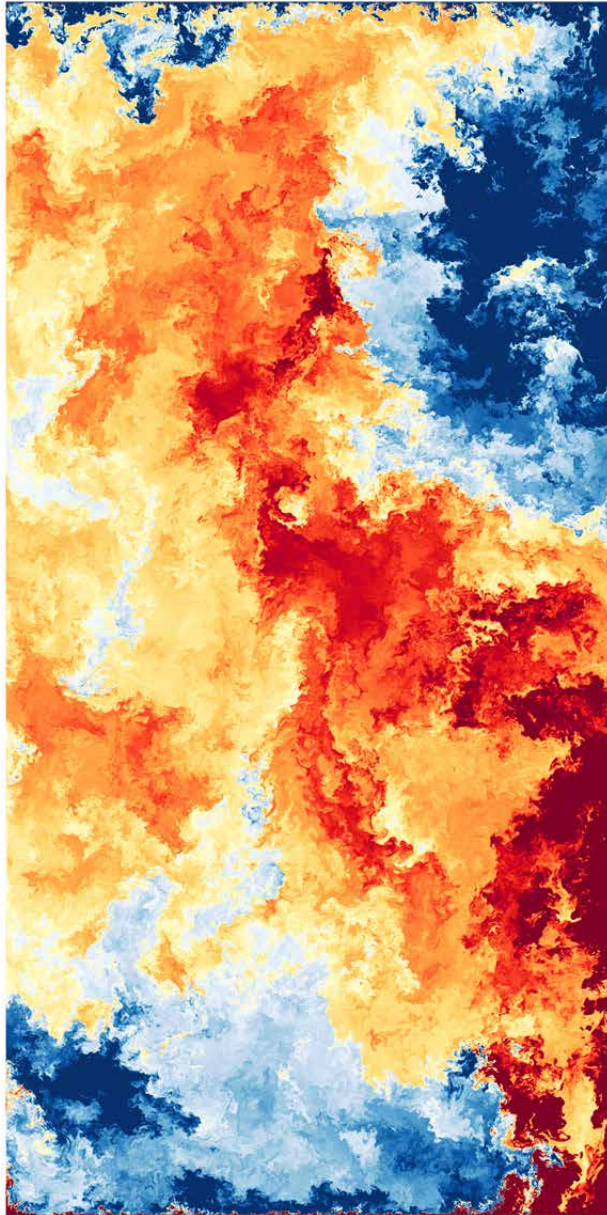


Zoom 64 times



Rayleigh-Bénard convection

Cold

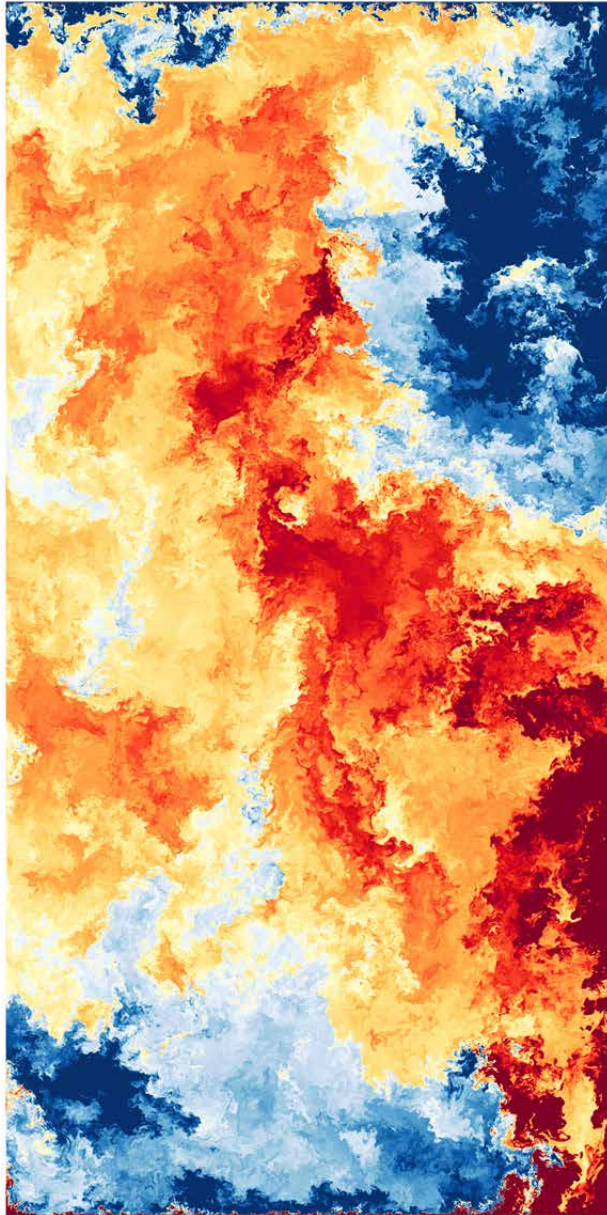


Hot



Rayleigh-Bénard convection

Cold

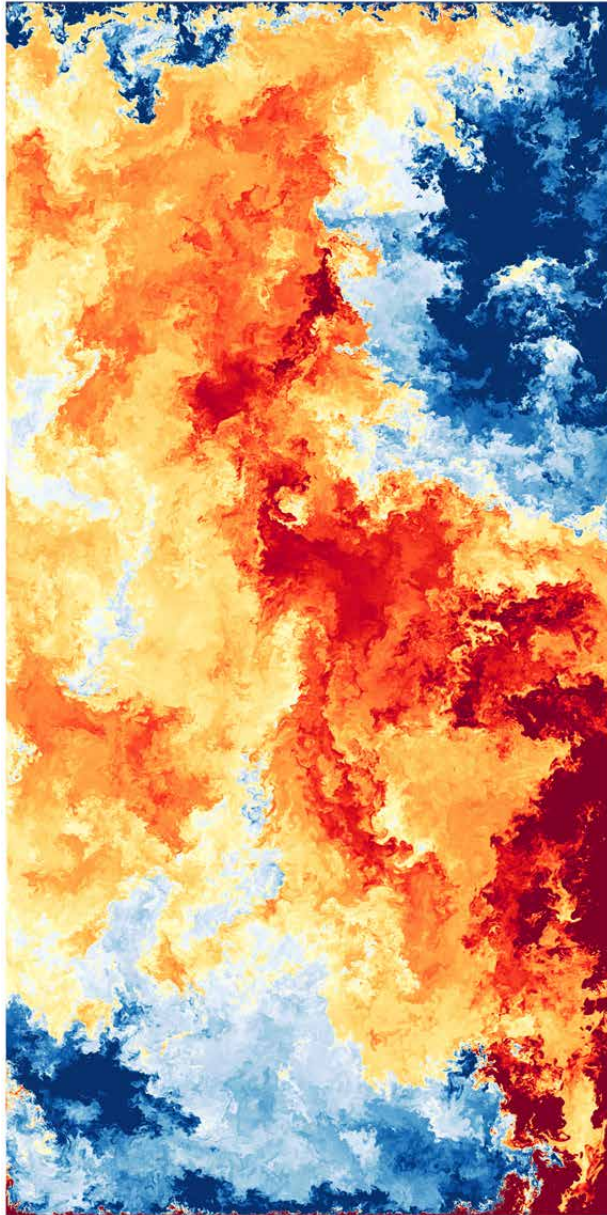


Hot

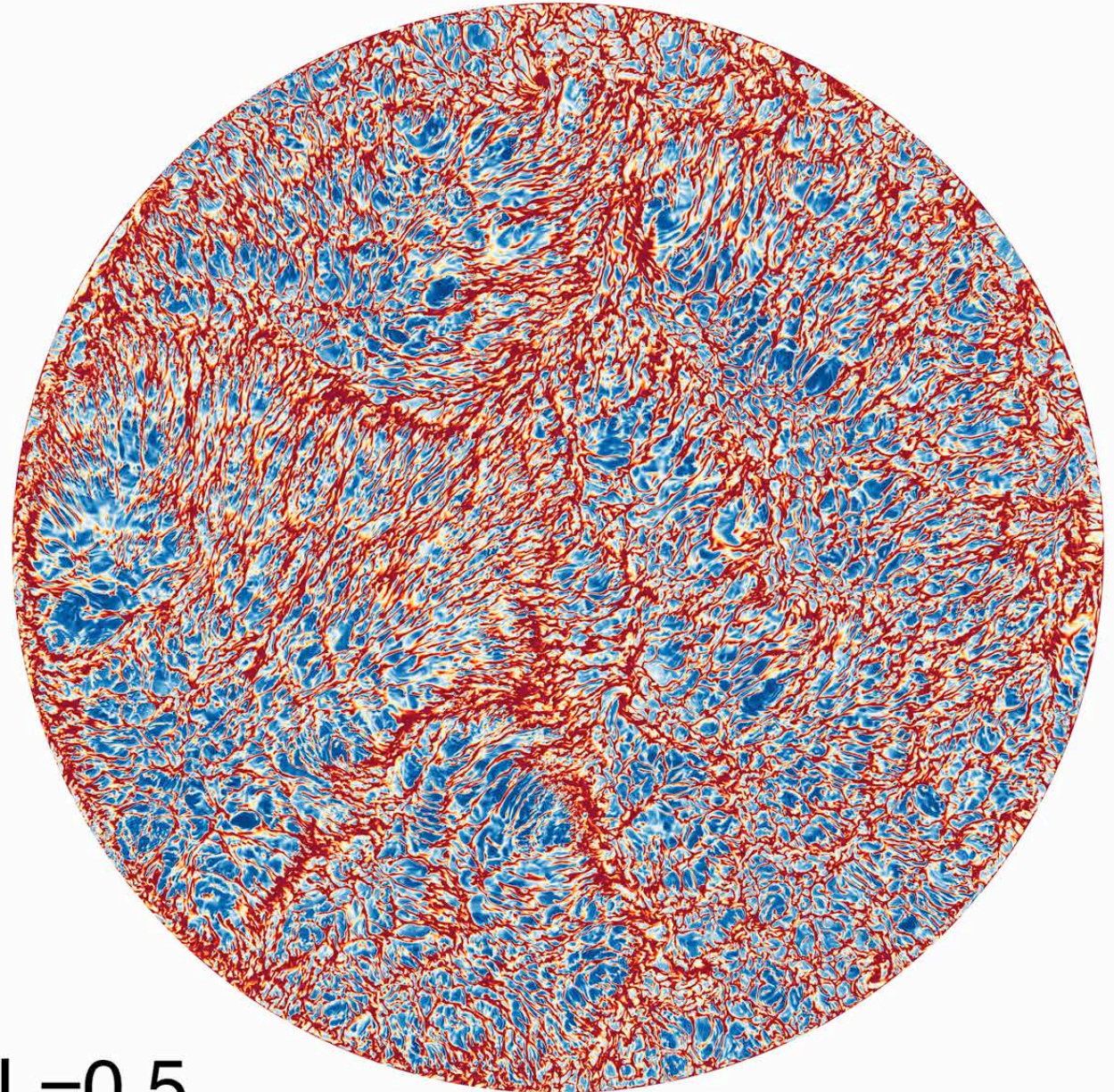


Rayleigh-Bénard convection

Cold



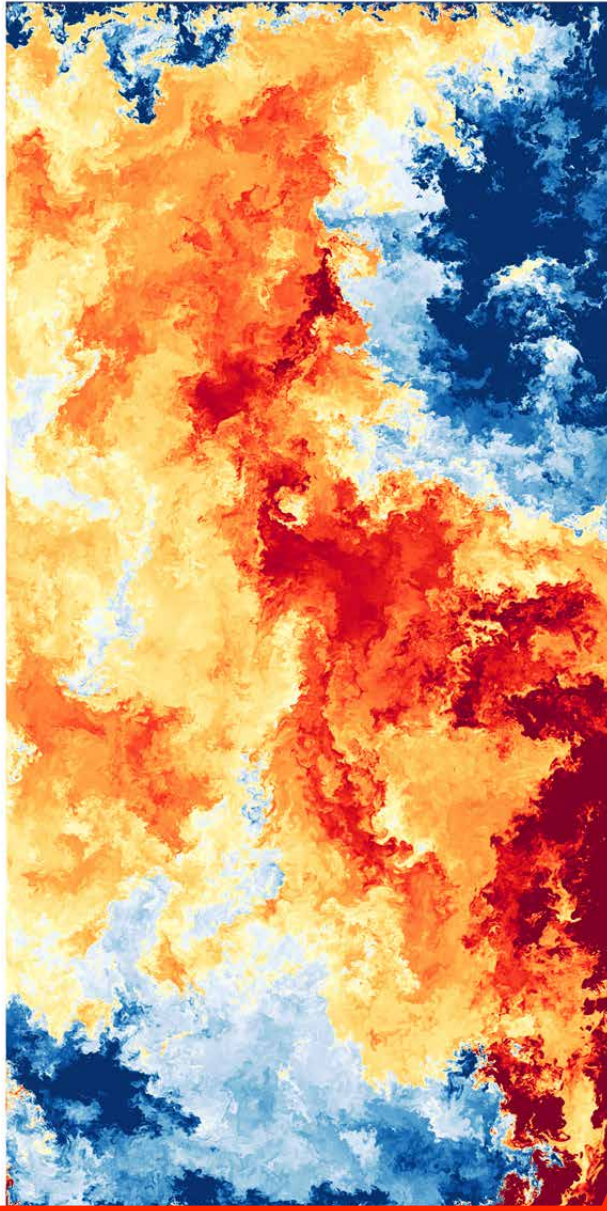
Hot



$D/L=0.5$

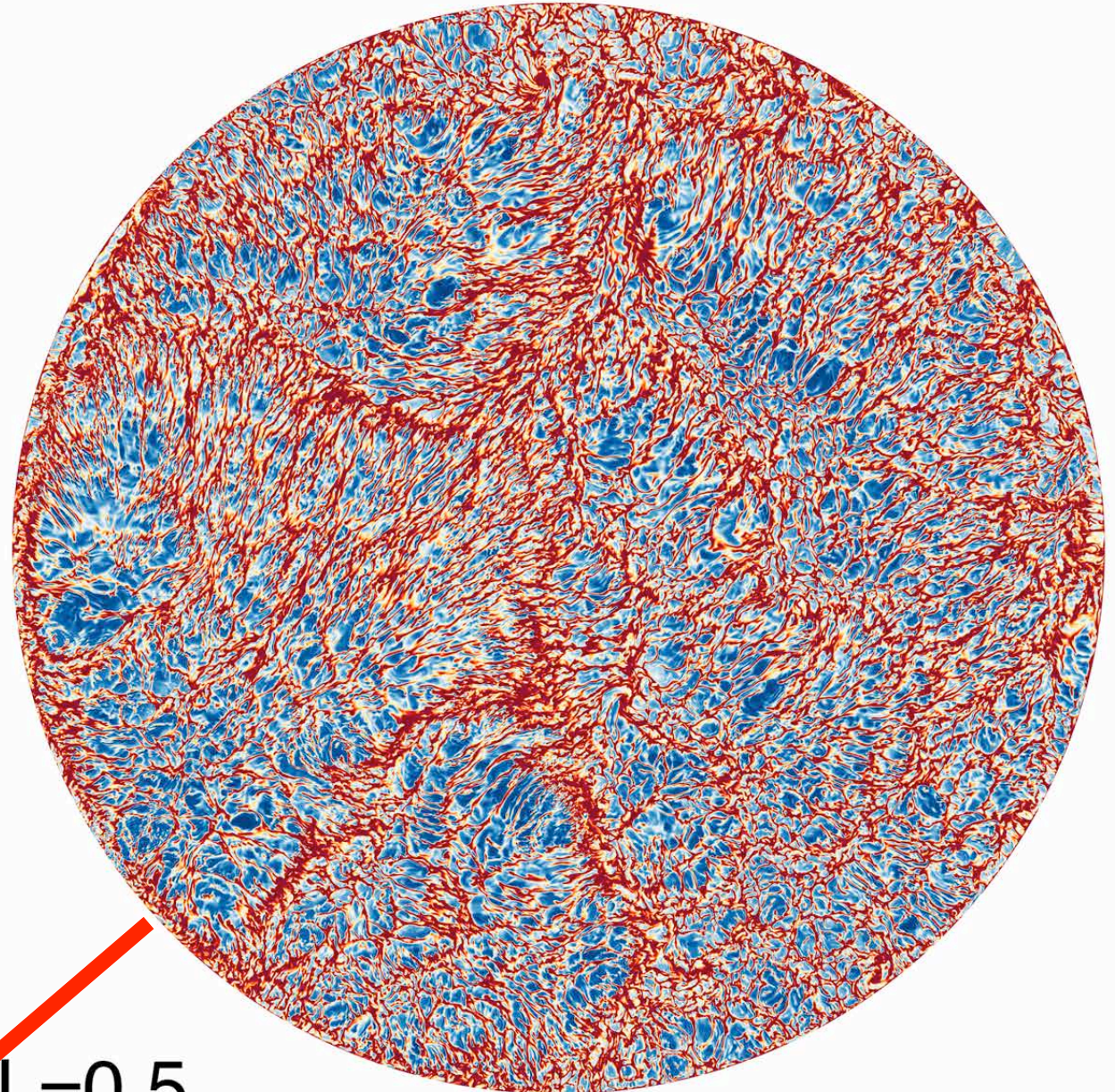
Rayleigh-Bénard convection

Cold

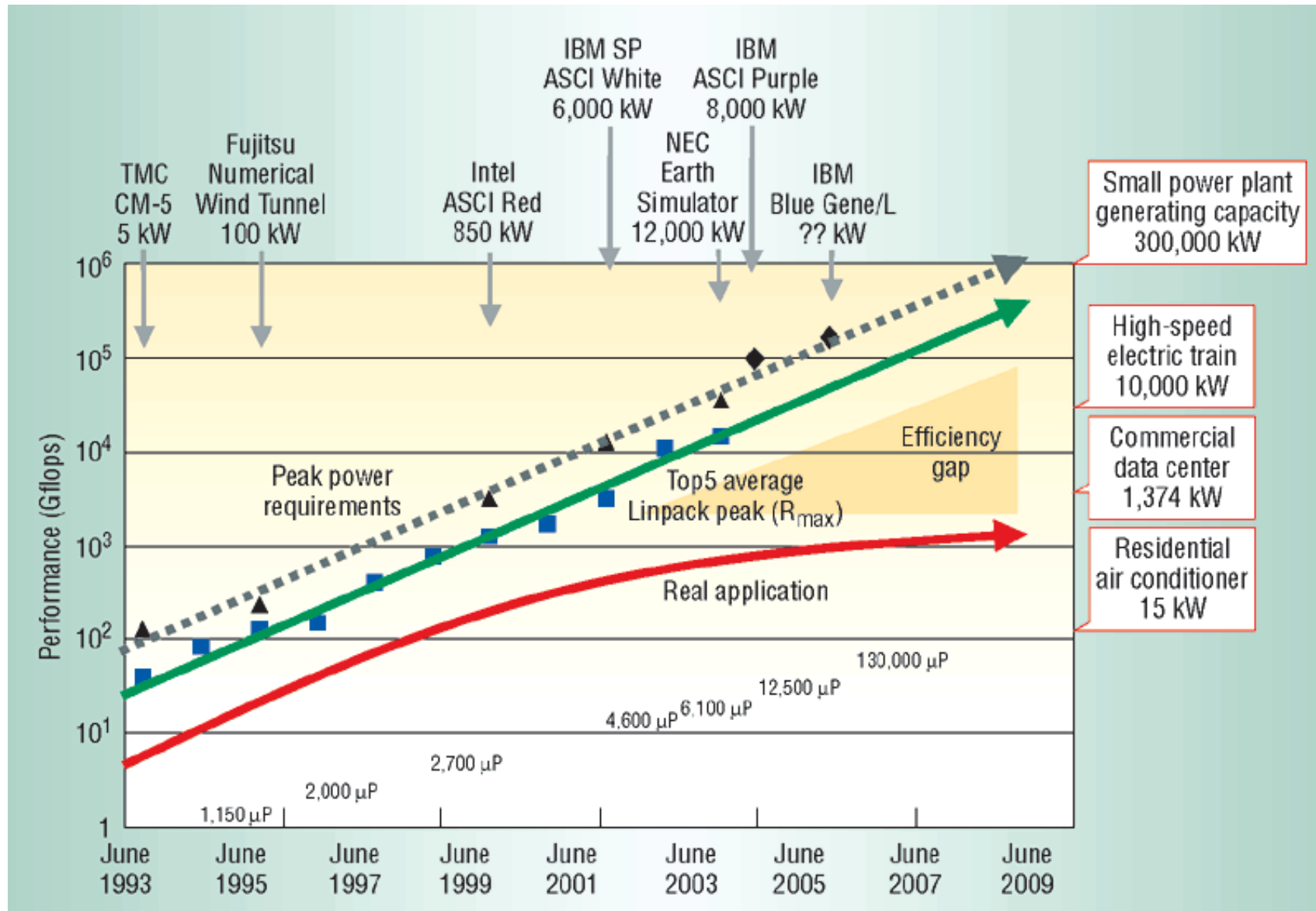


Hot

$D/L=0.5$



Massively parallel supercomputer



Kirk W. Cameron, Rong Ge, Xizhou Feng, High-Performance, Power-Aware Distributed Computing for Scientific Application, *Computer*, vol. 38, no. , pp. 40-47, November 2005

OpenMP versus MPI

OpenMP

- Pro's

- Relatively easy to implement
- Incremental on a loop per loop basis

- Con's

- Works only on shared memory architecture (typically max 32 cores)

