Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Università degli Studi di Padova

On the evolution of Poisson solvers

F.Xavier Trias[1], Àdel Alsalti-Baldellou[1,2]

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[2]Department of Civil, Environmental and Architectural Engineering, University of Padova



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On the evolution of Poisson solvers for extreme-scale CFD simulations

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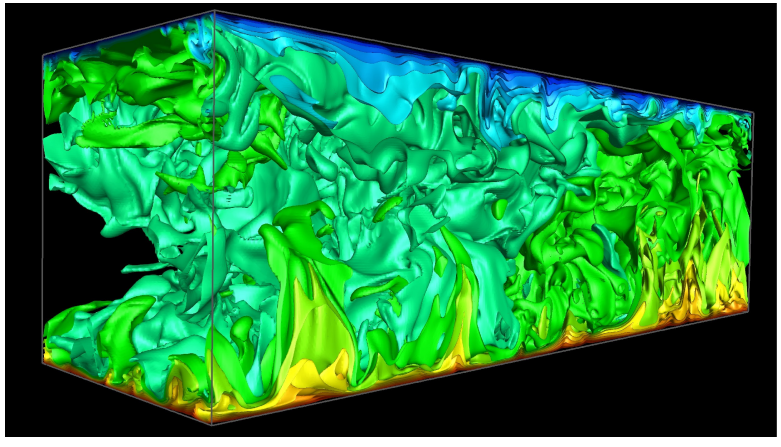

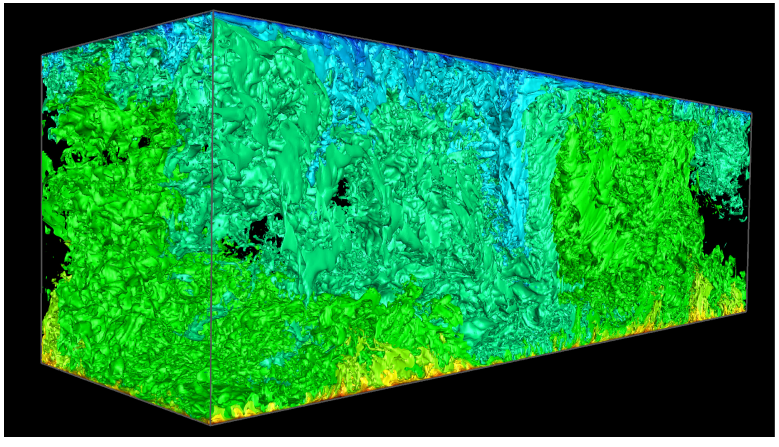

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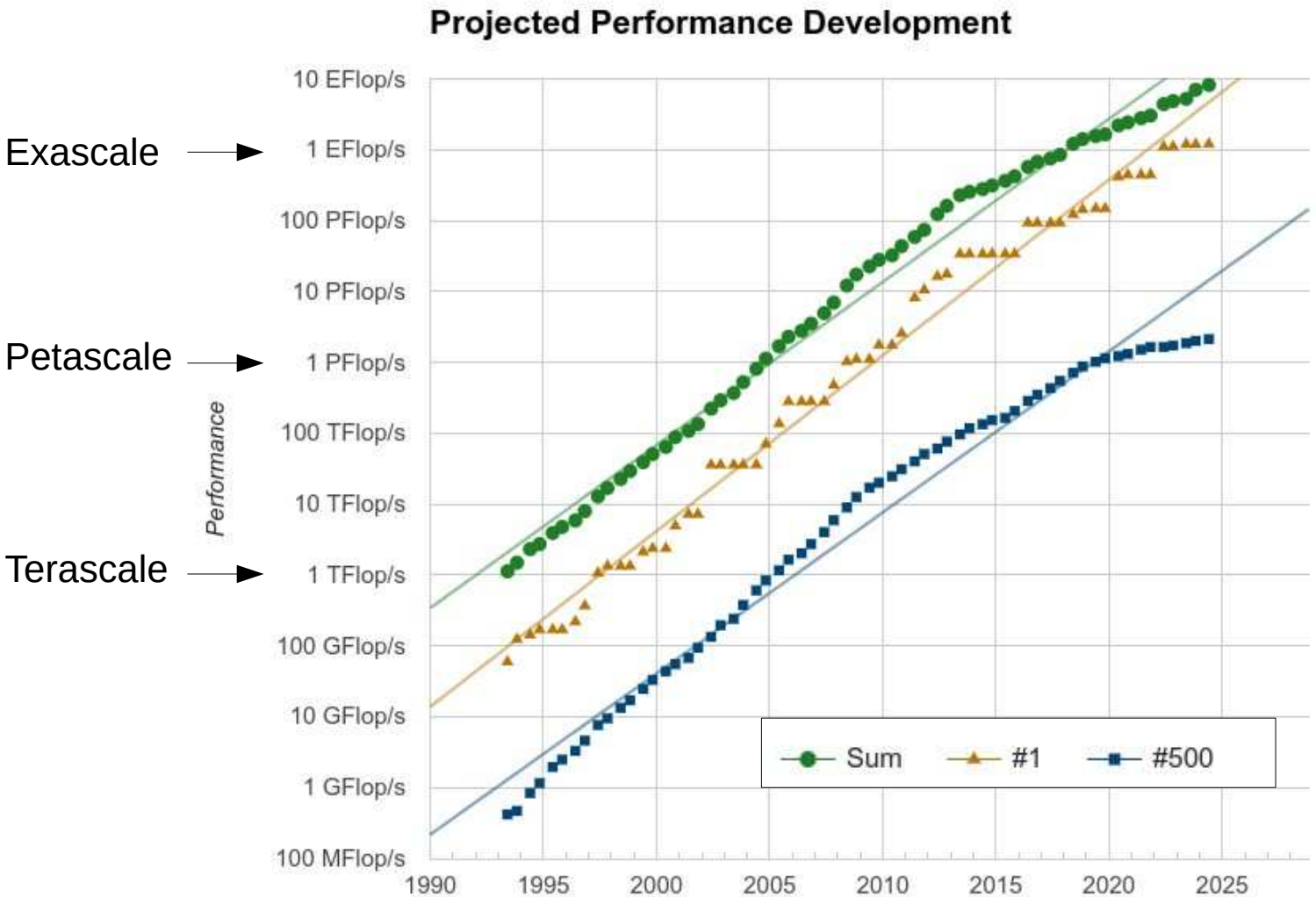
4. Solver convergence
5. Results
6. Conclusions