MPI

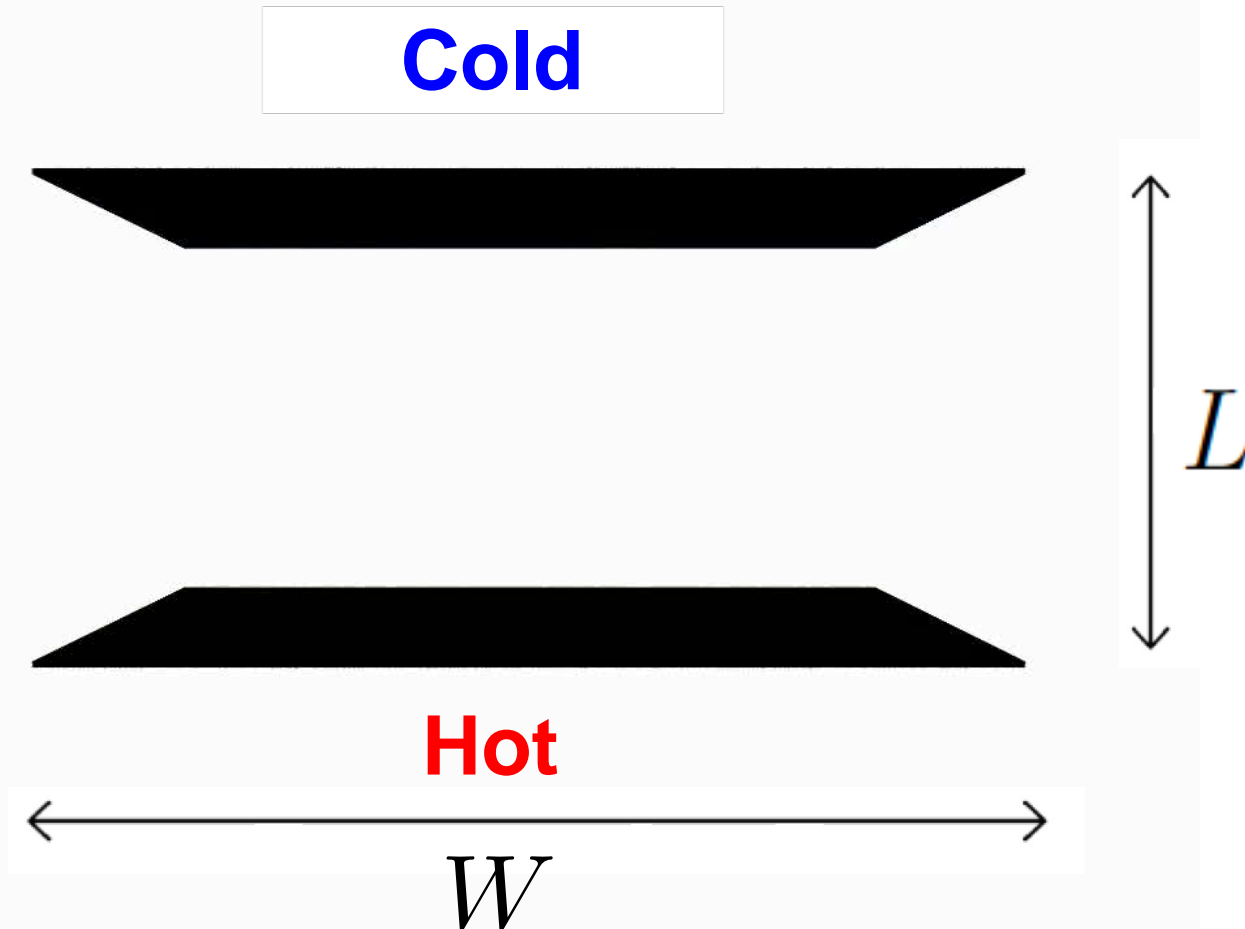
- Pro's

- Works for all systems
- up to an arbitrary number of cores

- Con's

- More work to implement

Rayleigh-Bénard convection



Control parameters

Aspect ratio

$$\Gamma = \frac{W}{L}$$

Rayleigh number

$$Ra = \frac{\beta g L^3 \Delta}{\nu \kappa}$$

Prandtl number

$$Pr = \frac{\nu}{\kappa}$$

Rayleigh-Bénard convection

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} + g\beta T \hat{z} \\ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \kappa \nabla^2 T \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

Rayleigh-Bénard convection

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Introduce the following dimensionless parameters

$$\begin{aligned}\tilde{x} &= x/H \\ \tilde{\mathbf{u}} &= \mathbf{u}/U\end{aligned}$$

Rayleigh-Bénard convection

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} + g\beta T \hat{z} \\ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \kappa \nabla^2 T \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

Introduce the following dimensionless parameters

$$\begin{aligned}\tilde{x} &= x/H \\ \tilde{\mathbf{u}} &= \mathbf{u}/U \\ \tilde{t} &= tU/H\end{aligned}$$

Rayleigh-Bénard convection

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= -\nabla p + \nu \nabla^2 \mathbf{u} + g\beta T \hat{z} \\ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \kappa \nabla^2 T \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

Introduce the following dimensionless parameters

$$\begin{aligned}\tilde{x} &= x/H \\ \tilde{\mathbf{u}} &= \mathbf{u}/U \\ \tilde{t} &= tU/H \\ \tilde{\theta} &= T/\Delta\end{aligned}$$

Rayleigh-Bénard convection

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Introduce the following dimensionless parameters

$$\begin{aligned}\tilde{x} &= x/H \\ \tilde{\mathbf{u}} &= \mathbf{u}/U \\ \tilde{t} &= tU/H \\ \tilde{\theta} &= T/\Delta \\ \tilde{p} &= p/U^2\end{aligned}$$

Rayleigh-Bénard convection

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} + g\beta T \hat{z}$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \kappa \nabla^2 T$$

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

$$\frac{\partial \tilde{\mathbf{u}}}{\partial \tilde{t}} + (\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\mathbf{u}} = -\tilde{\nabla} \tilde{p} + \frac{\nu}{\overline{UH}} \tilde{\nabla}^2 \tilde{\mathbf{u}} + \frac{g\beta \Delta H}{U^2} \tilde{T} \hat{z}$$

$$\frac{\partial \tilde{\theta}}{\partial \tilde{t}} + (\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\theta} = \frac{\kappa}{\overline{UH}} \tilde{\nabla}^2 \tilde{\theta}$$

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

Rayleigh-Bénard convection

$$\begin{aligned} \frac{\partial \tilde{\mathbf{u}}}{\partial \tilde{t}} + (\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\mathbf{u}} &= -\tilde{\nabla} \tilde{p} + \frac{\nu}{UH} \tilde{\nabla}^2 \tilde{\mathbf{u}} + \frac{g\beta\Delta H}{U^2} \tilde{\Gamma} \hat{z} \\ \frac{\partial \tilde{\theta}}{\partial \tilde{t}} + (\tilde{\mathbf{u}} \cdot \tilde{\nabla}) \tilde{\theta} &= \frac{\kappa}{UH} \tilde{\nabla}^2 \tilde{\theta} \\ \tilde{\nabla} \cdot \tilde{\mathbf{u}} &= 0 \end{aligned}$$

Setting buoyancy scale order 1 a convenient velocity scale is found: the so called free-fall velocity $U = \sqrt{g\beta\Delta H}$ as typical velocity.

$$\begin{aligned} \frac{\nu}{UH} &= \sqrt{\frac{Pr}{Ra}} & \text{With} & & Pr &= \frac{\nu}{\kappa} \\ \frac{\kappa}{UH} &= \frac{1}{\sqrt{Pr Ra}} & & & Ra &= \frac{\beta g L^3 \Delta}{\nu \kappa} \end{aligned}$$

Rayleigh-Bénard convection

$$\frac{D\mathbf{u}}{Dt} = -\nabla P + \left(\frac{Pr}{Ra}\right)^{1/2} \nabla^2 \mathbf{u} + \theta \hat{z}$$

$$\frac{D\theta}{Dt} = \frac{1}{(Pr Ra)^{1/2}} \nabla^2 \theta$$

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

With

$$Pr = \frac{\nu}{\kappa} \quad Ra = \frac{\beta g L^3 \Delta}{\nu \kappa}$$

AFiD code for wall bounded turbulence

Navier-Stokes equations with Boussinesq approximation
and additional equation for temperature

$$\begin{aligned}\frac{D\mathbf{u}}{Dt} &= -\nabla P + \left(\frac{Pr}{Ra}\right)^{1/2} \nabla^2 \mathbf{u} + \theta \hat{z} \\ \frac{D\theta}{Dt} &= \frac{1}{(Pr Ra)^{1/2}} \nabla^2 \theta \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

With

$$Pr = \frac{\nu}{\kappa} \quad Ra = \frac{\beta g L^3 \Delta}{\nu \kappa}$$

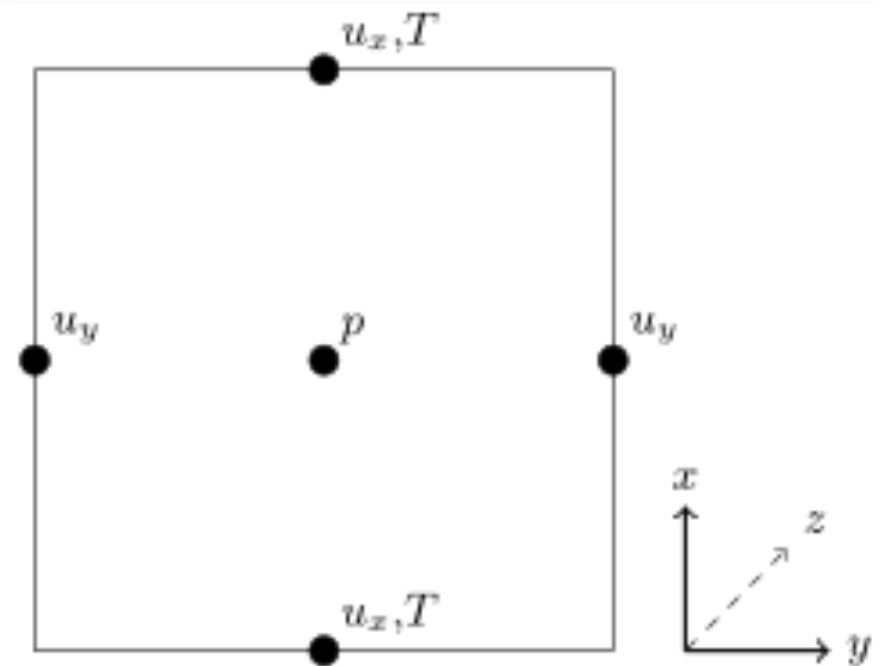
Two horizontal periodic directions (y-z), vertical direction (x) is wall-bounded

Mesh is equally spaced in the horizontal directions, stretched in the vertical direction

AFiD code: Numerical scheme

Conservative centered finite difference

- Staggered grid
- Fractional step
- Time marching: low-storage RK3
(Verzicco and Orlandi, JCP 1996)
(Orlandi, Fluid Flow Phenomena)



AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G} p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

AFiD code: Numerical scheme

At each sub-step:

- 1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G} p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

H - Explicit terms

AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G} p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

H - Explicit terms

Ai - Viscous terms in different computational direction

AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\underbrace{\gamma_l H^j}_{\uparrow} + \underbrace{\rho_l H^{j-1}}_{\uparrow} - \alpha_l \mathcal{G} p^j + \alpha_l (\underbrace{\mathcal{A}_x^j}_{\uparrow} + \underbrace{\mathcal{A}_y^j}_{\uparrow} + \underbrace{\mathcal{A}_z^j}_{\uparrow}) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

H - Explicit terms

Gradient operator

Ai - Viscous terms in different computational direction

AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G} p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

H - Explicit terms

Gradient operator

Ai - Viscous terms in different computational direction

\mathbf{u}^* intermediate, non-solenoidal velocity field \mathbf{u}

AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

Time integration coefficients: depend on the used scheme

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_H H^j + \rho_l T^{j-1} - \alpha_l \nabla p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

H - Explicit terms

Gradient operator

Ai - Viscous terms in different computational direction

\mathbf{u}^* intermediate, non-solenoidal velocity field \mathbf{u}

AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G} p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

2) Pressure correction is calculated solving the following Poisson equation

$$\nabla^2 \phi = \frac{1}{\alpha_l \Delta t} (\nabla \cdot \mathbf{u}^*),$$

AFiD code: Numerical scheme

At each sub-step:

1) Intermediate non-solenoidal velocity field is calculated using non-linear, viscous, buoyancy and pressure at the current time sub-step

$$\frac{\mathbf{u}^* - \mathbf{u}^j}{\Delta t} = \left[\gamma_l H^j + \rho_l H^{j-1} - \alpha_l \mathcal{G}p^j + \alpha_l (\mathcal{A}_x^j + \mathcal{A}_y^j + \mathcal{A}_z^j) \frac{(\mathbf{u}^* + \mathbf{u}^j)}{2} \right]$$

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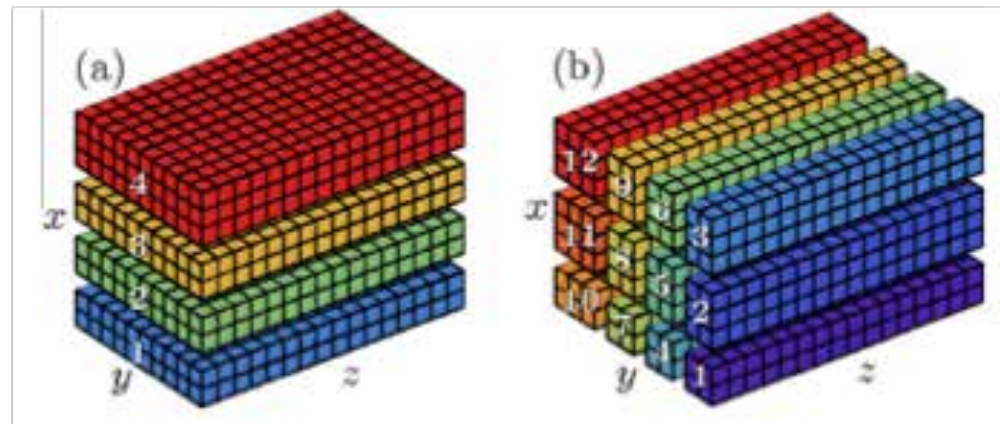
3) The velocity and pressure are then updated using:

$$\begin{aligned} \mathbf{u}^{j+1} &= \mathbf{u}^* - \alpha_l \Delta t (\mathcal{G}\phi), \\ p^{j+1} &= p^j + \phi - \frac{\alpha_l \Delta t}{2Re} (\mathcal{L}\phi), \end{aligned}$$

Making \mathbf{u}^{j+1} divergence free

AFiD code: Parallel implementation

- For large Ra numbers (large temperature difference), the implicit integration of the viscous terms in the horizontal directions becomes unnecessary (prevents solving tridiagonal matrices in the horizontal directions)
- This simplifies the parallel implementation:
 - Only the Poisson solver requires global communication
- The code uses a pencil-type decomposition, more general than a slab-type one



- The pencil decomposition is based on the Decomp2D library (www.2decomp.org)

AFiD code: Poisson solver

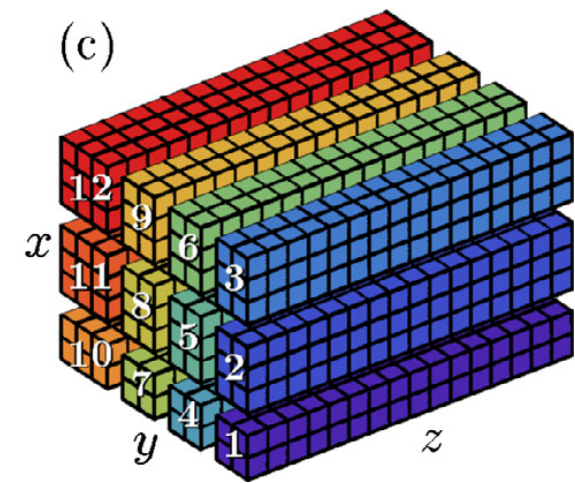
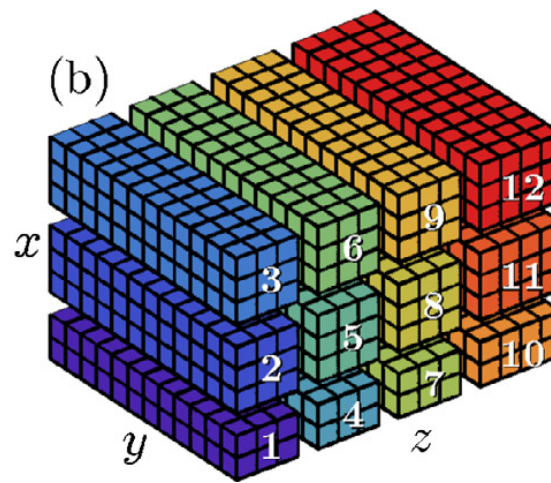
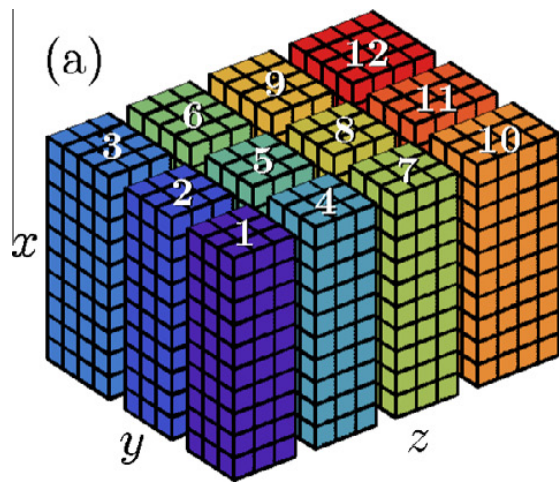
- The solution of the Poisson equation is always the critical part in incompressible solvers
- Direct solver:
 - Fourier decomposition in the horizontal plane
 - Tridiagonal solver in the normal direction

$$\left(\frac{\partial^2}{\partial x^2} - \omega_{y,j}^2 - \omega_{z,k}^2 \right) \mathcal{F}(\phi) = \mathcal{F} \left[\frac{1}{\alpha_l \Delta t} (\mathcal{D}\mathbf{u}^*) \right]$$

$$\omega_{y,j} = \begin{cases} \left(1 - \cos \left[\frac{2\pi(j-1)}{N_y} \right] \right) \Delta_y^{-2} & : \text{for } j \leq \frac{1}{2} N_y + 1 \\ \left(1 - \cos \left[\frac{2\pi(N_y-j+1)}{N_y} \right] \right) \Delta_y^{-2} & : \text{otherwise} \end{cases}$$

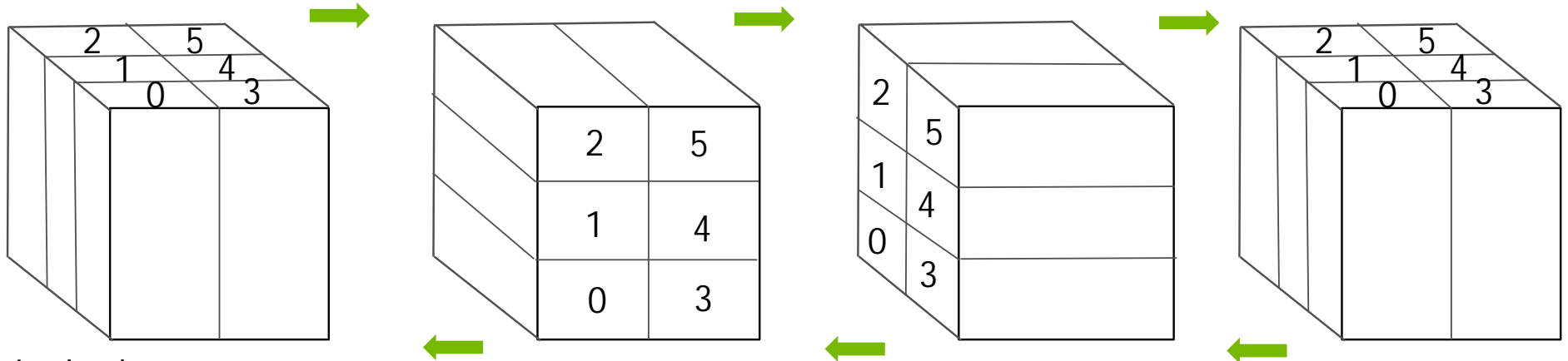
AFiD code: Poisson solver

- 1) FFT the r.h.s along y - (b) (from real $NX \times NY \times NZ$ to complex $NX \times (NY+1)/2 \times NZ$)
- 2) FFT the r.h.s. along z - (c) (from complex $NX \times (NY+1)/2 \times NZ$ to complex $NX \times (NY+1)/2 \times NZ$)
- 3) Solve tridiagonal system in x for each y and z wavenumber - (a)
- 4) Inverse FFT the solution along z - (c) (from complex $NX \times (NY+1)/2 \times NZ$ to complex $NX \times (NY+1)/2 \times NZ$)
- 5) Inverse FFT the solution along y - (b) (from complex $NX \times (NY+1)/2 \times NZ$ to real $NX \times NY \times NZ$)

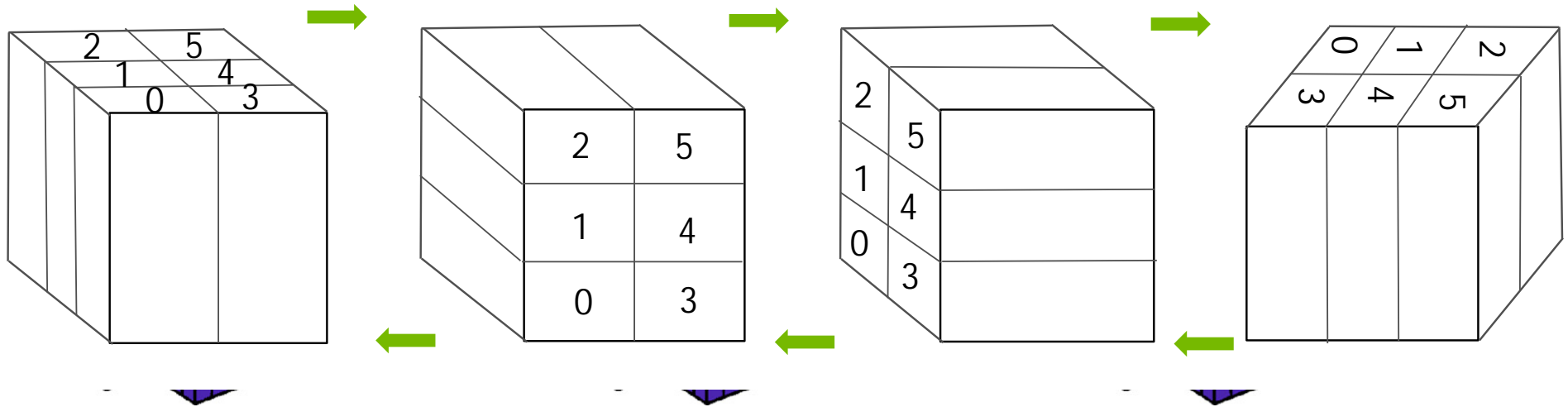


AFiD code: Poisson solver

Transpose



Improved scheme



AFiD Code — Libraries

CPU

I/O: HDF5

FFT: FFTW (guru plan)

Linear algebra:
BLAS+LAPACK

Distributed memory: MPI,
2DDecomp with additional
x-z and z-x transpose

GPU

I/O: HDF5

FFT: CUFFT

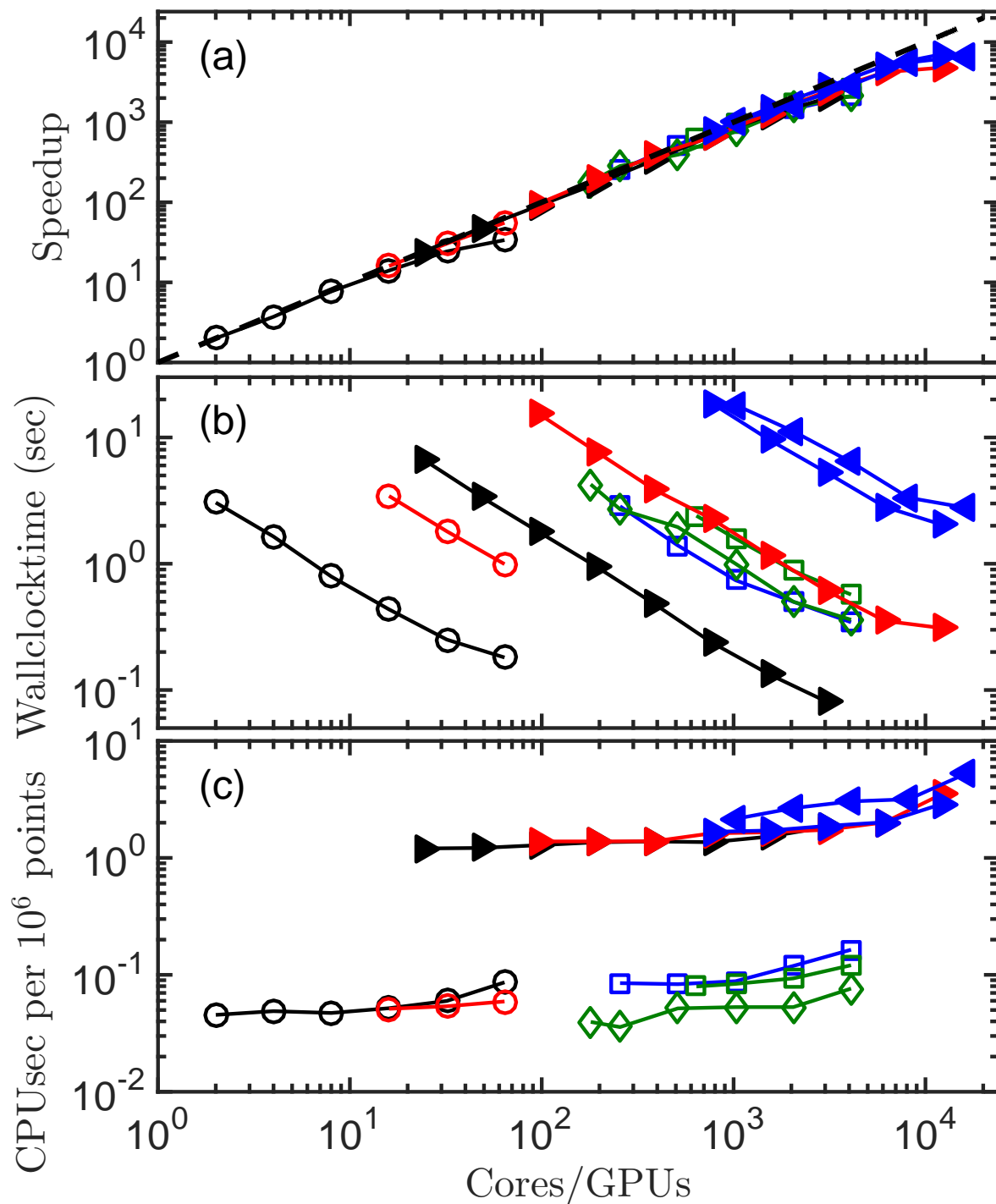
Linear algebra: custom
kernels

Distributed memory: MPI,
2DDecomp with improved
x-z and z-x transpose

Manycore: CUDA Fortran

Available through Github on
www.afid.eu

Scaling of AFiD code



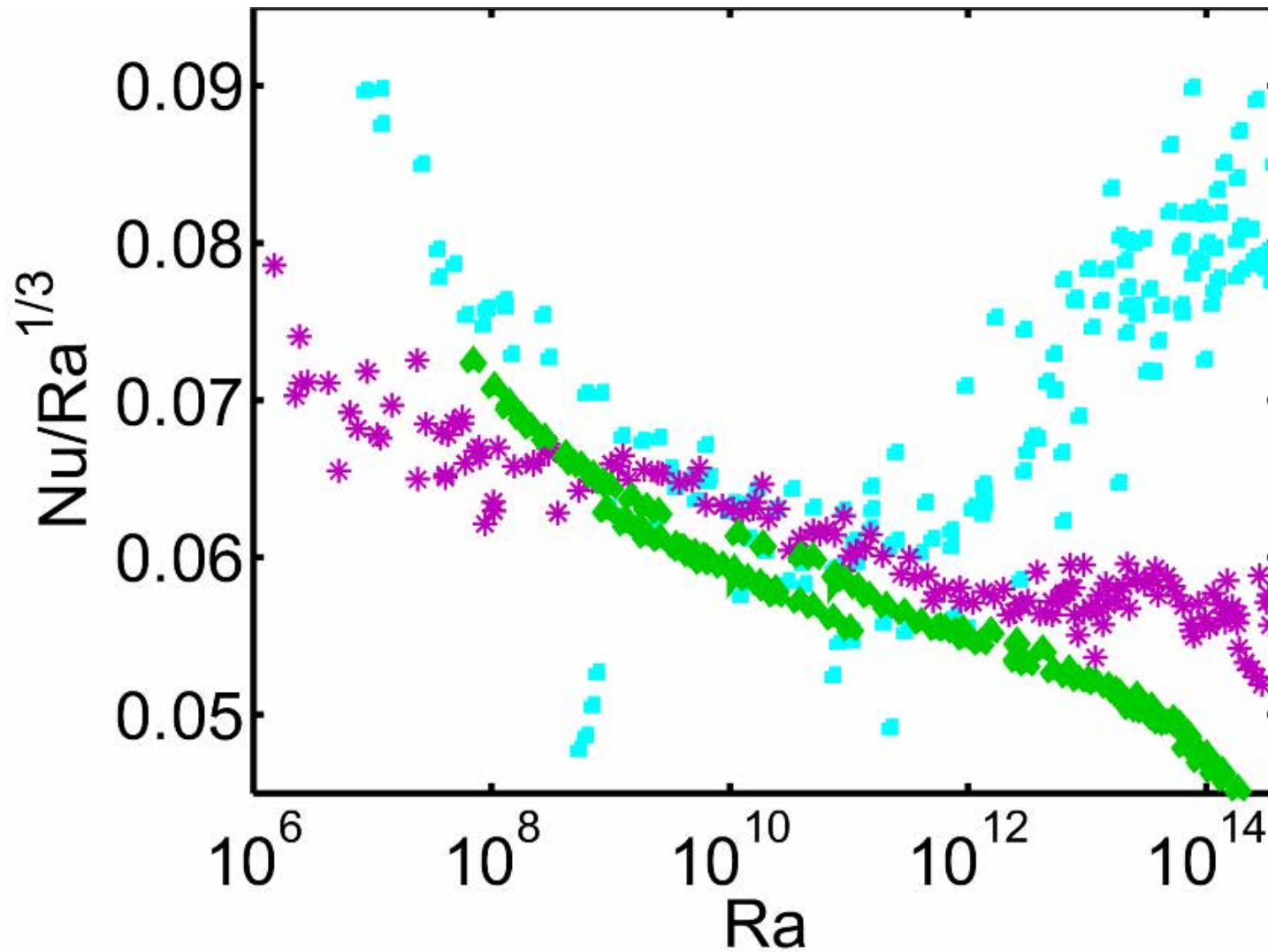
CPU

- ▶ 512³ (Haswell)
- ▶ 1024³ (Haswell)
- ▶ 2048³ (Haswell)
- ▶ 2048³ (Sandy Bridge)

GPU

- 512³ (K40m)
- 1024³ (K40m)
- 2048³ (K20X)
- 2048 × 3072² (K20X)
- ◇ 2048 × 3072² (P100)

Compensated Nusselt Number



Experiments

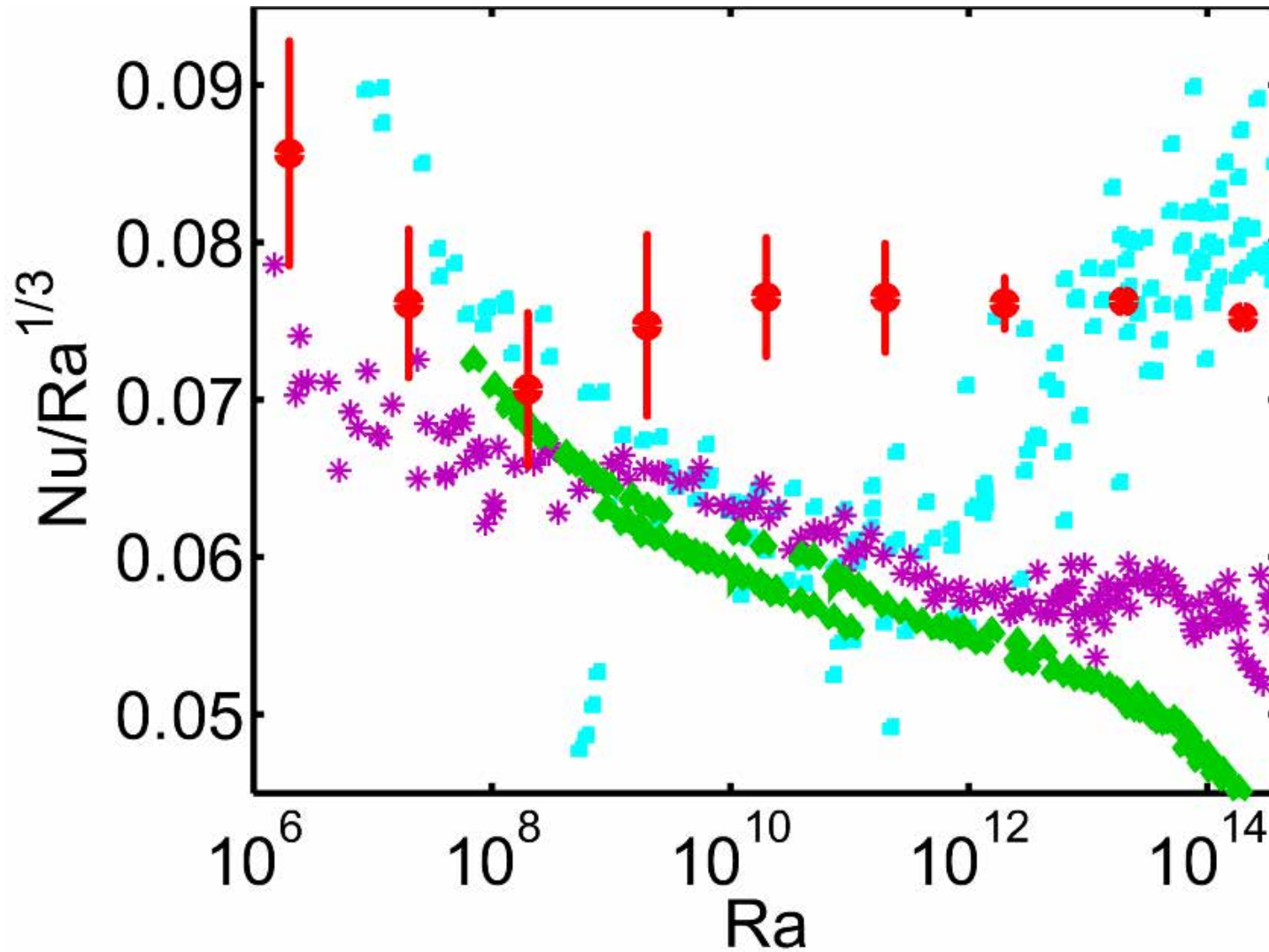
Chavanne
et al. (2001)

Niemela
et al. (2000)

Funfschilling
et al. (2009)

$\Gamma = 0.5, Pr = 0.7$

Compensated Nusselt Number



Experiments

Chavanne
et al. (2001)

Niemela
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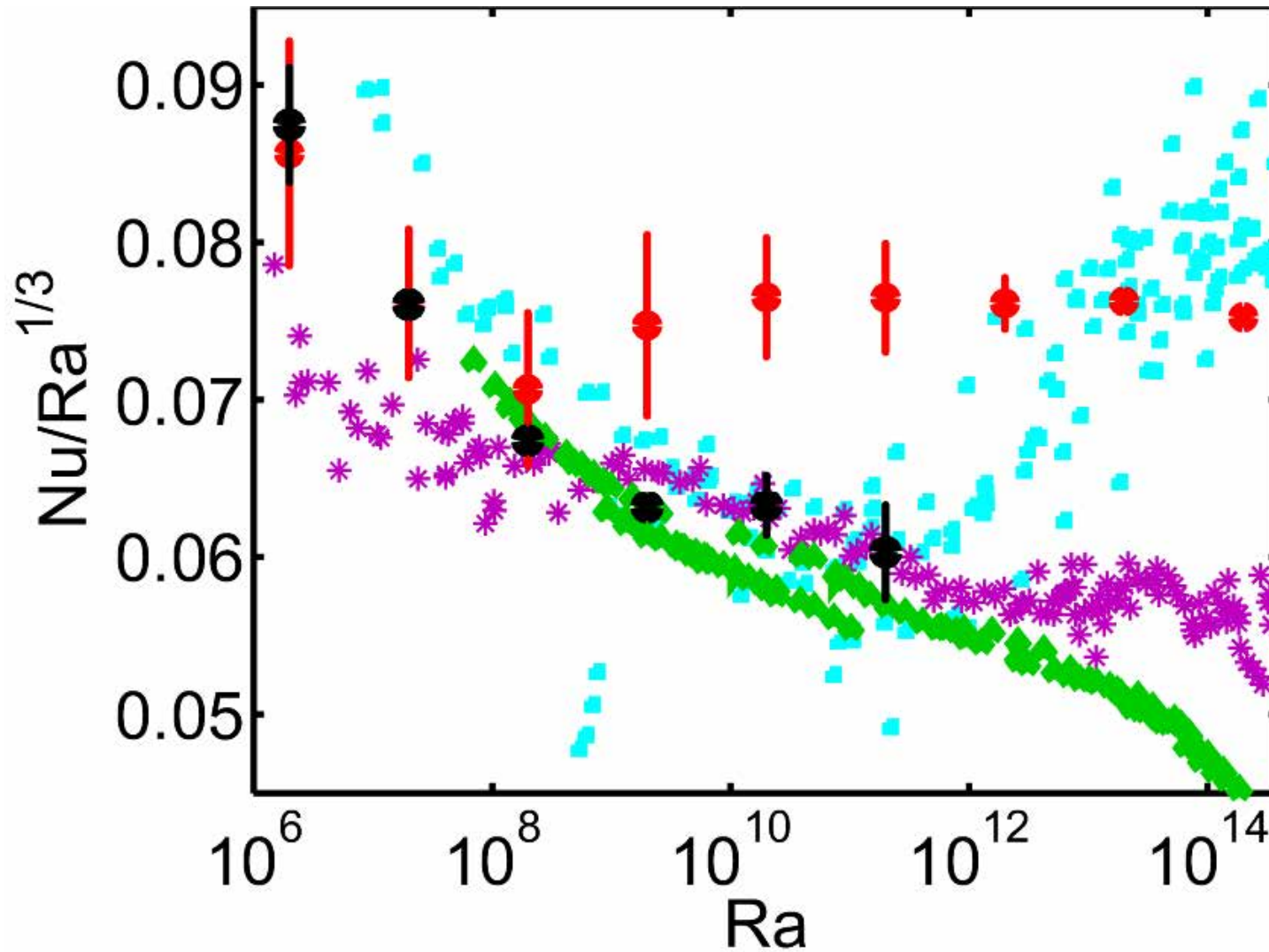
Funfschilling
et al. (2009)

Simulations

Amati *et al.*
(2005)

$\Gamma = 0.5, Pr = 0.7$

Compensated Nusselt Number



$\Gamma = 0.5, Pr = 0.7$

Experiments

Chavanne
et al. (2001)

Niemela
et al. (2000)

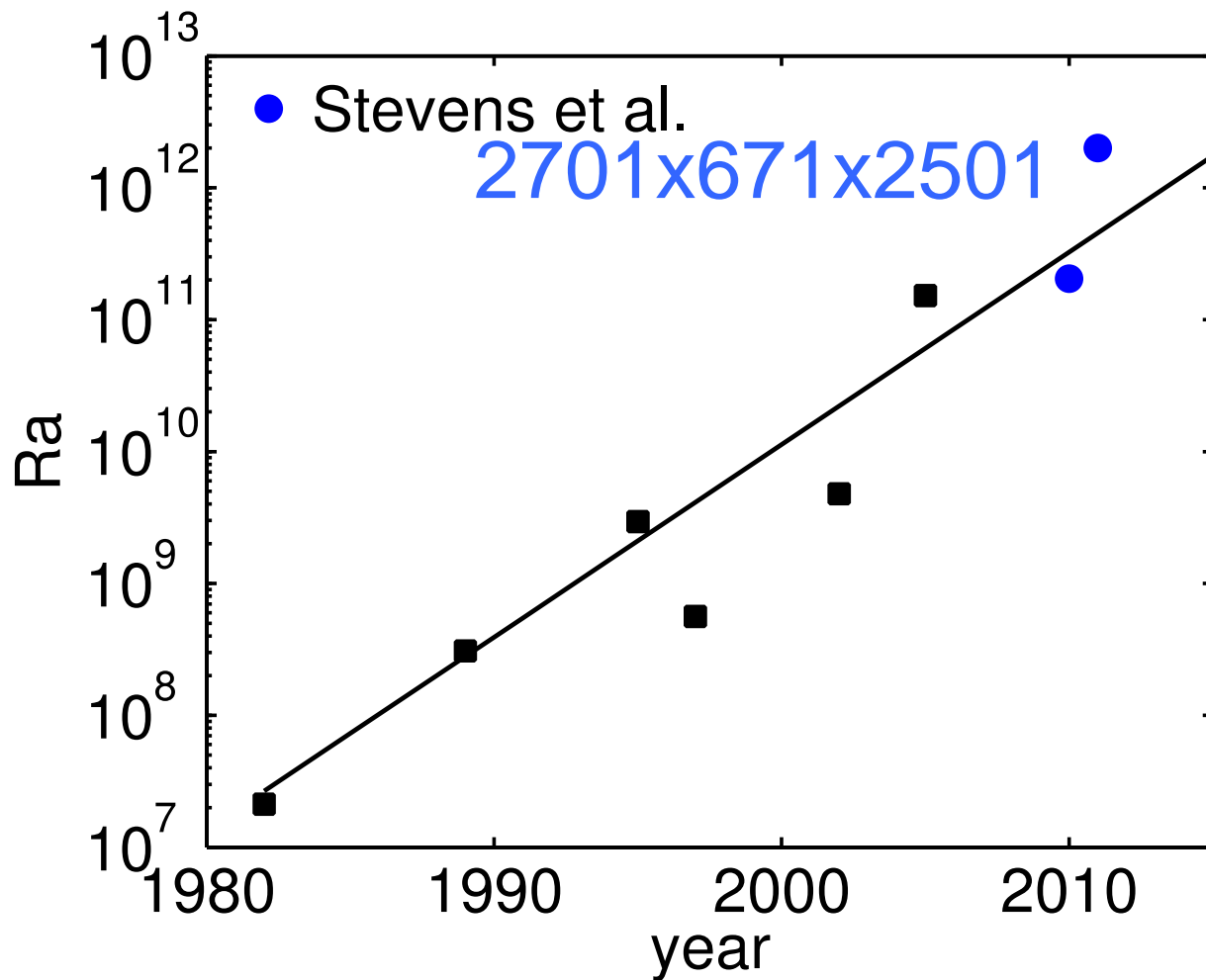
Funfschilling
et al. (2009)

Simulations

Amati *et al.*
(2005)

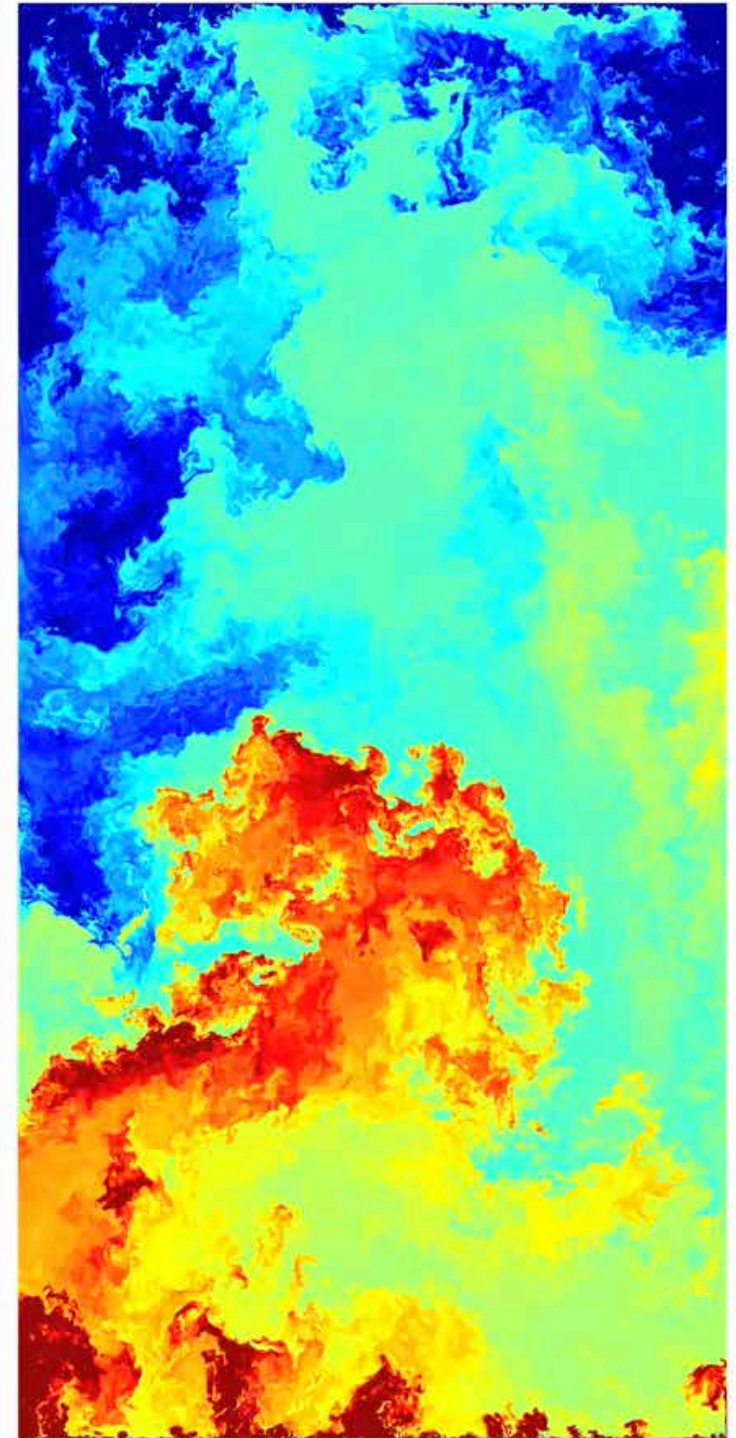
Stevens *et al.*
(2009)