Tera, Peta, Exa,..., Zetta, Yotta



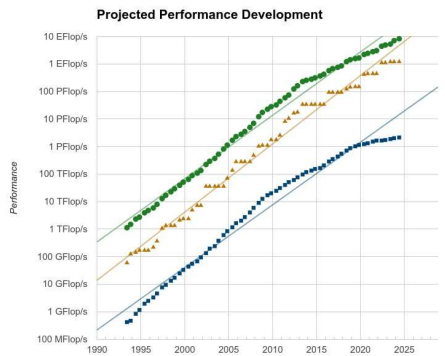
Source: `www.top500.org`

Tera, Peta, Exa,..., Zetta, Yotta

~10 years

	PetaFLOPS		#1 in LINPACK	#1 in HPCG	Cutting-edge CFD simulation	'Routine' CFD simulation
Zetta	10^6					
Exa	10^3	14 years	**2022** (Frontier)			
Peta	1		**2008** (Roadrunner)	**2018** (Summit)		
Tera	10^{-3}	11 years	**1997** (ASCI Red)	No data		





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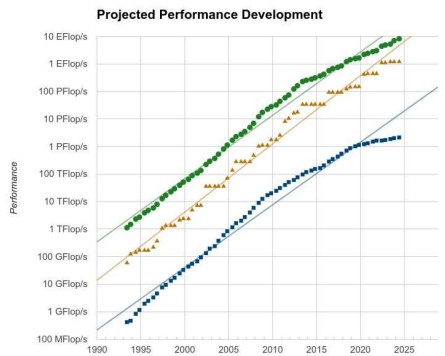

Tera, Peta, Exa,..., Zetta, Yotta

~10 years ~5 years

	PetaFLOPS		#1 in LINPACK	#1 in HPCG	Cutting-edge CFD simulation	'Routine' CFD simulation
Zetta	10^6		2037	2047	2052	
Exa	10^3	14 years	**2022** (Frontier)	2032	2037	
Peta	1		**2008** (Roadrunner)	**2018** (Summit)	2023	
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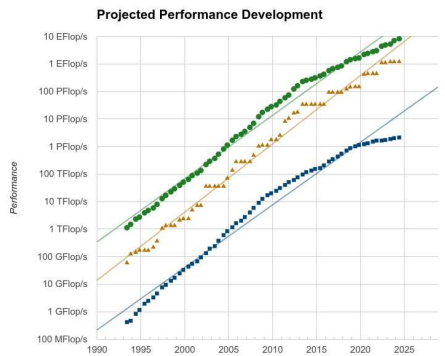
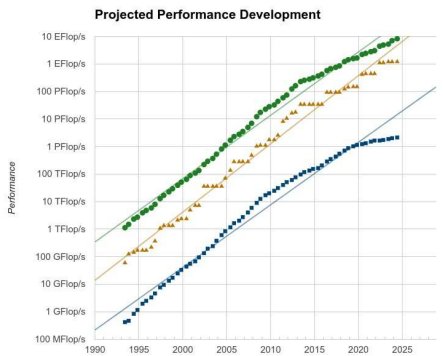