Rayleigh Bénard convection: Direct numerical Simulations

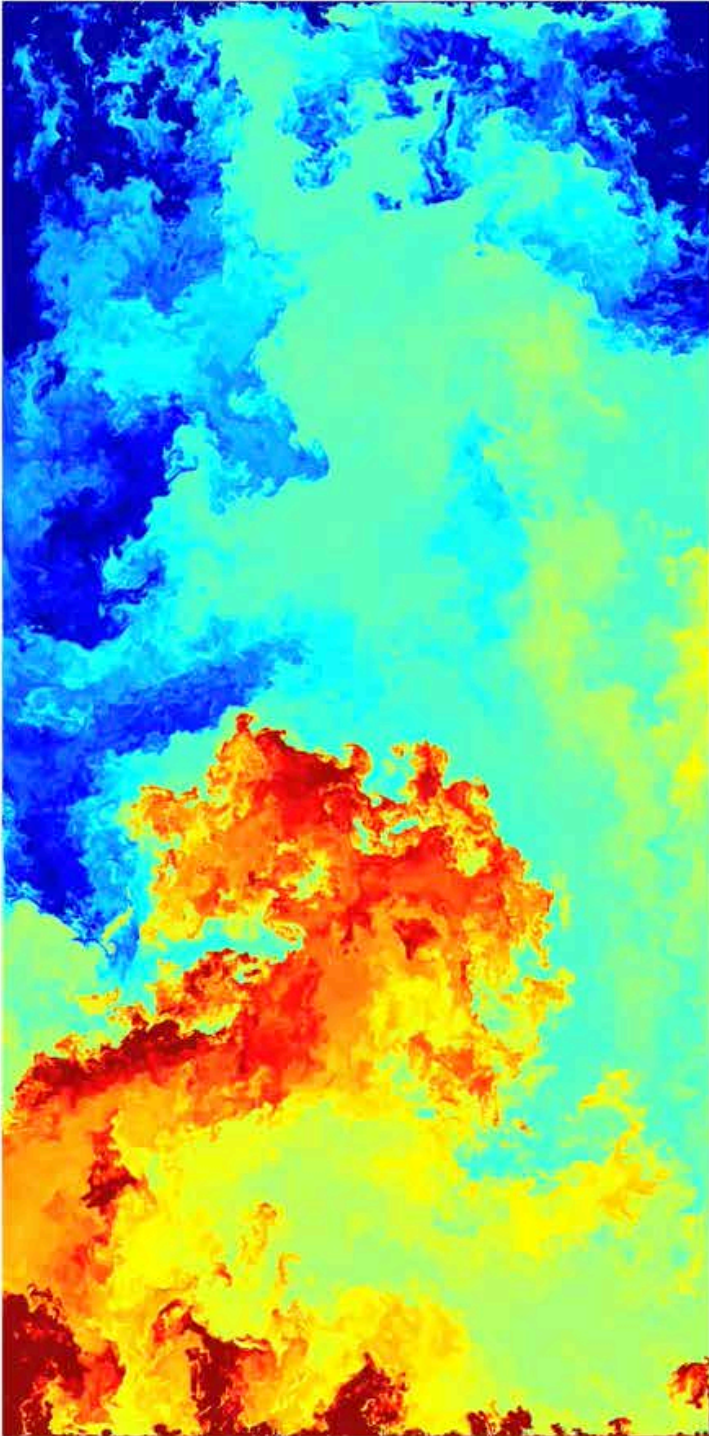


Stevens, Verzicco, Lohse, JFM 643, 495–507 (2010)
Stevens, Lohse, Verzicco, JFM 688, 31-43 (2011)

3D flow



3D flow



Largest DNS

$$Ra = 2 \cdot 10^{12}$$

$$Pr = 0.7$$

$$\Gamma = 0.5$$

3D

2012

Simulation details for $Ra = 2 \times 10^{12}$

- grid = $N_\phi \times N_r \times N_z = 2701 \times 671 \times 2501$
- 10^7 DEISA CPU hours = 1000 years!
(devoted machine in Stuttgart)
- corresponds to 750 Huygens cores
- Upscaling presently limited by ratio
 $\#cores / N_z$

Grid resolution

Smallest scales must be resolved, i.e. the Kolmogorov (velocity scale) and the Batchelor scale (temperature scale) have to be fully resolved.

$$h \leq \pi \eta = \pi L \left(\frac{Pr^2}{RaNu} \right)^{1/4} \quad \text{for } Pr \leq 1 ,$$

$$h \leq \pi \eta_T = \pi L \left(\frac{1}{RaPrNu} \right)^{1/4} \quad \text{for } Pr \geq 1 ,$$

Note that the flow has to be solved properly in all directions, i.e. $h = \max(\Delta x, \Delta y, \Delta z)$

Stevens, Verzicco, Lohse, JFM 643, 495–507 (2010).

How to verify resolution?

- Check whether the relevant length scales are properly resolved by calculating them from the kinetic and thermal dissipation rates.
- Kinetic energy dissipation rate

$$\epsilon_u(\vec{x}) = \nu |\nabla \mathbf{u}|^2$$

- Thermal energy dissipation rate

$$\epsilon_\theta(\vec{x}) = \kappa |\nabla \theta|^2$$

- These can be checked from exact analytic relationships

Derivation of exact relations: ϵ_u

Multiply Boussinesq equation for u_i

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \nu \partial_j^2 u_i + \beta g \partial_{i3} \theta \quad (1)$$

with u_i :

$$\partial_t \frac{u^2}{2} = -\partial_j \left(u_j \frac{u^2}{2} \right) - u_i \partial_i p + \nu u_i \partial_j^2 u_i + \beta g \theta u_3 \quad (2)$$

Derivation of exact relations: ϵ_u

Multiply Boussinesq equation for u_i

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \nu \partial_j^2 u_i + \beta g \partial_{i3} \theta \quad (1)$$

with u_i :

$$\partial_t \frac{u^2}{2} = -\partial_j \left(u_j \frac{u^2}{2} \right) - u_i \partial_i p + \nu u_i \partial_j^2 u_i + \beta g \theta u_3 \quad (2)$$

Apply product rule for the second but last term:

$$\nu u_i \partial_j^2 u_i = \nu \partial_j (u_i \partial_j u_i) - \nu \partial_j u_i \partial_j u_i \quad (3)$$

Derivation of exact relations: ϵ_u

Multiply Boussinesq equation for u_i

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \nu \partial_j^2 u_i + \beta g \partial_{i3} \theta \quad (1)$$

with u_i :

$$\partial_t \frac{u^2}{2} = -\partial_j \left(u_j \frac{u^2}{2} \right) - u_i \partial_i p + \nu u_i \partial_j^2 u_i + \beta g \theta u_3 \quad (2)$$

Apply product rule for the second but last term:

$$\nu u_i \partial_j^2 u_i = \nu \partial_j (u_i \partial_j u_i) - \nu \partial_j u_i \partial_j u_i \quad (3)$$

Summarize terms which can be written as divergence:

$$\partial_t \frac{u^2}{2} = -\partial_i \left(u_i \frac{u^2}{2} + u_i p - \nu \left[\partial_i \frac{u^2}{2} \right] \right) - \nu \partial_j u_i \partial_j u_i + \beta g \theta u_3 \quad (4)$$

Derivation of exact relations: ϵ_u

Multiply Boussinesq equation for u_i

$$\partial_t u_i + u_j \partial_j u_i = -\partial_i p + \nu \partial_j^2 u_i + \beta g \partial_{i3} \theta \quad (1)$$

with u_i :

$$\partial_t \frac{u^2}{2} = -\partial_j \left(u_j \frac{u^2}{2} \right) - u_i \partial_i p + \nu u_i \partial_j^2 u_i + \beta g \theta u_3 \quad (2)$$

Apply product rule for the second but last term:

$$\nu u_i \partial_j^2 u_i = \nu \partial_j (u_i \partial_j u_i) - \nu \partial_j u_i \partial_j u_i \quad (3)$$

Summarize terms which can be written as divergence:

$$\partial_t \frac{u^2}{2} = -\partial_i \left(u_i \frac{u^2}{2} + u_i p + \nu \left[\partial_i \frac{u^2}{2} \right] \right) - \nu \partial_j u_i \partial_j u_i + \beta g \theta u_3 \quad (4)$$

Apply stationarity, i.e. $lhs = 0$, and volume average: With Gauss's theorem the first term on the rhs vanishes as $u = 0$ at all boundaries. Thus

$$\epsilon_u = \nu \langle \partial_j u_i \partial_j u_i \rangle_V = \beta g \langle \theta u_3 \rangle_V = \beta g \frac{1}{L} \int_0^L \langle \theta u_3 \rangle_A dz \quad (5)$$

Derivation of exact relations: ϵ_u

Use the definition of Nu to write

$$\langle \theta u_3 \rangle_A = k \Delta L^{-1} Nu + k \partial_3 \langle \theta \rangle_A \quad (6)$$

and perform the integration over z

$$\epsilon_u = \beta g \left(\kappa \Delta L^{-1} Nu + \frac{\kappa}{L} [\langle \theta \rangle_A]_0^L \right) \quad (7)$$

Derivation of exact relations: ϵ_u

Use the definition of Nu to write

$$\langle \theta u_3 \rangle_A = k\Delta L^{-1}Nu + k\partial_3 \langle \theta \rangle_A \quad (6)$$

and perform the integration over z

$$\epsilon_u = \beta g \left(\kappa\Delta L^{-1}Nu + \frac{\kappa}{L} [\langle \theta \rangle_A]_0^L \right) \quad (7)$$

$$\epsilon_u = \beta g \left(\kappa\Delta L^{-1}Nu + \frac{\kappa}{L} \left[-\frac{\Delta}{2} - \frac{\Delta}{2} \right]_0^L \right) \quad (8)$$

$$\epsilon_u = \frac{\beta g \kappa \Delta}{L} (Nu - 1) \quad (9)$$

Derivation of exact relations: ϵ_u

Use the definition of Nu to write

$$\langle \theta u_3 \rangle_A = k\Delta L^{-1}Nu + k\partial_3 \langle \theta \rangle_A \quad (6)$$

and perform the integration over z

$$\epsilon_u = \beta g \left(\kappa\Delta L^{-1}Nu + \frac{\kappa}{L} [\langle \theta \rangle_A]_0^L \right) \quad (7)$$

$$\epsilon_u = \beta g \left(\kappa\Delta L^{-1}Nu + \frac{\kappa}{L} \left[-\frac{\Delta}{2} - \frac{\Delta}{2} \right]_0^L \right) \quad (8)$$

$$\epsilon_u = \frac{\beta g \kappa \Delta}{L} (Nu - 1) \quad (9)$$

$$\epsilon_u = \frac{\nu^3 Pr^{-2} Ra}{L^4} (Nu - 1) \quad (10)$$

Derivation of exact relations: ϵ_θ

Multiply Boussinesq equation for θ

$$\partial_t \theta + u_i \partial_i \theta = \kappa \partial_i \partial_i \theta \quad (11)$$

with θ and obtain

$$\partial_t \frac{\theta^2}{2} + \partial_i \left(\frac{\theta^2}{2} u_i \right) = \kappa \theta \partial_i \partial_i \theta = \kappa \partial_i (\theta \partial_i \theta) - \kappa (\partial_i \theta)^2 \quad (12)$$

Derivation of exact relations: ϵ_θ

Multiply Boussinesq equation for θ

$$\partial_t \theta + u_i \partial_i \theta = \kappa \partial_i \partial_i \theta \quad (11)$$

with θ and obtain

$$\partial_t \frac{\theta^2}{2} + \partial_i \left(\frac{\theta^2}{2} u_i \right) = \kappa \theta \partial_i \partial_i \theta = \kappa \partial_i (\theta \partial_i \theta) - \kappa (\partial_i \theta)^2 \quad (12)$$

Apply stationarity and volume average, apply Gauss's theorem: Both terms on lhs vanish, the second because $u = 0$ at the boundary. It remains

$$\epsilon_\theta = \kappa \langle (\partial_i \theta)^2 \rangle = \frac{\kappa}{V} \int_V \partial_i (\theta \partial_i \theta) dV = \frac{\kappa}{V} \int_S \langle \theta \partial_i \theta \rangle_A dA_i \quad (13)$$

The surface integral can only contribute at the top and at the bottom, because there is no heat flux through the side walls.

Derivation of exact relations: ϵ_θ

$$\epsilon_\theta = \kappa \langle (\partial_i \theta)^2 \rangle = \frac{\kappa}{V} \int_V \partial_i (\theta \partial_i \theta) dV = \frac{\kappa}{V} \int_S \langle \theta \partial_i \theta \rangle_A dA_i \quad (13)$$

Area/Volume = $A/V = 1/L$. Thus

$$\epsilon_\theta = \frac{\kappa}{L} [\langle \theta \partial_3 \theta \rangle_A]_{bottom}^{top} = \frac{\kappa}{L} \left(-\frac{\Delta}{2} \partial_3 \langle \theta \rangle_{A,top} - \frac{\Delta}{2} \partial_3 \langle \theta \rangle_{A,bottom} \right) \quad (14)$$

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Now realize that the Nusselt number and also the dimensional heat flux

$$H = \kappa \Delta L^{-1} Nu = \langle u_3 \theta \rangle_A - \kappa \partial_3 \langle \theta \rangle_A \quad (15)$$

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For $z = 0$ or $z = L$ $u_3 = 0$ and therefore

$$H = -\kappa \partial_3 \langle \theta \rangle_{A,top} = -\kappa \partial_3 \langle \theta \rangle_{A,bottom} \quad (16)$$

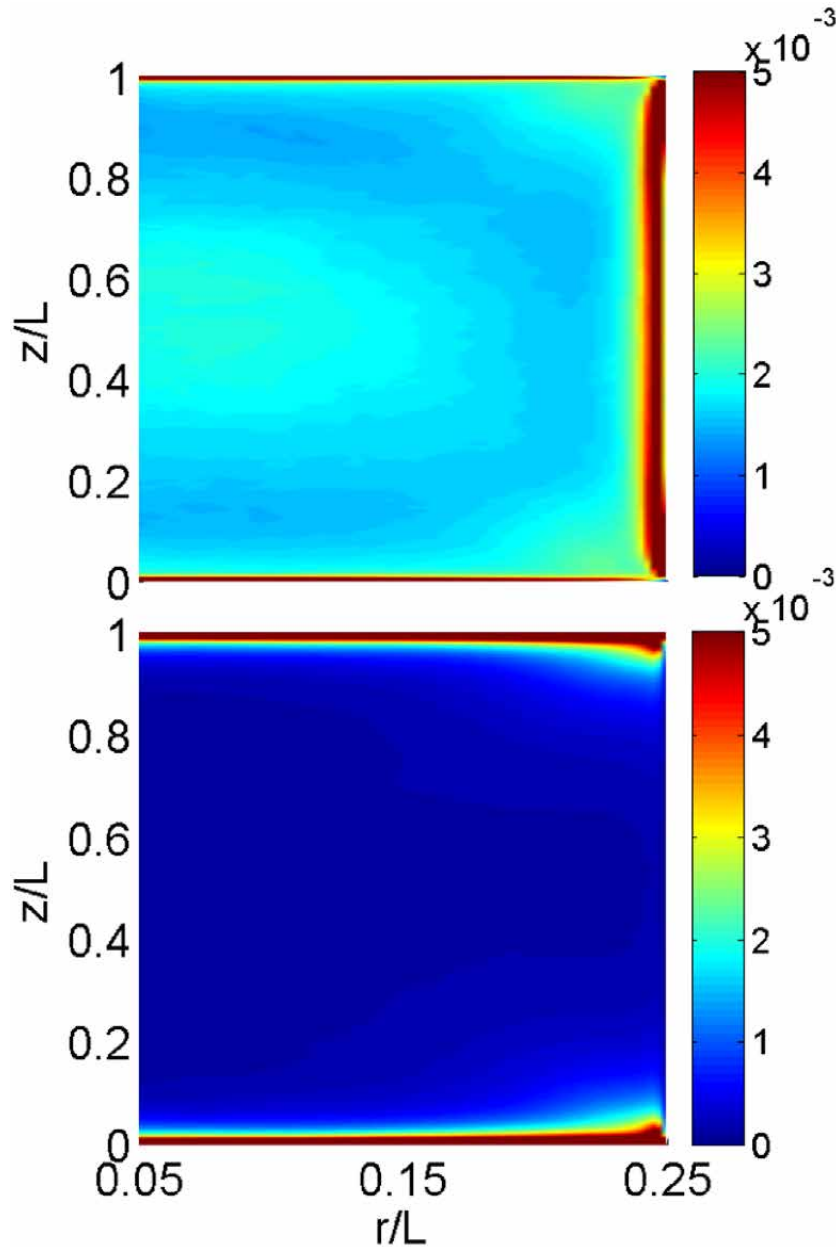
It follows the desired relation

$$\epsilon_\theta = \frac{\Delta H}{L} = \kappa \frac{\Delta^2}{L^2} Nu \quad (17)$$

Check relations in simulations

Ra	$N_\theta \times N_r \times N_z$	Nu	Nu_h	max-diff	N_{BL}	$\frac{\ell_{max,g}}{\eta}$	$\frac{\ell_{max,p}}{\eta}$	$\frac{\langle \epsilon_u \rangle}{\nu^3 Ra Pr^{-2} / L^4 + 1}$	$\frac{\langle \epsilon_\theta \rangle}{\kappa \Delta^2 / L^2}$
2×10^6	$97 \times 49 \times 129$	10.85	10.92	0.32 %	18	0.42	–	–	–
2×10^6	$97 \times 49 \times 129$	10.68	10.32	0.35 %	18	0.42	0.51	0.973	0.978
2×10^6	$129 \times 65 \times 193$	10.56	10.86	0.15 %	27	0.31	0.39	0.972	0.986
2×10^6	$193 \times 97 \times 257$	11.02	11.03	0.44 %	35	0.21	0.26	0.974	0.991
2×10^7	$129 \times 49 \times 193$	20.52	20.56	0.36 %	17	0.66	–	–	–
2×10^7	$193 \times 97 \times 257$	20.54	20.69	0.70 %	31	0.46	0.64	0.989	0.987
2×10^7	$289 \times 129 \times 353$	20.64	20.53	0.36 %	42	0.34	0.43	0.984	0.991
2×10^8	$97 \times 49 \times 193$	40.57	40.71	0.02 %	10	1.84	2.82	1.007	0.926
2×10^8	$193 \times 65 \times 257$	39.42	39.52	0.02 %	13	0.92	1.41	0.992	0.950
2×10^8	$257 \times 97 \times 385$	39.41	39.10	0.79 %	19	0.70	1.11	0.995	0.973
2×10^9	$129 \times 65 \times 257$	89.07	88.25	0.02 %	6	3.01	4.57	1.001	0.858
2×10^9	$193 \times 65 \times 257$	84.49	84.46	0.45 %	7	1.99	3.10	1.002	0.879
2×10^9	$193 \times 65 \times 257$	84.10	83.66	0.51 %	7	1.98	3.06	1.000	0.877
2×10^9	$385 \times 97 \times 385$	79.75	78.70	0.70 %	10	1.15	1.47	0.999	0.935
2×10^9	$513 \times 129 \times 513$	79.60	78.89	0.45 %	17	0.93	1.22	1.006	0.962
2×10^{10}	$129 \times 97 \times 385$	201.08	201.21	1.01 %	12	6.56	10.88	1.006	0.878
2×10^{10}	$513 \times 129 \times 513$	171.79	169.58	2.09 %	19	1.59	2.83	0.994	0.927
2×10^{10}	$385 \times 257 \times 1025$	173.13	173.30	0.98 %	29	2.12	–	–	–
2×10^{11}	$769 \times 193 \times 769$	387.07	387.53	2.18 %	16	2.31	–	–	–
2×10^{11}	$769 \times 257 \times 1025$	373.64	368.88	2.03 %	18	2.28	6.34	0.9883	0.9058
2×10^{11}	$1081 \times 351 \times 1301$	352.67	364.75	4.15 %	26	1.60	3.96	1.0244	0.9318

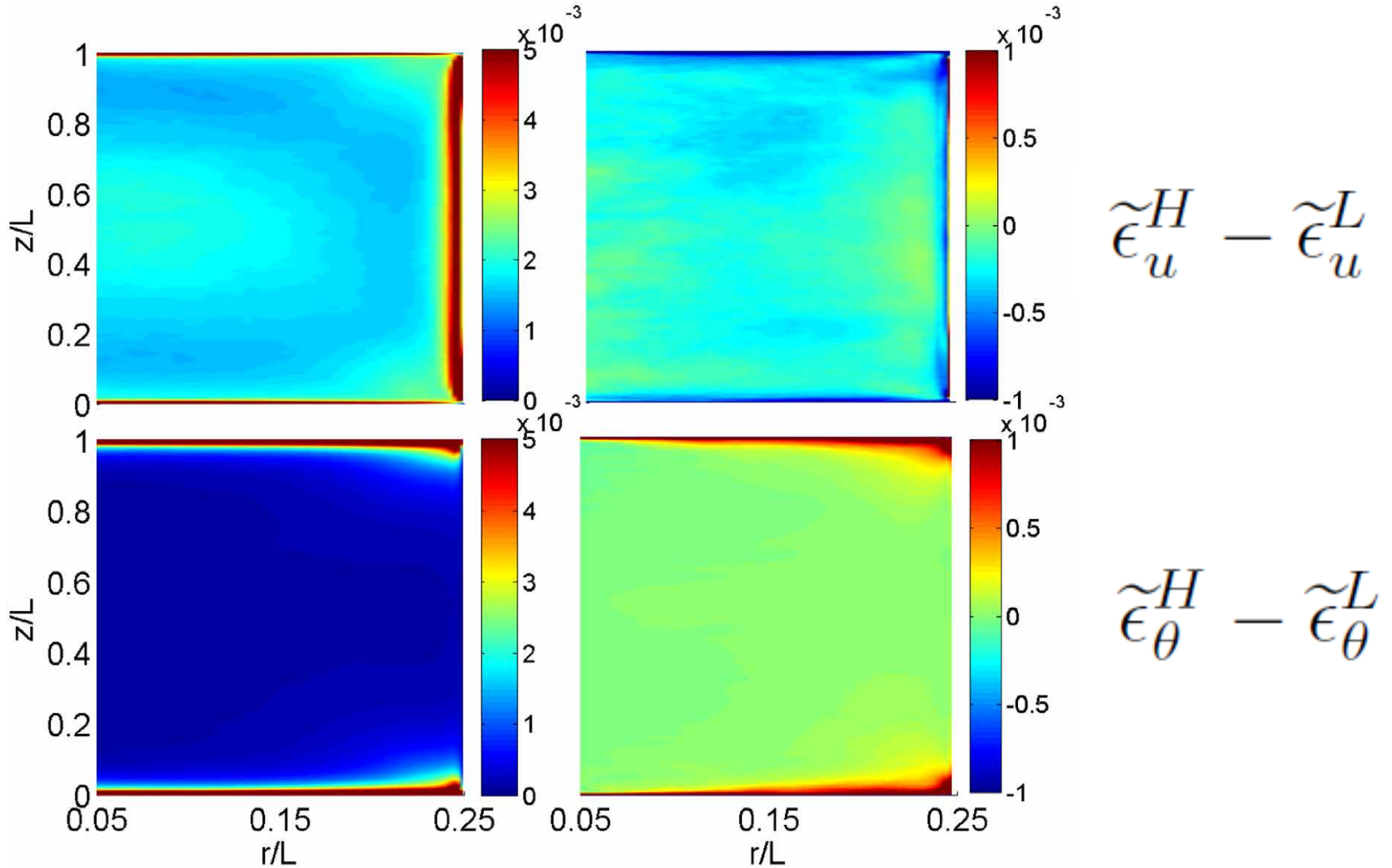
Dissipation rates (Ra = 2·10⁹)



$$\tilde{\epsilon}_u = \epsilon_u L^3 / U^2$$

$$\tilde{\epsilon}_\theta = \epsilon_\theta U / (\Delta^2 L)$$

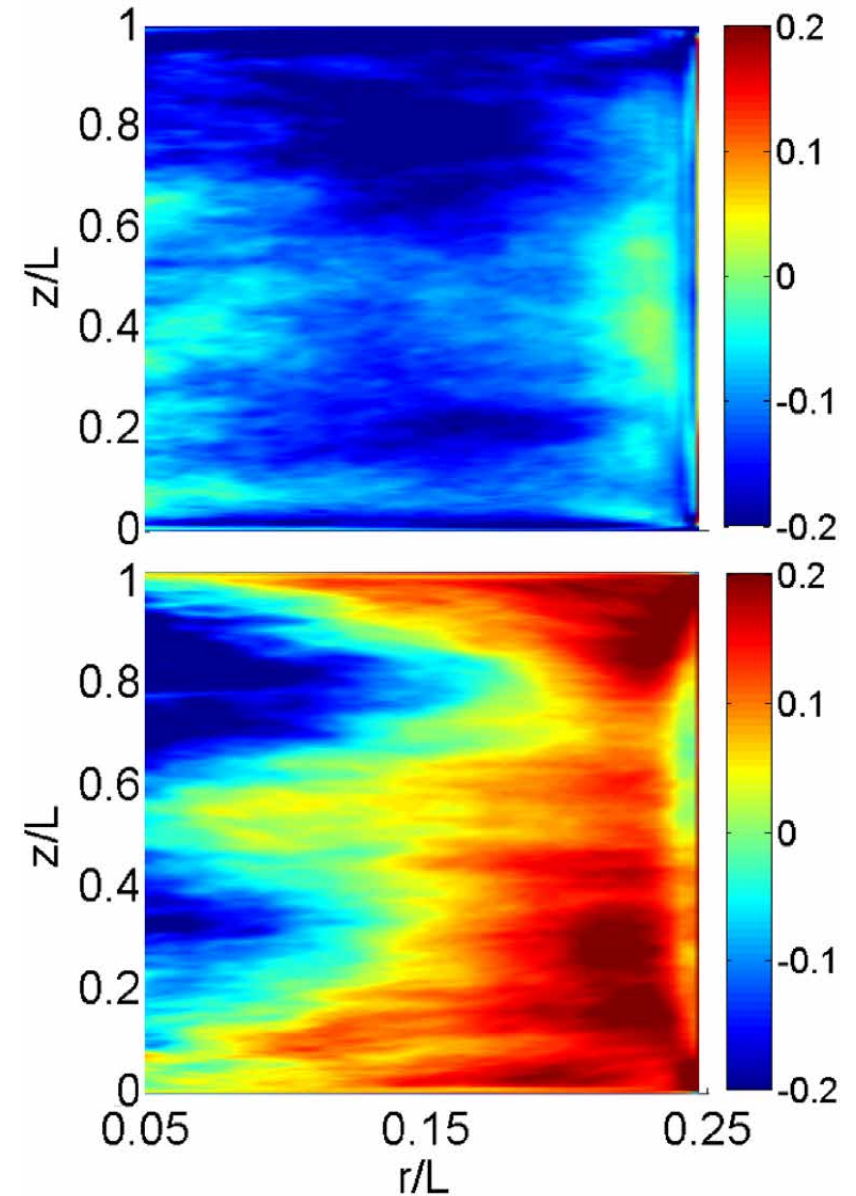
Dissipation rates ($Ra = 2 \cdot 10^9$)



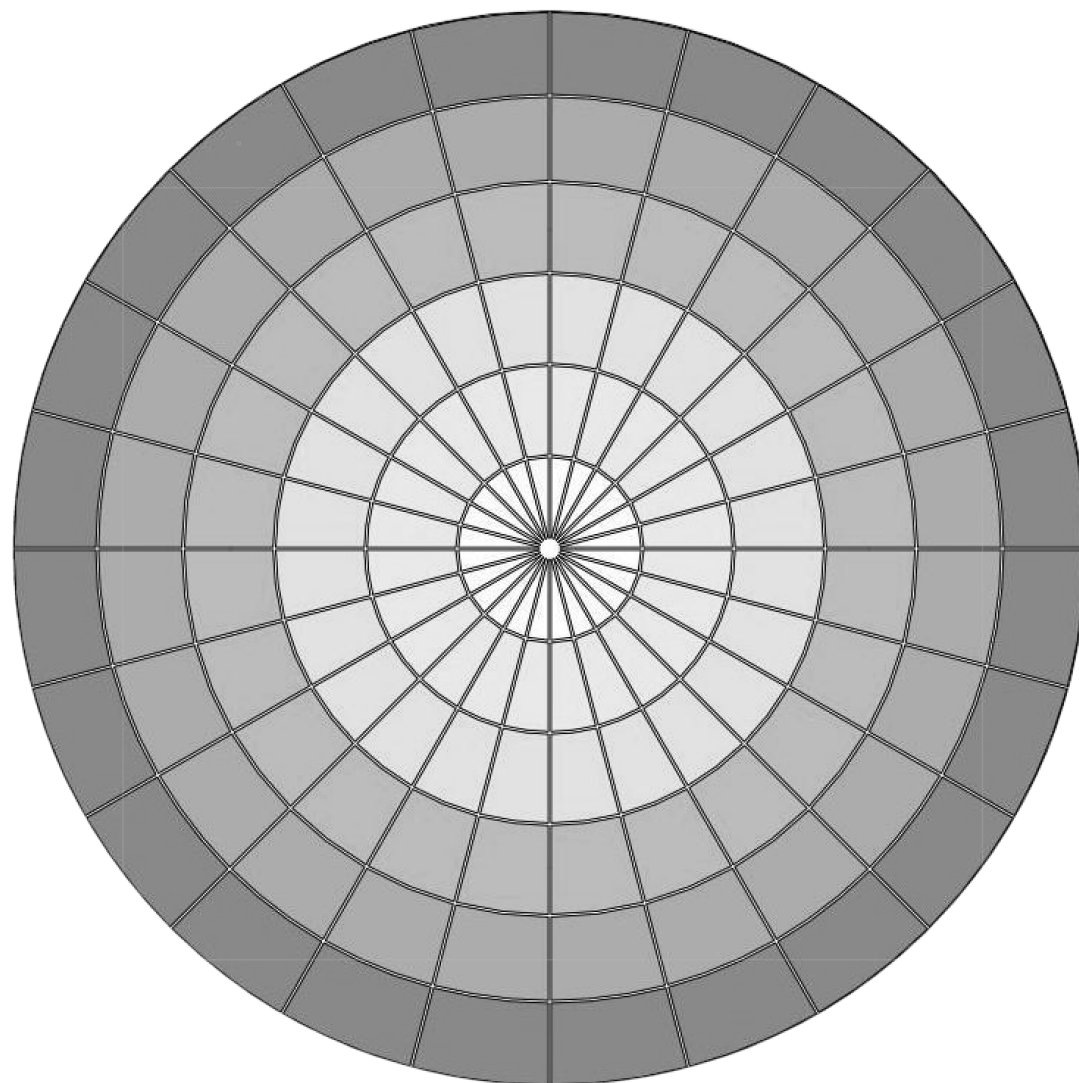
Dissipation rates ($Ra = 2 \cdot 10^9$)

$$\frac{\tilde{\epsilon}_u^H - \tilde{\epsilon}_u^L}{\tilde{\epsilon}_u^H}$$

$$\frac{\tilde{\epsilon}_\theta^H - \tilde{\epsilon}_\theta^L}{\tilde{\epsilon}_\theta^H}$$

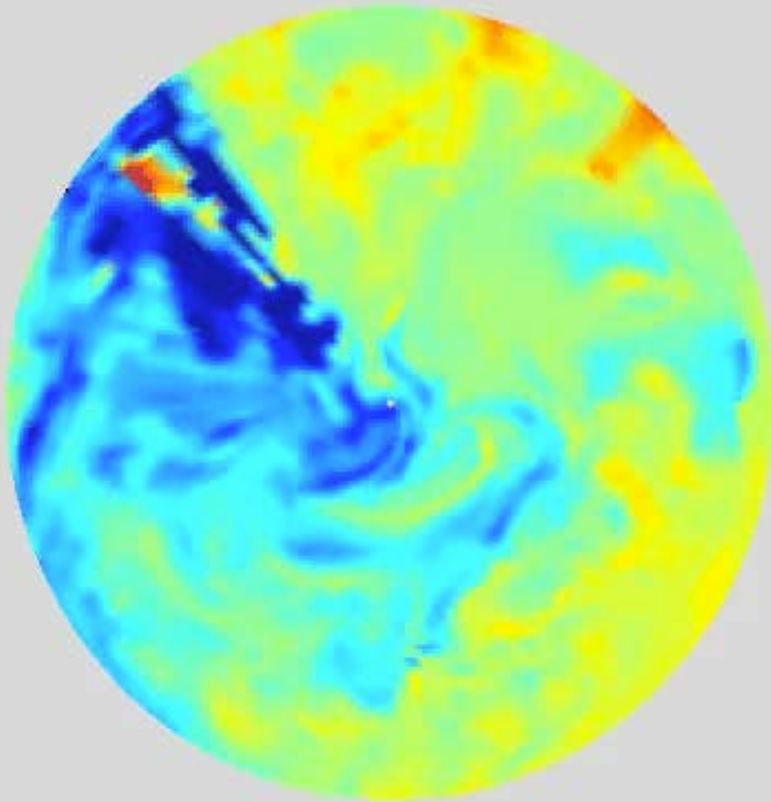


Sketch of grid



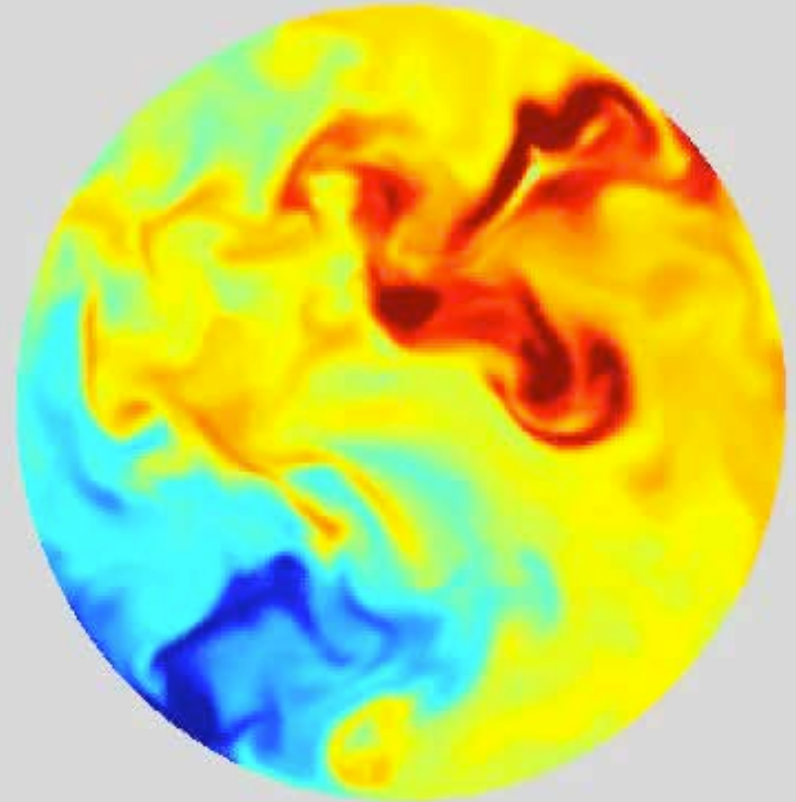
Movies at $Ra = 2 \cdot 10^9$ (midheight)

0.252192



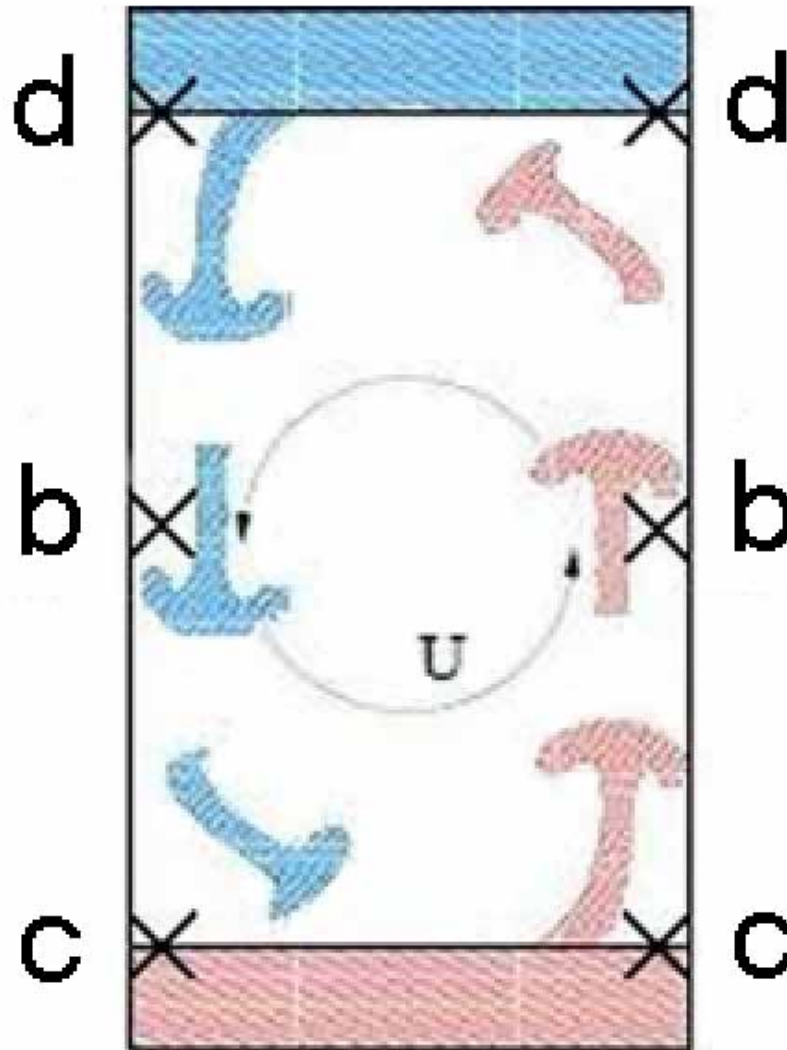
Low resolution

0.251046

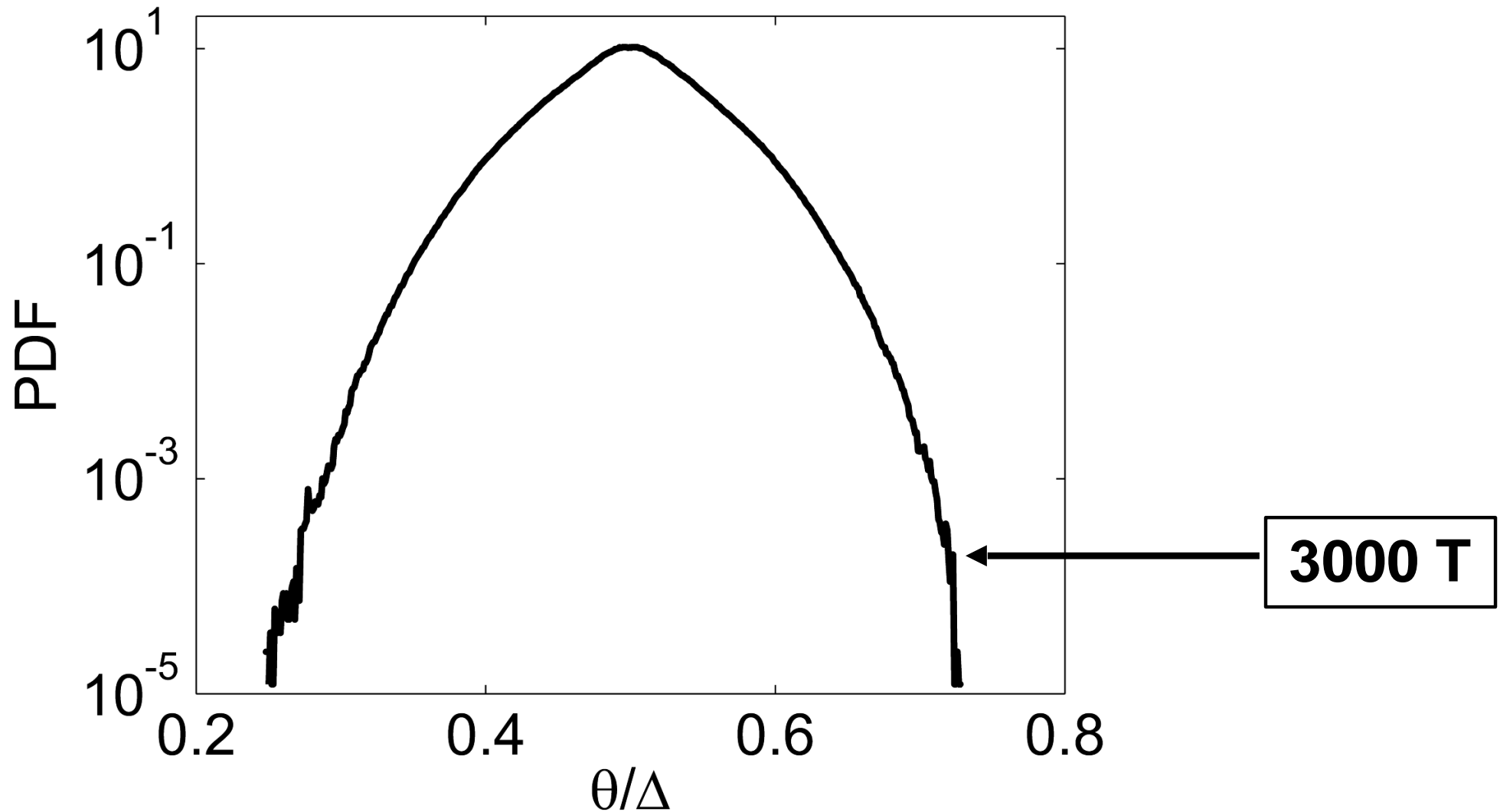


High resolution

PDF locations

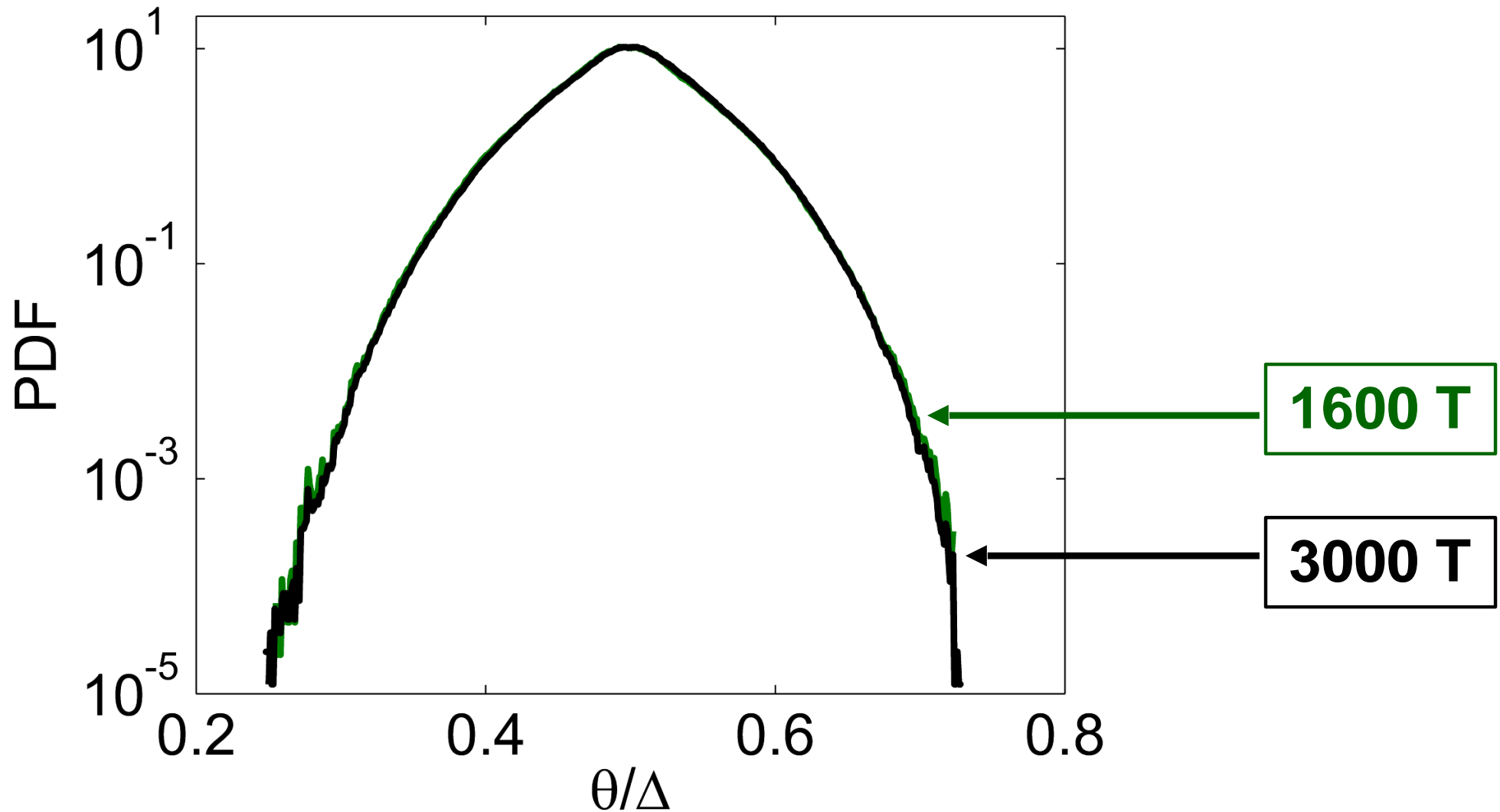


Mid height ($Ra = 2 \cdot 10^8$)