Tera, Peta, Exa,..., Zetta, Yotta

~10 years ~5 years ~10 years

	PetaFLOPS		#1 in LINPACK	#1 in HPCG	Cutting-edge CFD simulation	'Routine' CFD simulation
Zetta	10^6		2037	2047	2052	2062
Exa	10^3	14 years	**2022** (Frontier)	2032	2037	2047
Peta	1		**2008** (Roadrunner)	**2018** (Summit)	2023	2033
Tera	10^{-3}	11 years	**1997** (ASCI Red)	No data		

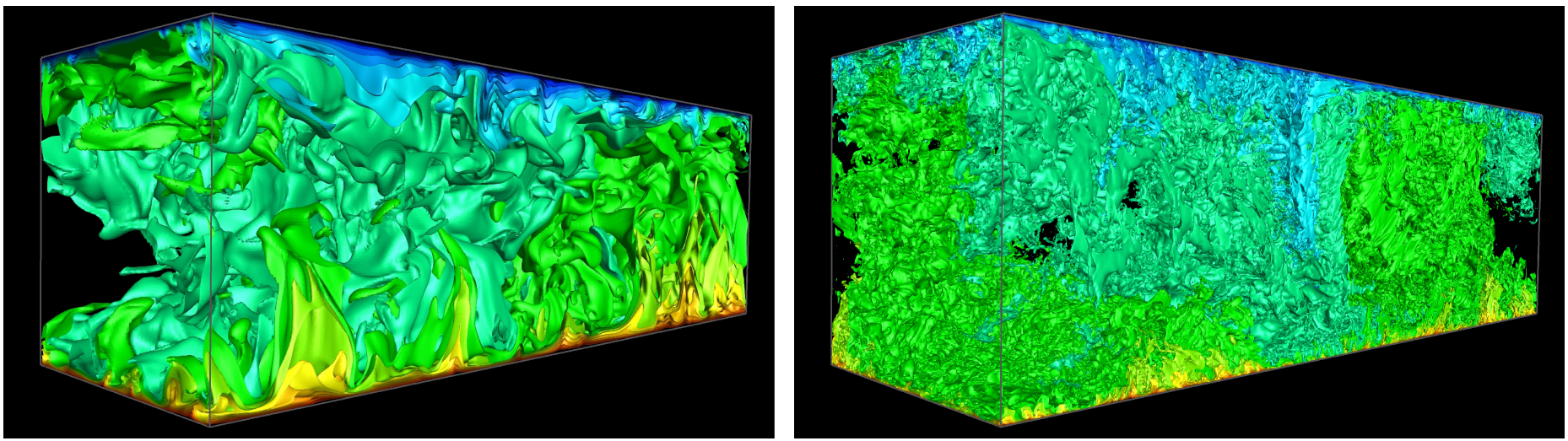




Motivation

Research question :

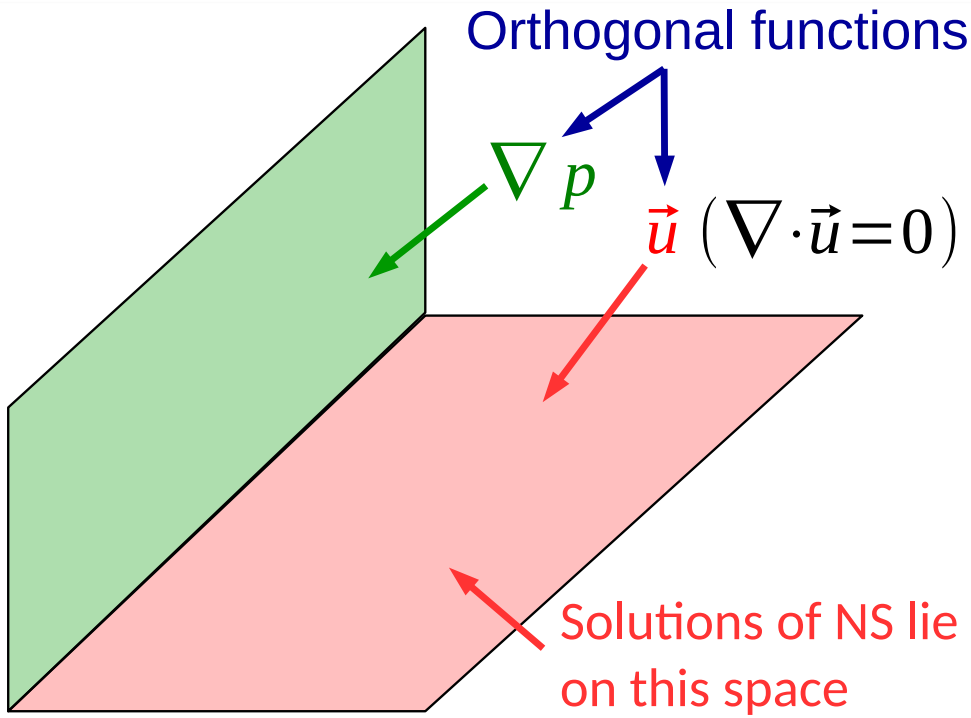
- Will the **complexity** of numerically solving **Poisson's equation** increase or decrease for **very large scale DNS/LES** simulations of incompressible turbulent flows?



DNS[1] of air-filled Rayleigh–Bénard convection at $Ra = 10^8$ and 10^{10}

[1] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow*. **Computers & Fluids**, 286:106473, 2025

Poisson's equation: a quick reminder



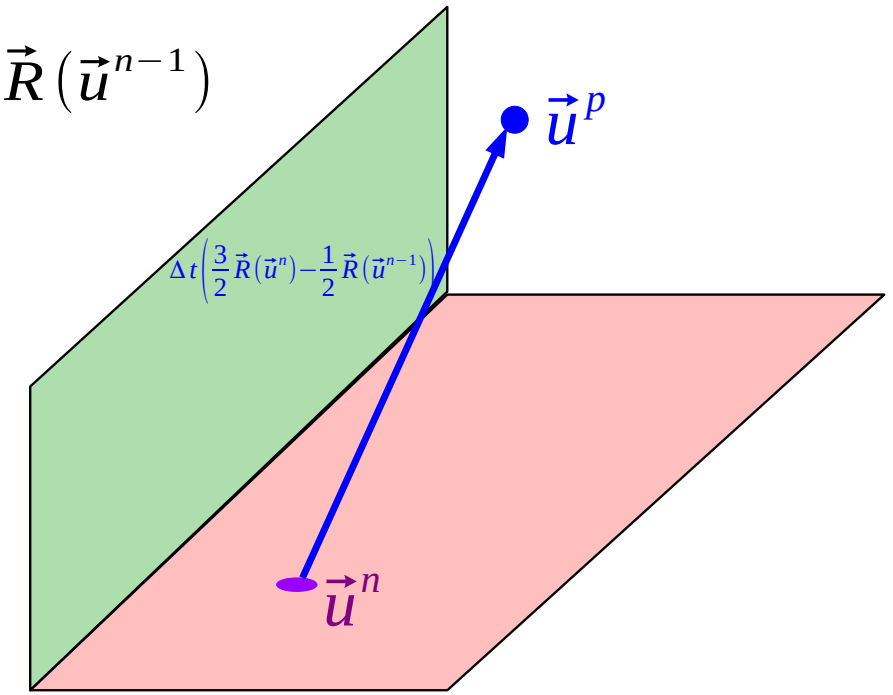
Semi-discrete (just in time) NS equations

$$\frac{\vec{u}^{n+1}-\vec{u}^{n}}{\Delta t}=\frac{3}{2}\vec{R}(\vec{u}^{n})-\frac{1}{2}\vec{R}(\vec{u}^{n-1})-\nabla p^{n+1}$$

$$\nabla\cdot\vec{u}^{n+1}=0$$

Poisson's equation: a quick reminder

Step 1: $\frac{\vec{u}^{p}-\vec{u}^{n}}{\Delta t}=\frac{3}{2}\vec{R}(\vec{u}^{n})-\frac{1}{2}\vec{R}(\vec{u}^{n-1})$



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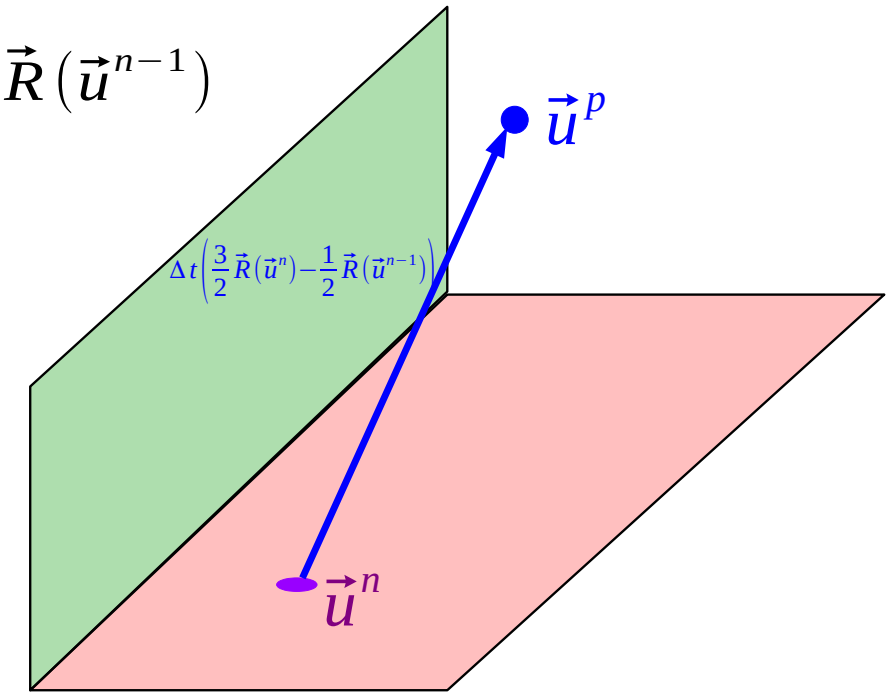