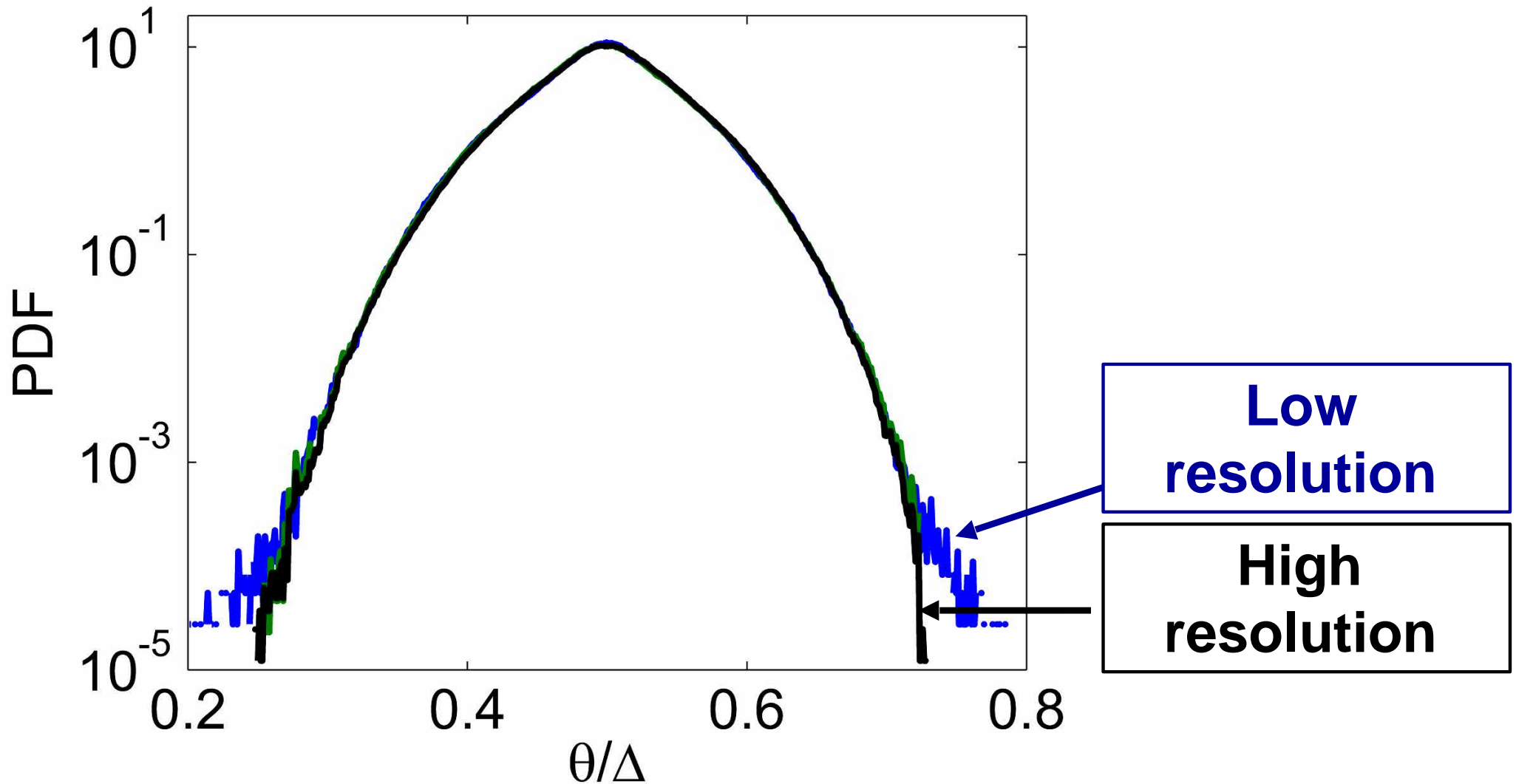
M.S. Emran, J. Schumacher, Fine-scale statistics of temperature and its derivatives in convective turbulence. *J. Fluid Mech.* 611, 13-34 (2008)

Mid height ($Ra = 2 \cdot 10^8$)



M.S. Emran, J. Schumacher, Fine-scale statistics of temperature and its derivatives in convective turbulence. *J. Fluid Mech.* 611, 13-34 (2008)

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M.S. Emran, J. Schumacher, Fine-scale statistics of temperature and its derivatives in convective turbulence. *J. Fluid Mech.* 611, 13-34 (2008)

New resolution criteria

Following Grötzbach (1983) we get

$$h \leq \pi\eta = \pi L \left(\frac{Pr^2}{RaNu} \right)^{1/4} \quad \text{for } Pr \leq 1,$$

$$h \leq \pi\eta_T = \pi L \left(\frac{1}{RaPrNu} \right)^{1/4} \quad \text{for } Pr \geq 1,$$

But not on the average grid size $d=(D_1D_2D_3)^{1/3}$, but by each grid dimension D_1, D_2, D_3 simultaneously!

Number of grid points in the boundary layer should be

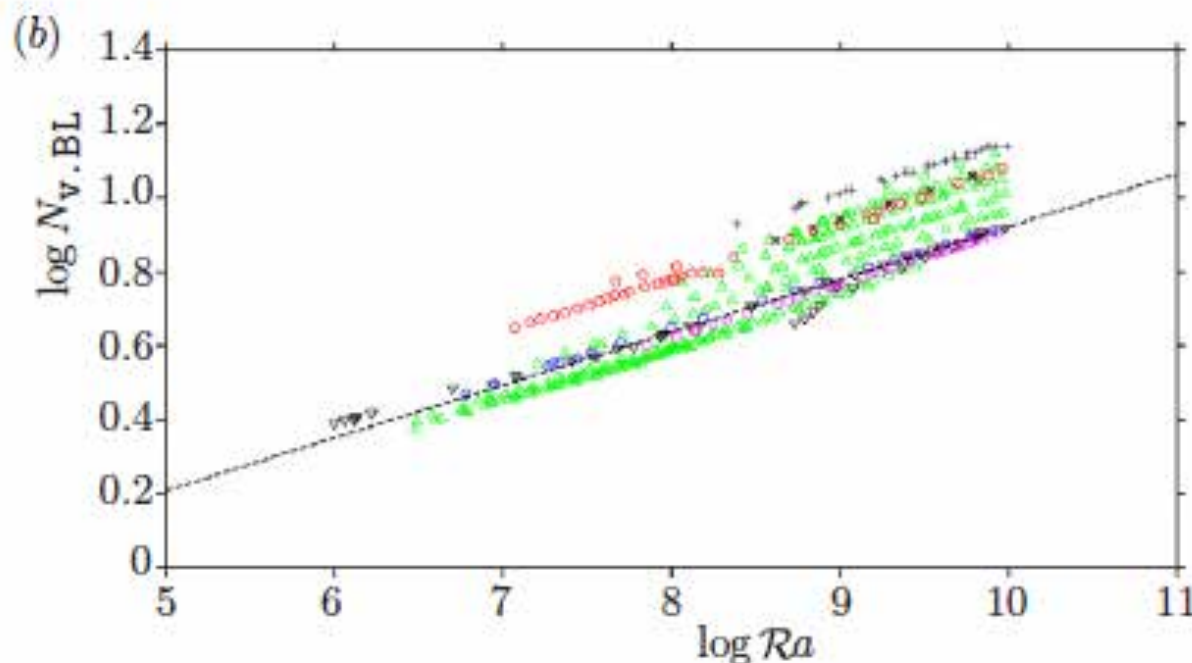
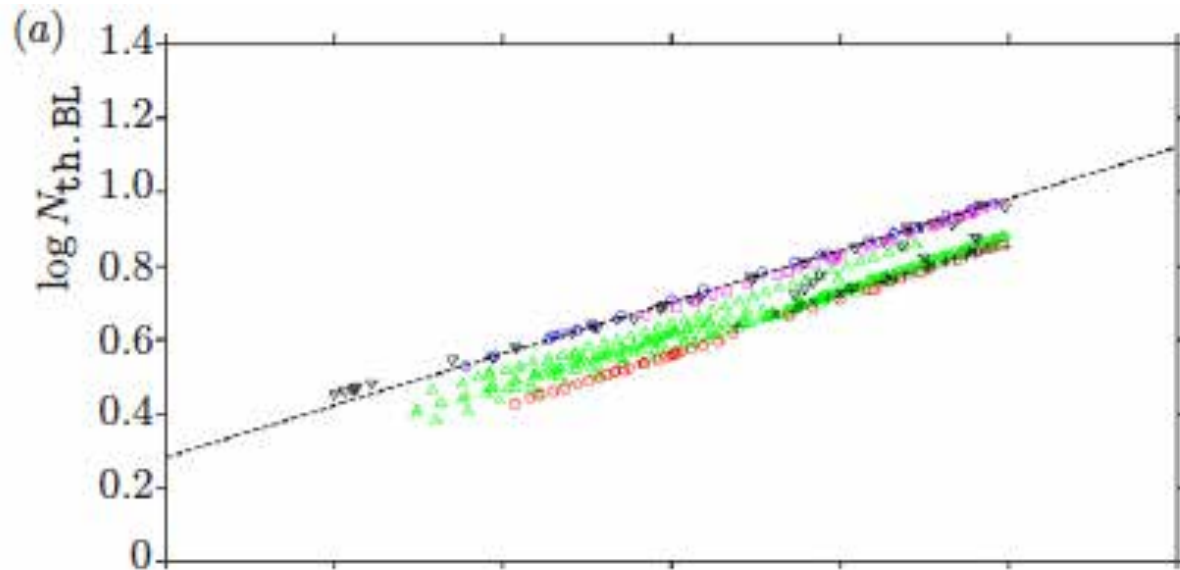
$$N_{\text{th.BL}} \approx 0.35Ra^{0.15}, \quad 10^6 \leq Ra \leq 10^{10},$$

$$N_{\text{v.BL}} \approx 0.31Ra^{0.15}, \quad 10^6 \leq Ra \leq 10^{10}.$$

Stevens, Verzicco, Lohse, **J. Fluid Mech.** 643, 495-507 (2010).

Shishkina, **Stevens**, Grossmann, Lohse, **New J. Phys.** 12, 075022 (2010).

Boundary layer resolution



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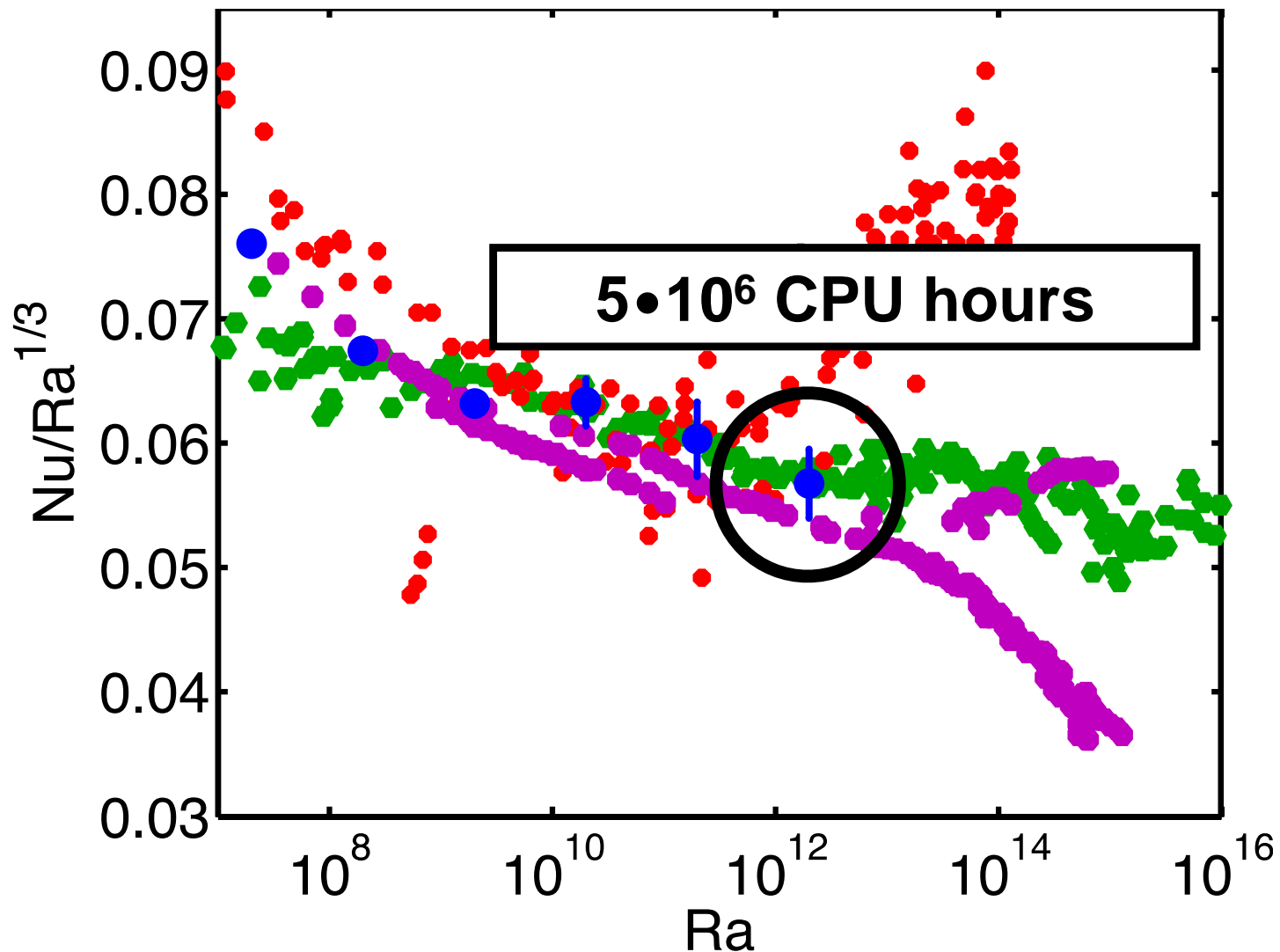
$$N_{\text{v.BL}} \approx 0.31 Ra^{0.15}, \quad 10^6 \leq Ra \leq 10^{10}.$$

For higher Ra this can easily be 20 or more, instead of the fixed value of 3-5 recommended by Grotzbach

Stevens, Verzicco, Lohse, J. Fluid Mech. 643, 495-507 (2010).

Shishkina, **Stevens, Grossmann, Lohse, New J. Phys.** 12, 075022 (2010).

RB convection ($\Gamma=0.5$)

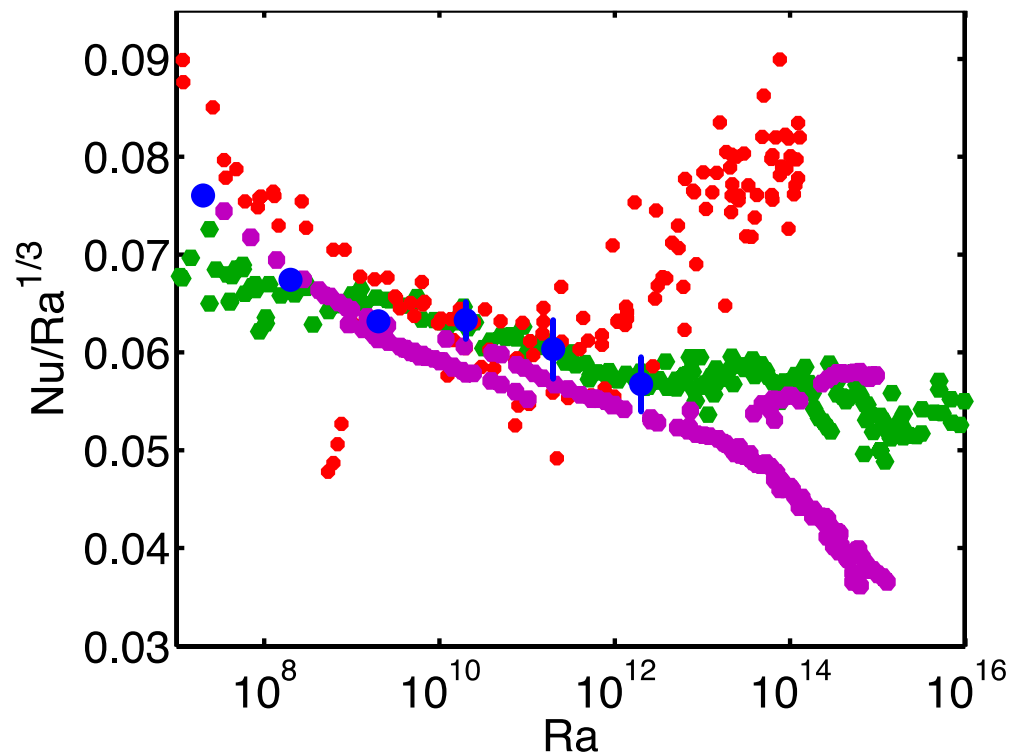


- E Niemela et al. (2000)
- E Chavanne et al. (2001)
- E Funfschilling et al. (2010)
- N Stevens et al. (2010-2011)

E=Experiments, N=Numerics

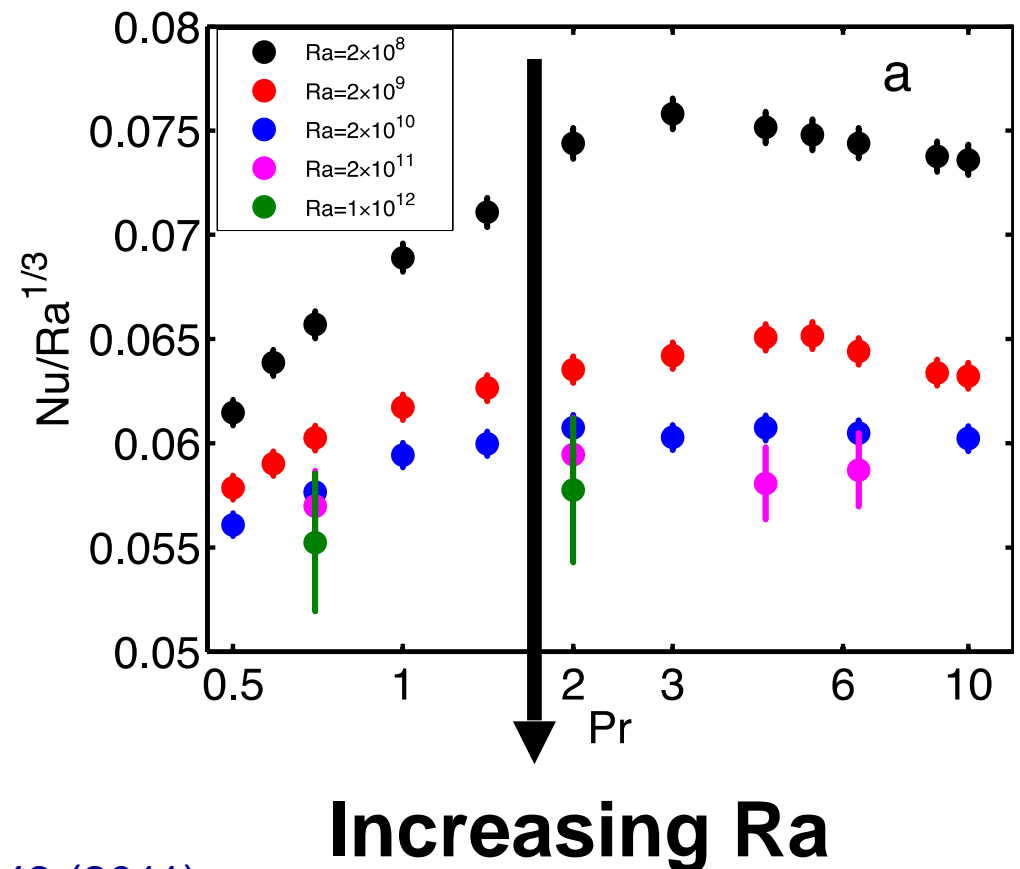
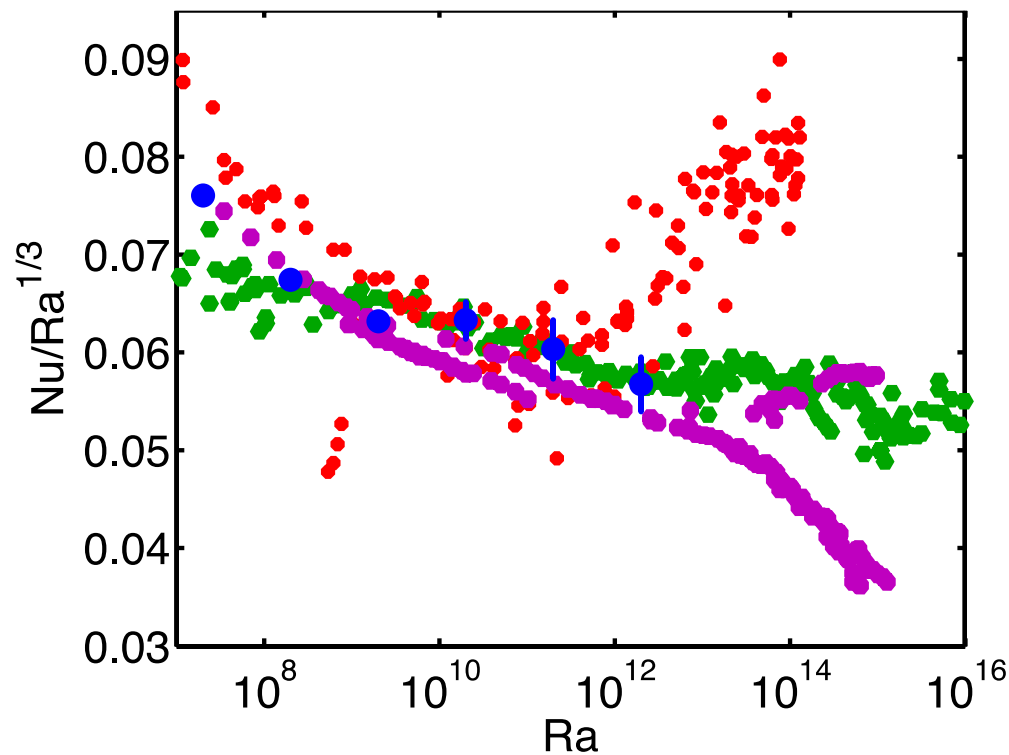
Why is there a discrepancy between experiments?