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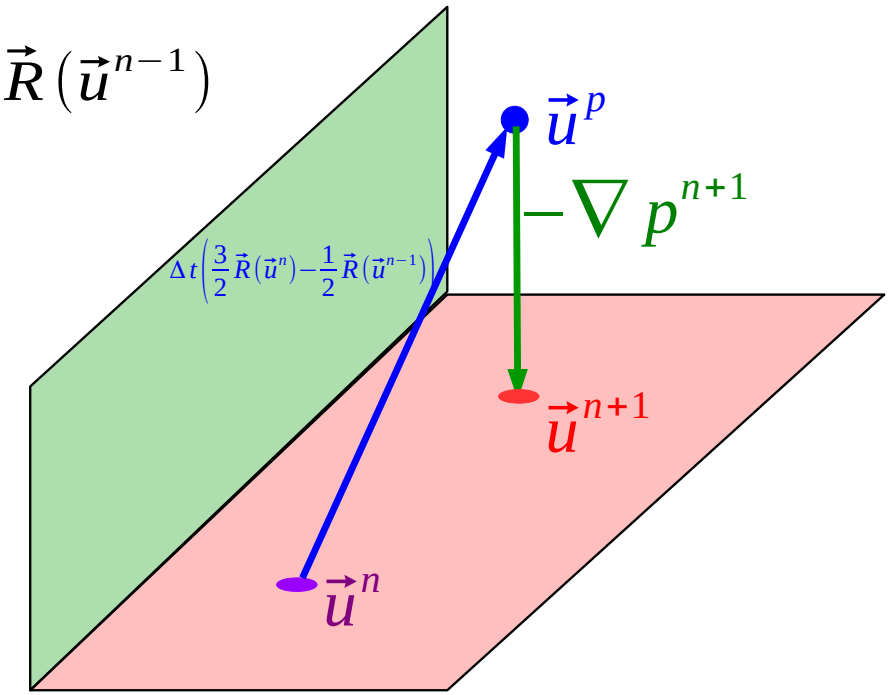
Step 3: $\vec{u}^{n+1}=\vec{u}^{p}-\Delta t\,\nabla p^{n+1}$



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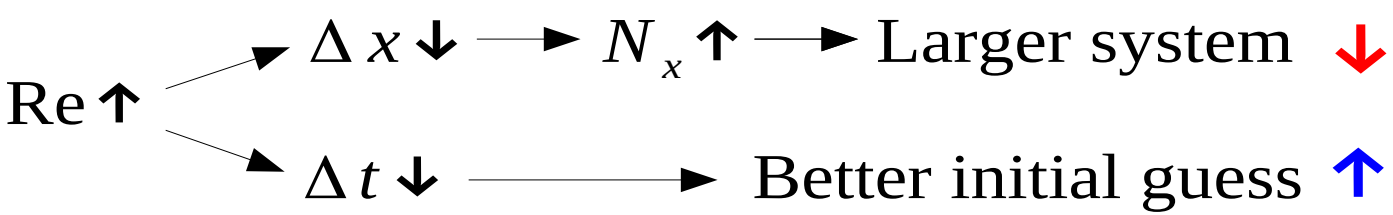
Poisson's equation: getting more tough or not?

Research question:

- Will the **complexity** of numerically solving **Poisson's equation** **increase** or **decrease** for **very large scale DNS/LES** simulations of incompressible turbulent flows?

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^p$$

Two competing effects: who (if any) will eventually win?



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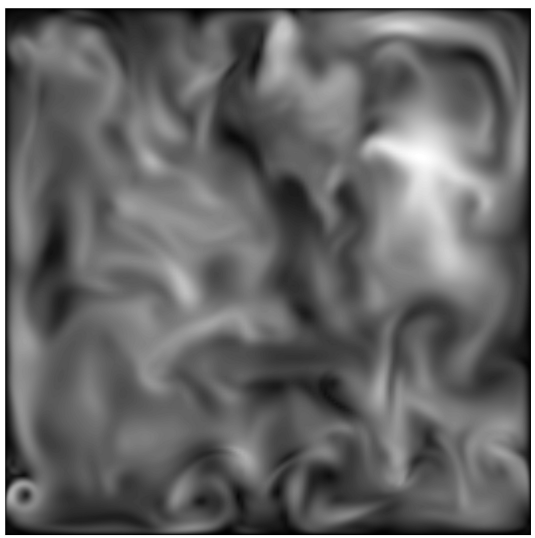
$Ra = 10^8$



[2] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *Flow topology dynamics in a 3D phase space for turbulent Rayleigh-Bénard convection*, **Phys.Rev.Fluids**, 5:024603, 2020.