- Prandtl number effect, i.e. different fluid properties



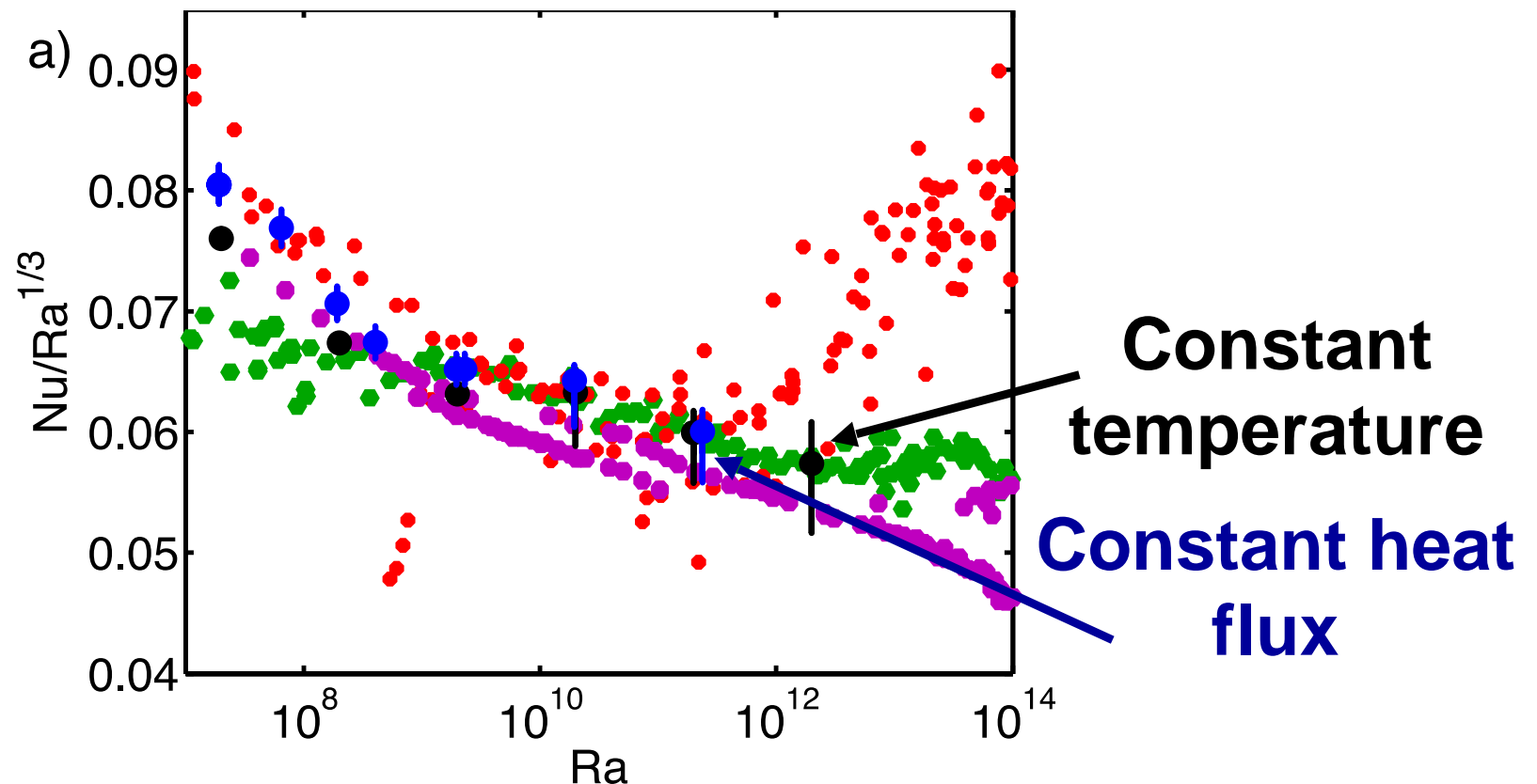
Why is there a discrepancy between experiments?

- Prandtl number effect, i.e. different fluid properties
 - Simulations confirm theoretical prediction that Nu becomes independent of Pr for high Ra

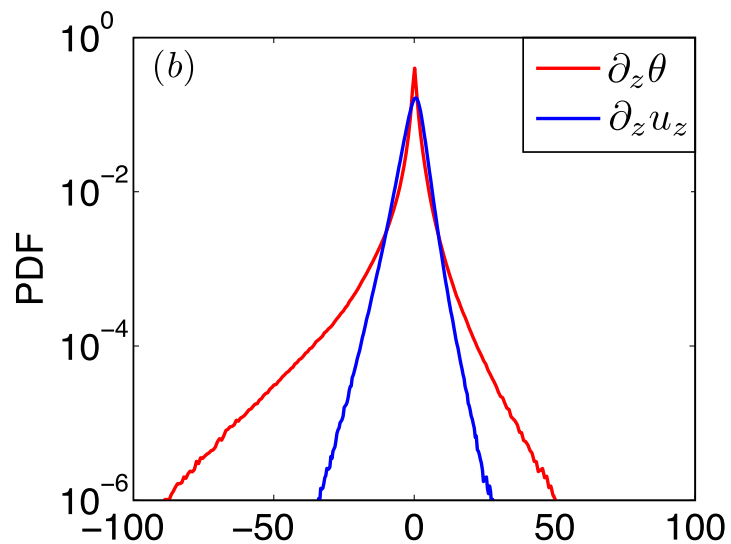
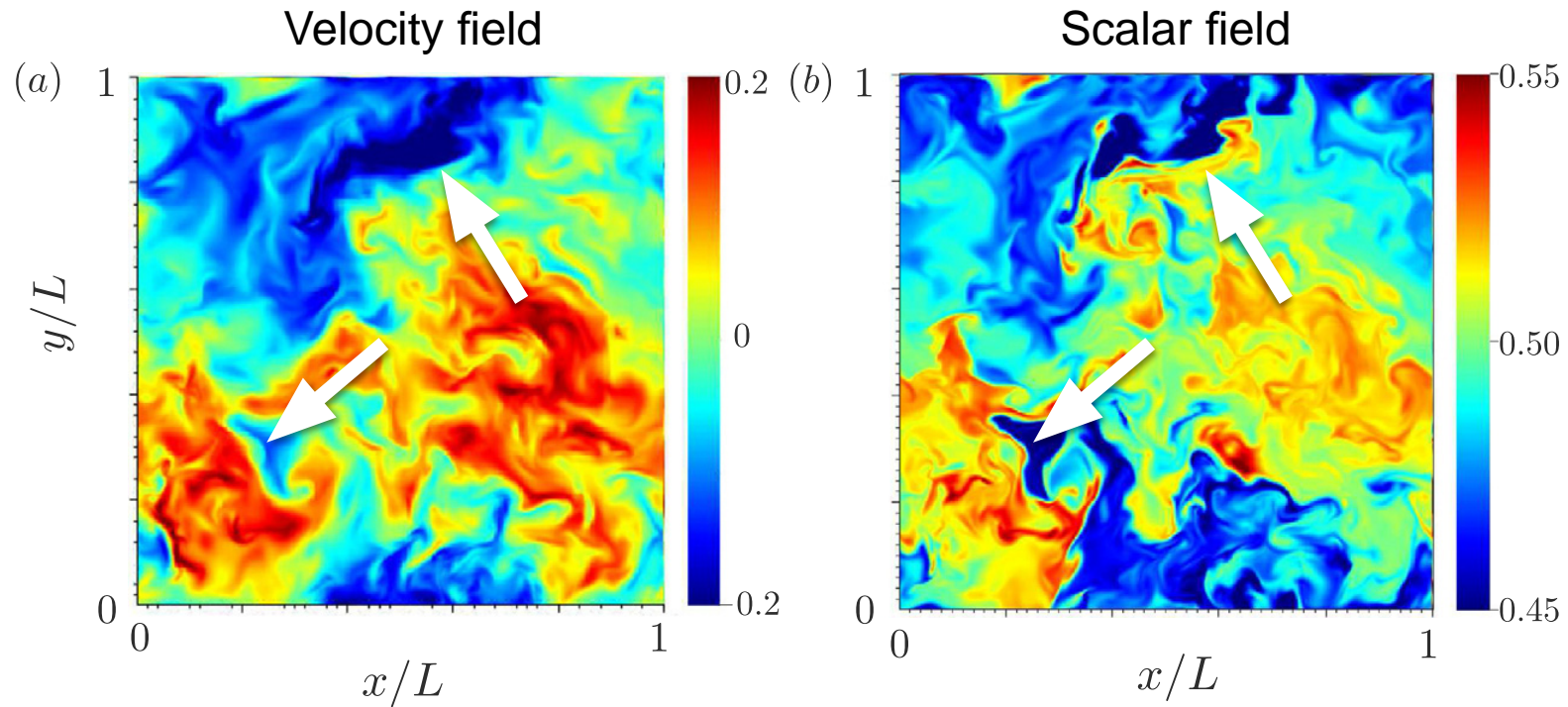


Why is there a discrepancy between experiments?

- ~~Prandtl number effect, i.e. different fluid properties~~
- Constant temperature versus constant heat flux boundary condition at the bottom plate

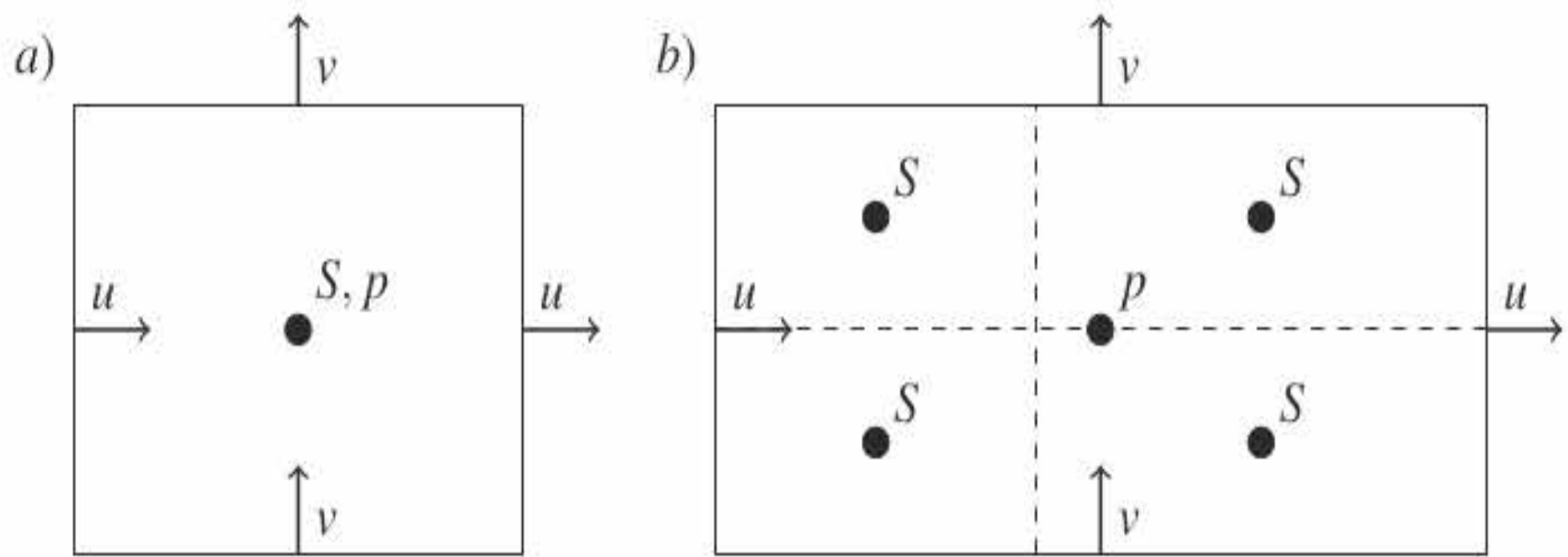


DNS for scalar turbulence requires care: sharp gradients!



Even if the diffusivities are equal ($Pr = 1$),
temperature shows much sharper fronts

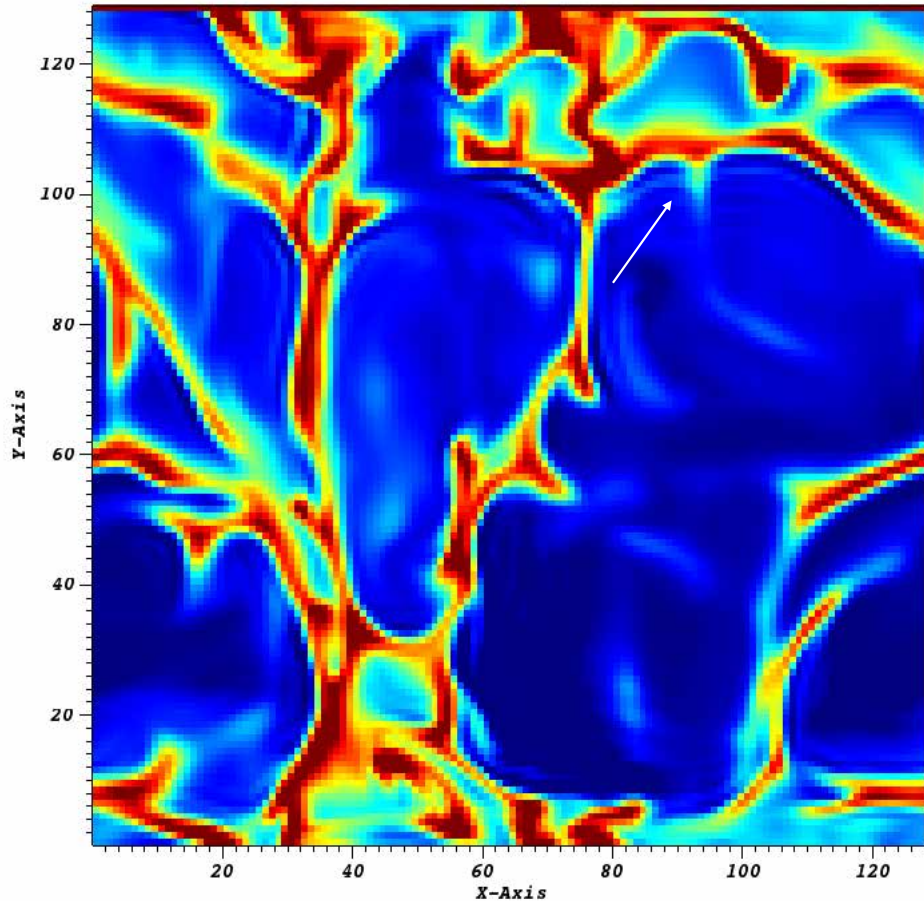
Different grids for scalar and momentum



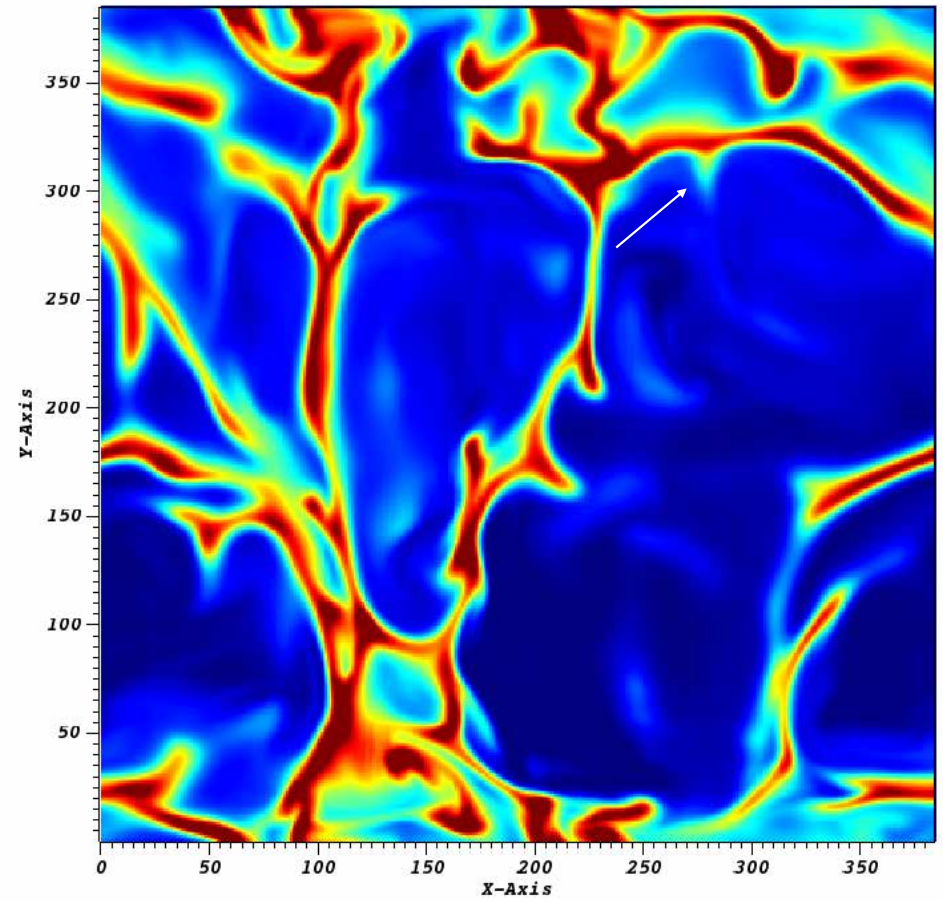
- Interpolation techniques for velocity in space
- Needs also sub-time stepping integration due to stability constraints

Refined scalar field resolution

Normal grid



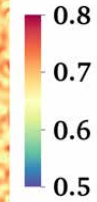
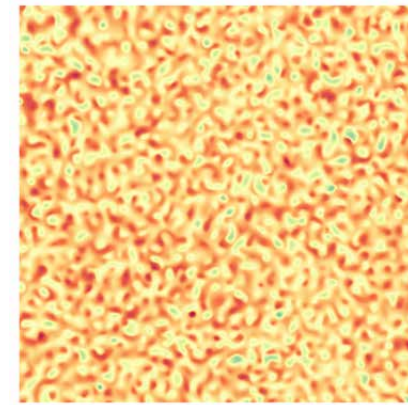
Refined grid



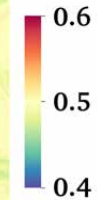
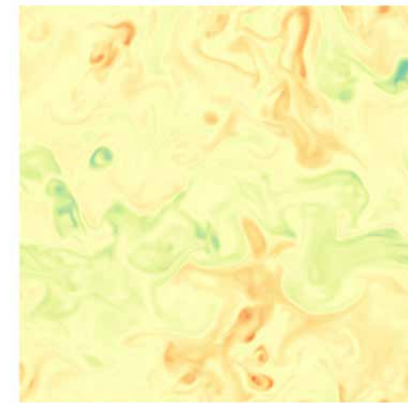
Savings from 2x CPU time for $Pr \sim 1$ to 4x CPU time for high Pr

Reduces memory use by 3x for medium-size problems

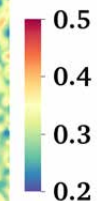
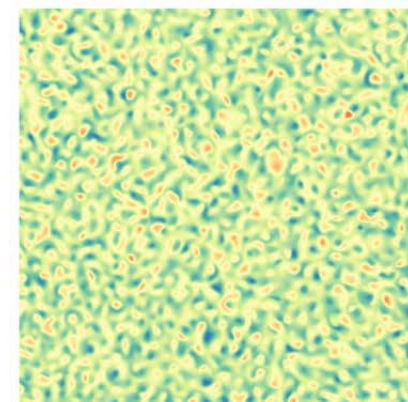
Double diffusive convection



$z/L = 0.9$



$z/L = 0.5$



$z/L = 0.1$

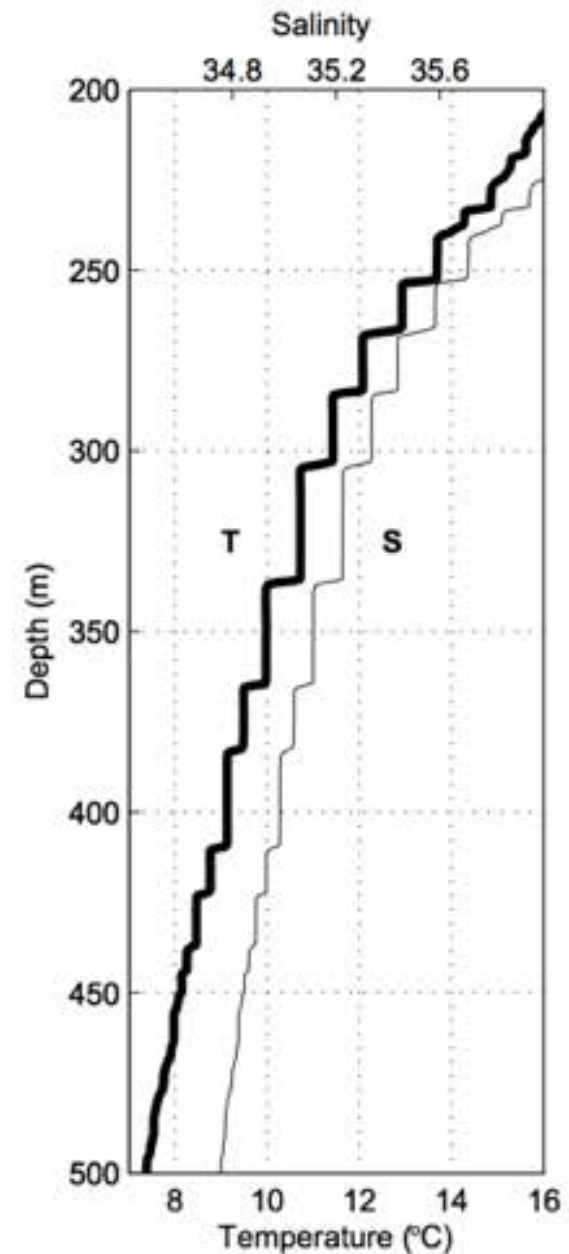
$Ra_S = 1 \times 10^{11}$

by Yantao Yang

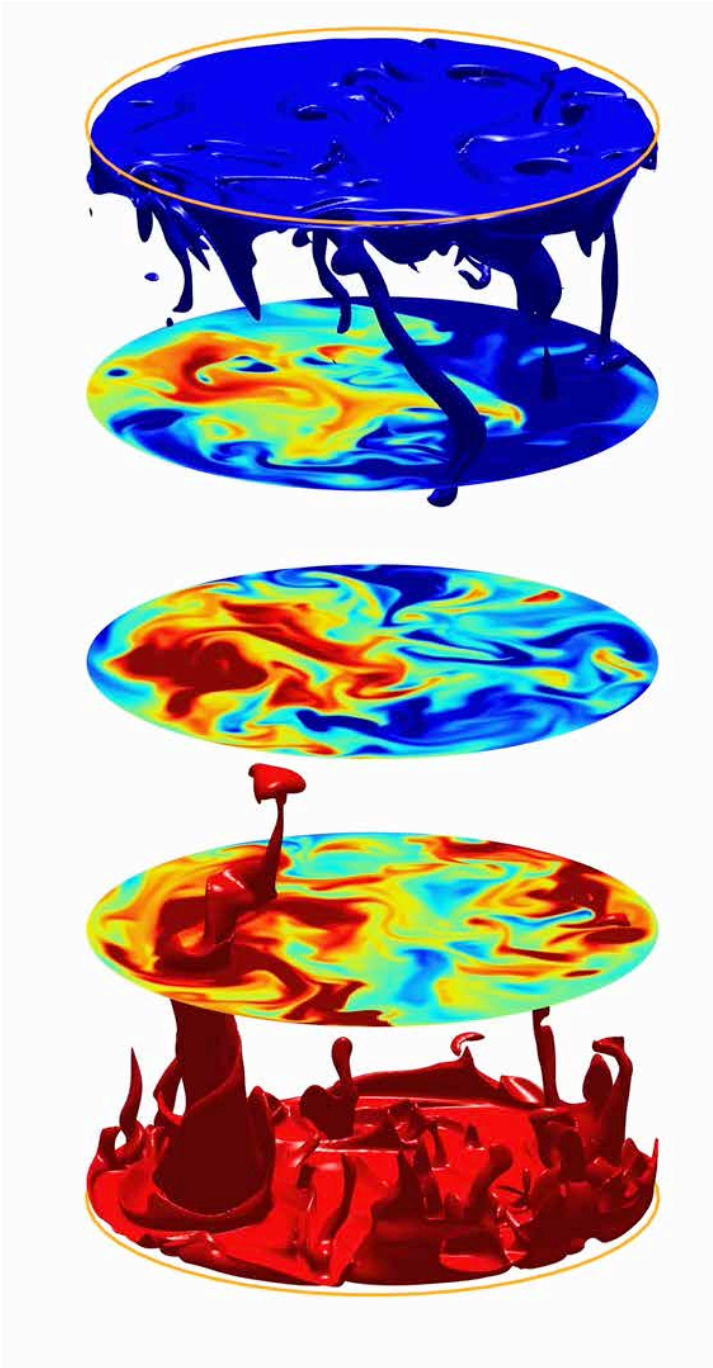
Double diffusive convection



$$Ra_S = 1 \times 10^{11}$$

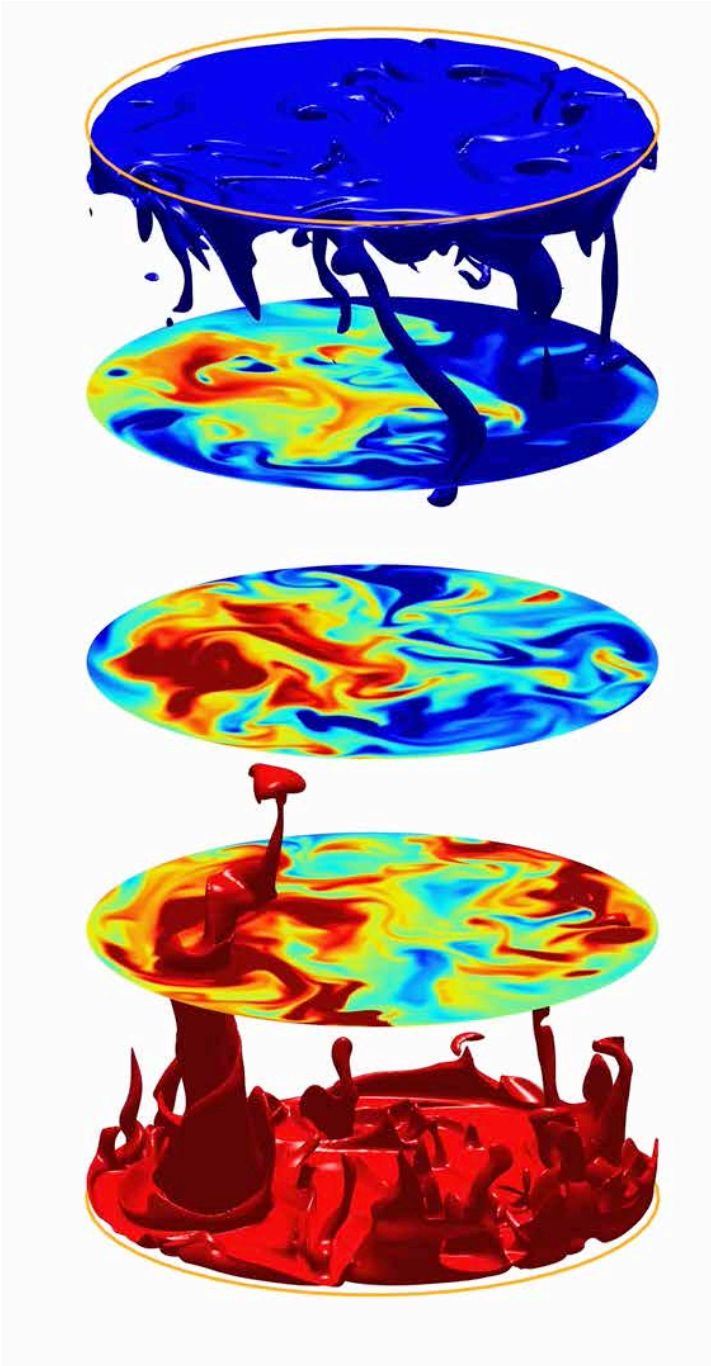


Rotating convection



Bubbly convection

Rotating convection

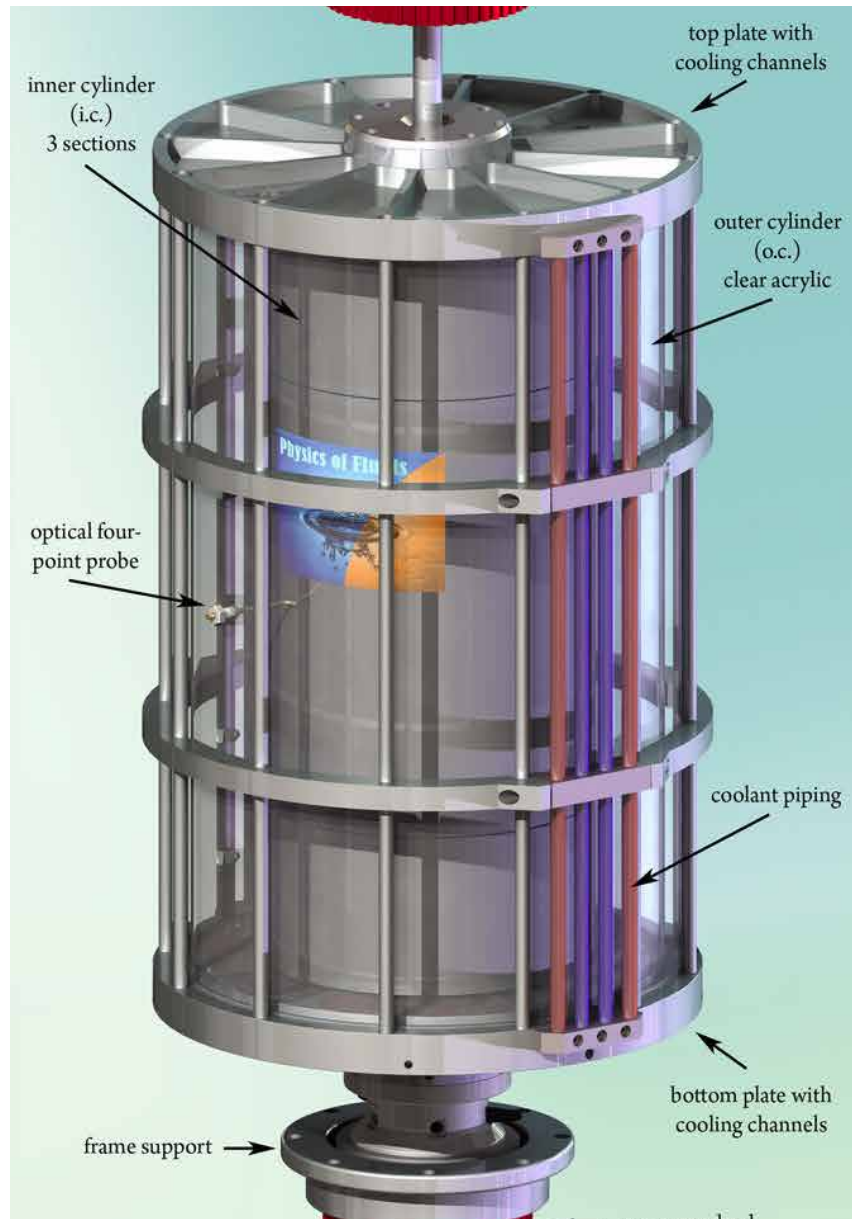


Bubbly convection



by Rajaram Lakkaraju

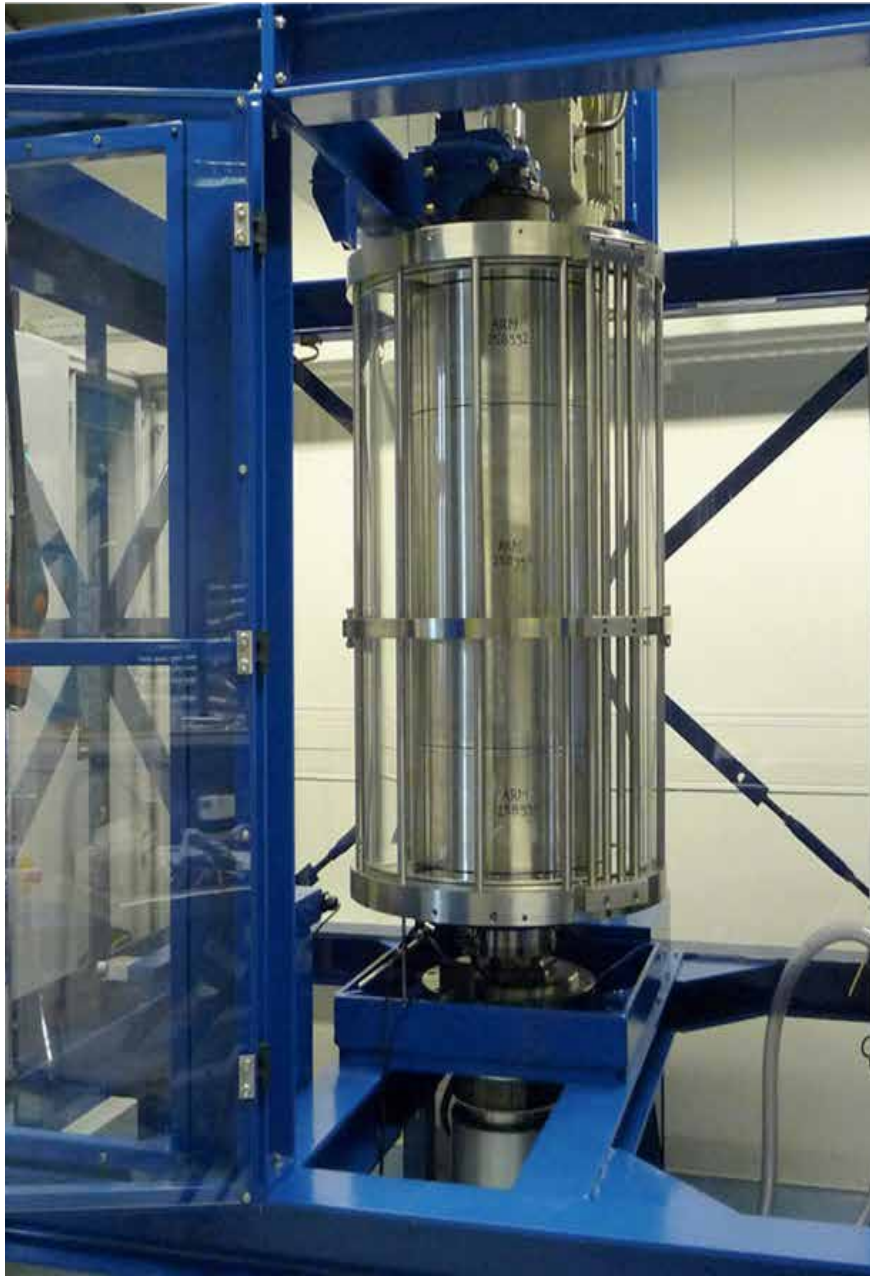
Taylor-Couette flow



Taylor-Couette flow



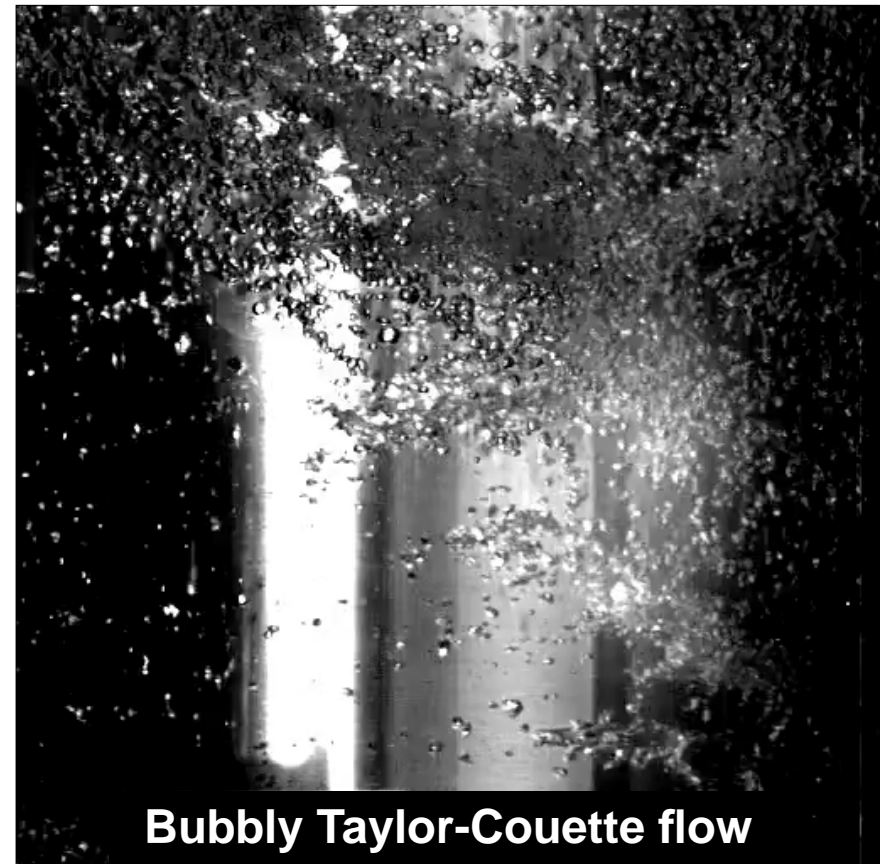
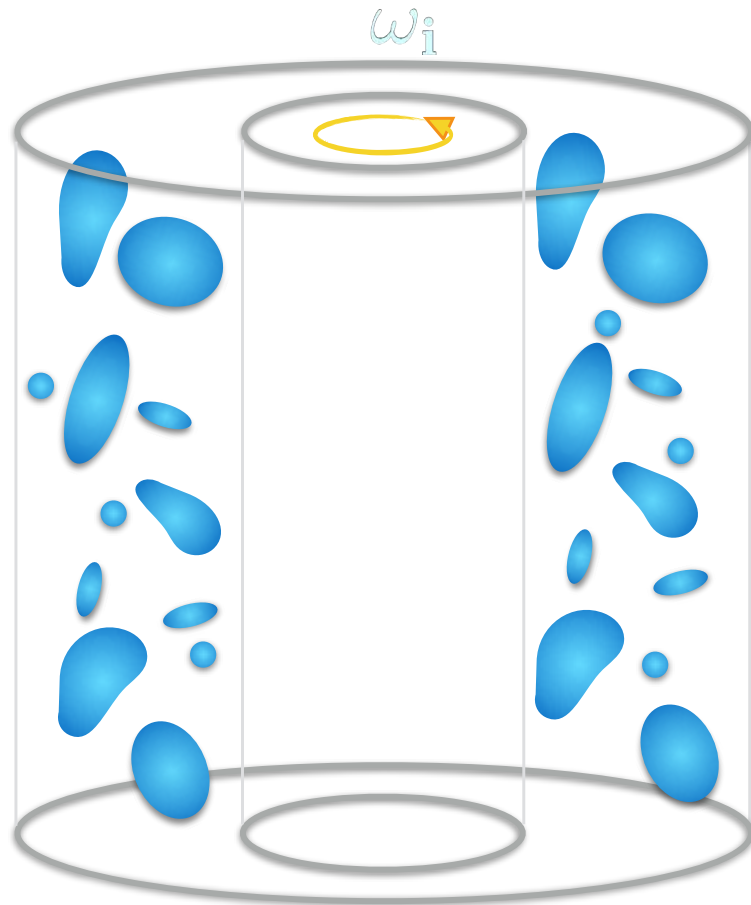
Taylor-Couette flow



by Rodolfo Ostilla and Xiaojuan Zhu

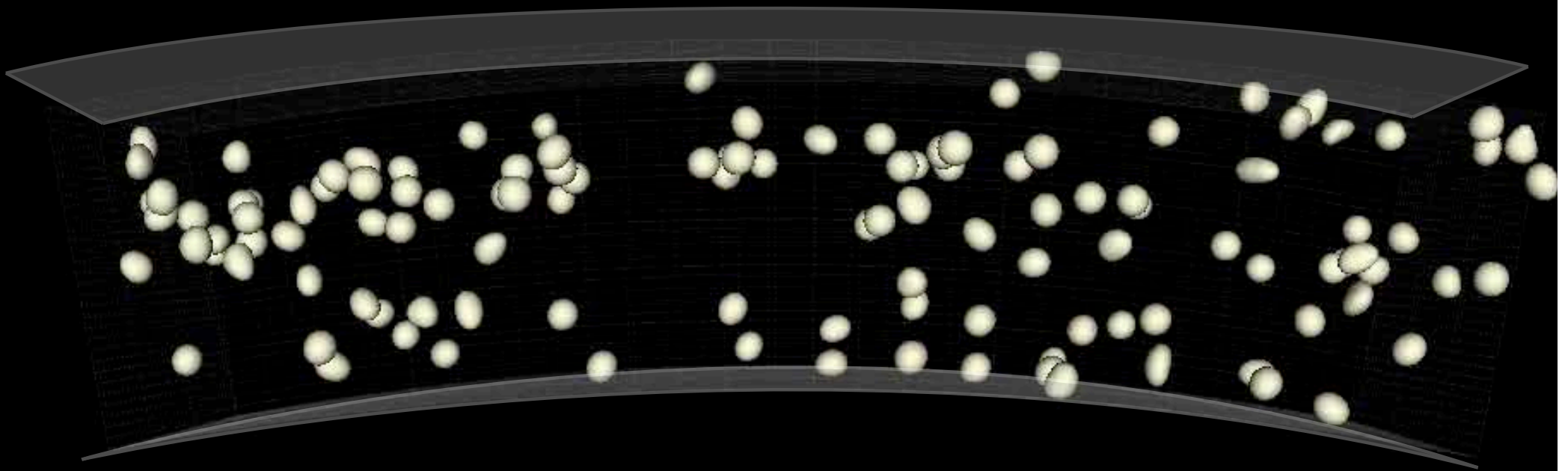
Understanding multi-component/phase flows

Two-phase Taylor-Couette flow



van Gils et al., JFM (2013)

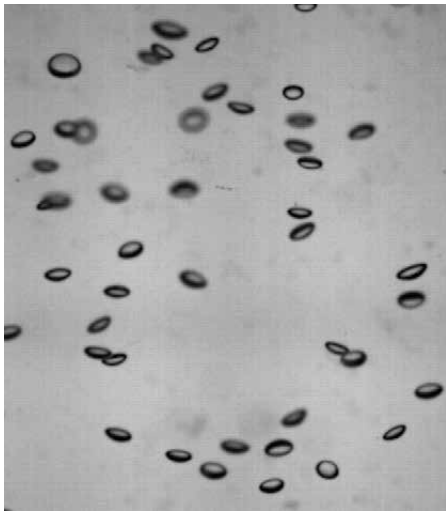
Two-phase Taylor-Couette simulation



by Vamsi Spandan

Deformability of bodies immersed in a flow

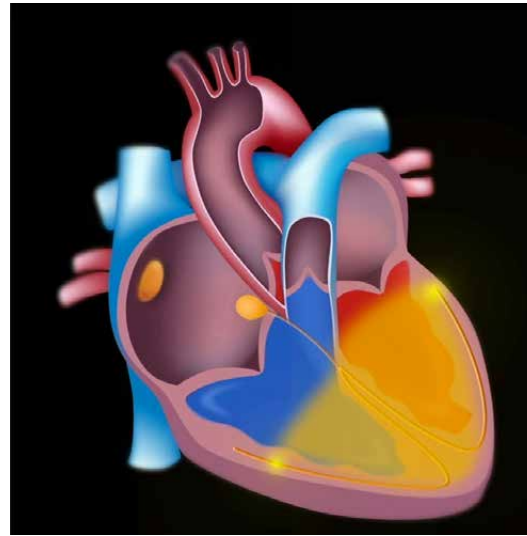
- Bubble/drop laden turbulent flows - atmosphere, oceans
- Flapping, bending bodies - flags, boat sails
- Biological flows - blood flow, heart-valves



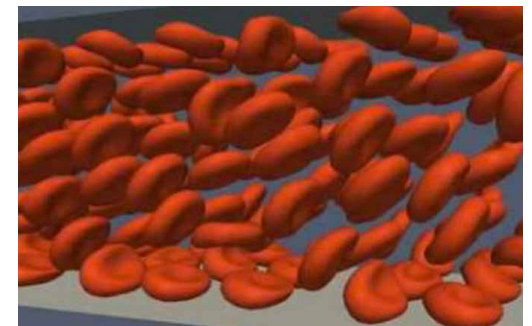
Bubbles



Sails



Heart



Red blood cells