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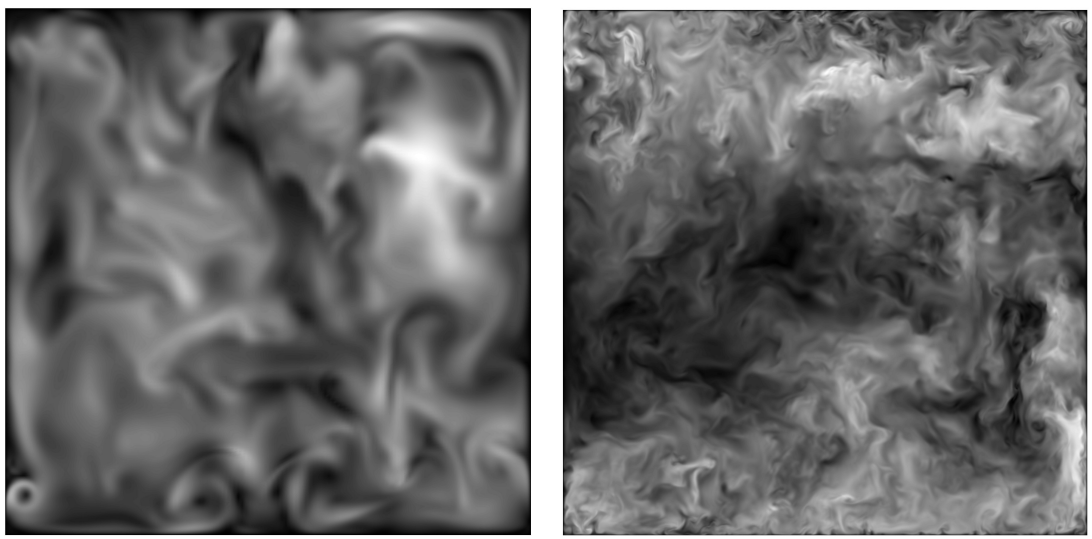

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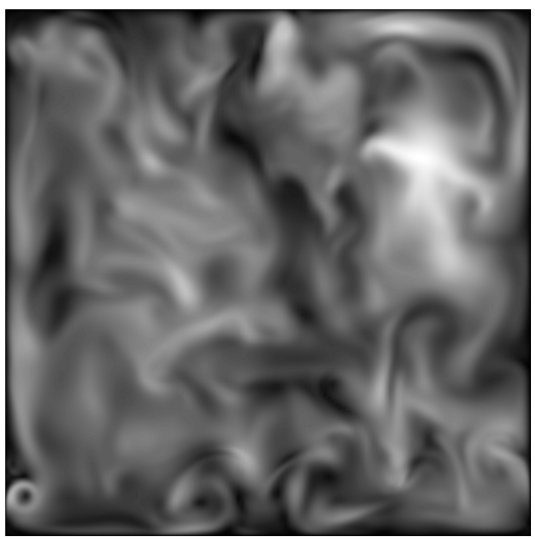
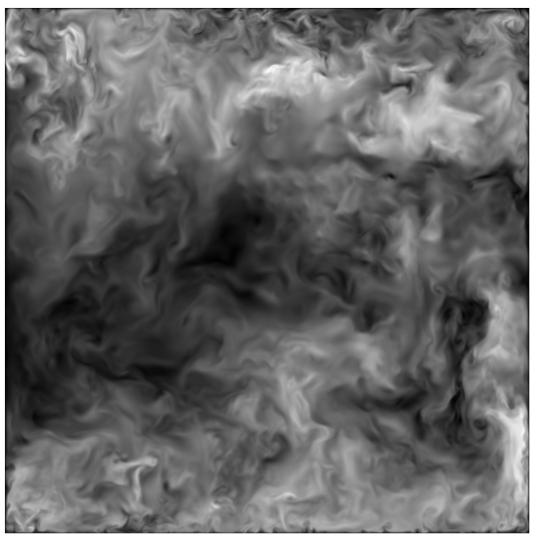
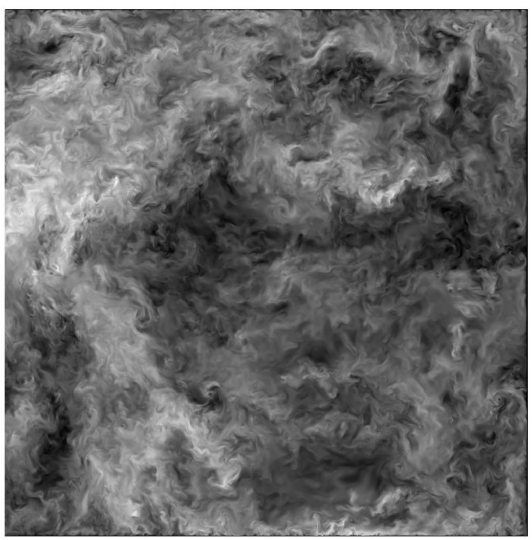

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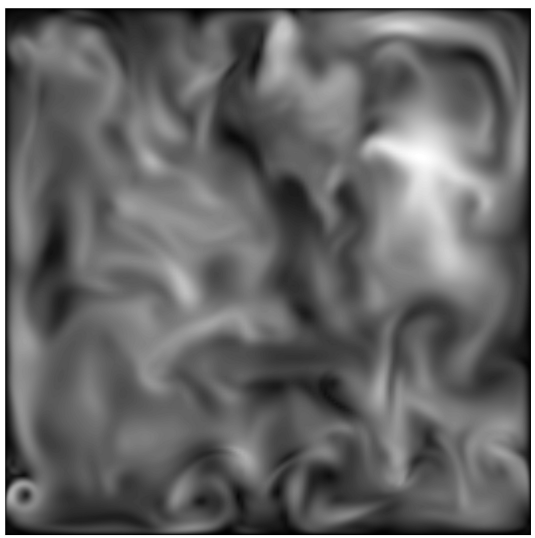
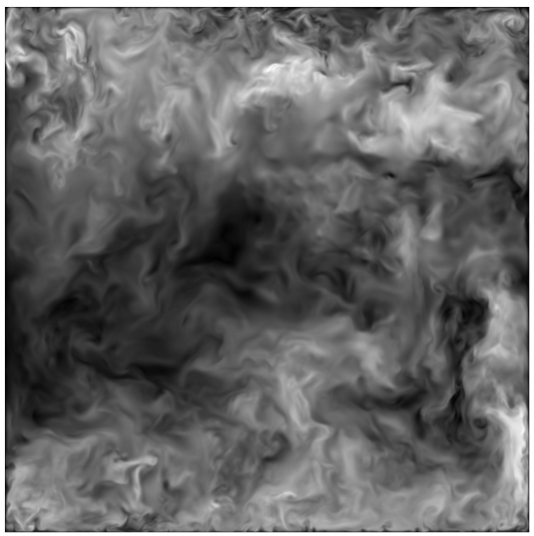
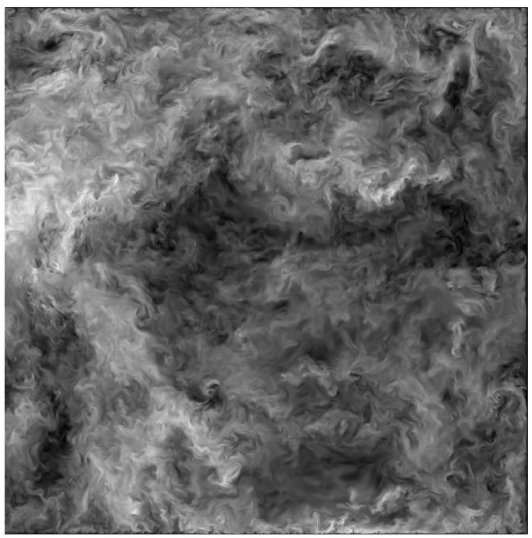
		
$208 \times 208 \times 400$	$768 \times 768 \times 1024$	$1662 \times 1662 \times 2048$
17.5M	**607M**	**5600M**

[2] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *Flow topology dynamics in a 3D phase space for turbulent Rayleigh-Bénard convection*, **Phys.Rev.Fluids**, 5:024603, 2020.

Smaller and smaller, but how much?

Two competing effects: who (if any) will eventually win?

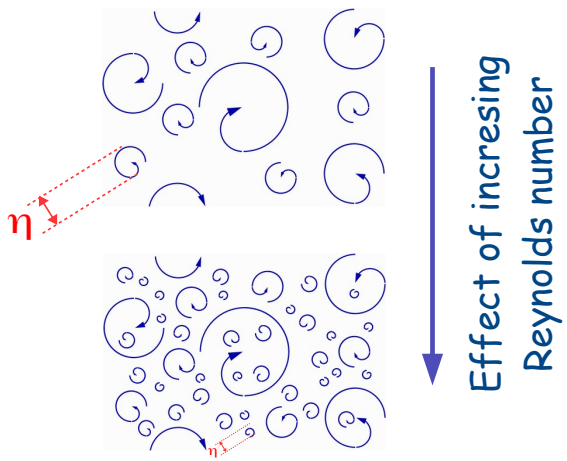
$$\mathrm{Re}\uparrow \;\begin{cases} \Delta x \downarrow \rightarrow N_x \uparrow \rightarrow \text{Larger system} \downarrow \\ \Delta t \downarrow \rightarrow \text{Better initial guess} \uparrow \end{cases}$$

From classical K41 theory:

$$\frac{1}{N_x^{\mathrm{K41}}} = \frac{\Delta x}{L_x} \sim \frac{\eta}{l} \propto \mathrm{Re}^{-3/4}$$

$$\frac{u}{U} \propto \mathrm{Re}^{-1/4}$$

l: biggest eddies (driving scale)
η: smallest eddies (Kolmogorov length scale)



Question:

how $\frac{\eta}{l}$ decreases with Re?

$$\frac{1}{N_t^{\mathrm{K41}}} = \frac{\Delta t}{t_{\mathrm{sim}}} \sim \frac{t_\eta}{t_l} \propto \frac{\eta}{l}\frac{U}{u} \propto \mathrm{Re}^{-3/4}\,\mathrm{Re}^{1/4} = \mathrm{Re}^{-1/2}$$

Smaller and smaller, but how much?

Two competing effects: who (if any) will eventually win?

$\mathrm{Re}\uparrow$ → $\Delta x \downarrow$ → $N_x \uparrow$ → Larger system ↓

$\mathrm{Re}\uparrow$ → $\Delta t \downarrow$ → Better initial guess ↑

From classical K41 theory:

$$\frac{1}{N_x^{\mathrm{K41}}} = \frac{\Delta x}{L_x} \sim \frac{\eta}{l} \propto \mathrm{Re}^{-3/4}$$

$$\frac{u}{U} \propto \mathrm{Re}^{-1/4}$$

From CFL condition:

$$\Delta t^{\mathrm{conv}} \sim \frac{\Delta x}{U} \qquad \Delta t^{\mathrm{diff}} \sim \frac{\Delta x^2}{\nu}$$

$$\frac{1}{N_t^{\mathrm{conv}}} \sim \frac{\Delta t^{\mathrm{conv}}}{t_l} \sim \frac{U}{l}\frac{l\,\mathrm{Re}^{-3/4}}{U} = \mathrm{Re}^{-3/4}$$

$$\frac{1}{N_t^{\mathrm{diff}}} \sim \frac{\Delta t^{\mathrm{diff}}}{t_l} \sim \frac{U}{l}\frac{l^2\left(\mathrm{Re}^{-3/4}\right)^2}{\nu} = \mathrm{Re}^{-1/2}$$

$$\frac{1}{N_t^{\mathrm{K41}}} = \frac{\Delta t}{t_{\mathrm{sim}}} \sim \frac{t_\eta}{t_l} \propto \frac{\eta}{l}\frac{U}{u} \propto \mathrm{Re}^{-3/4}\,\mathrm{Re}^{1/4} = \mathrm{Re}^{-1/2}$$

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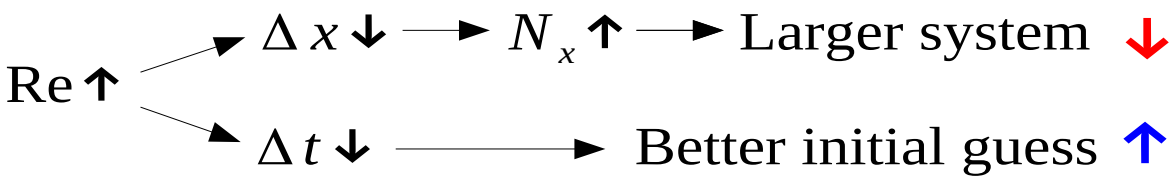


In summary:

$$\frac{1}{N_x^{\mathrm{K41}}} = \frac{\Delta x}{L_x} \sim \frac{\eta}{l} \propto \mathrm{Re}^{-3/4}$$

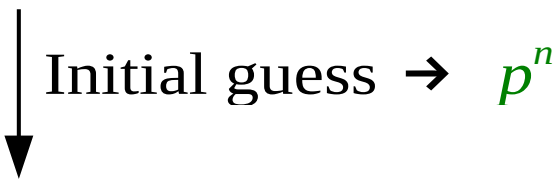
$$\frac{\Delta t}{t_l} \sim \mathrm{Re}^{\alpha}$$

$\alpha = -1/2$ (K41 or diffusion dominated)

$\alpha = -3/4$ (convection dominated)

Residual of Poisson's equation

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^{\,p}$$



$$r^o = \nabla^2 p^n - \frac{1}{\Delta t} \nabla \cdot u^{p,n+1}$$

Residual of Poisson's equation

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^{p}$$

Initial guess → p^n

$$r^o = \nabla^2 p^n - \frac{1}{\Delta t} \nabla \cdot u^{p,n+1} = \frac{1}{\Delta t} \nabla \cdot u^{p,n} - \frac{1}{\Delta t} \nabla \cdot u^{p,n+1} \approx \frac{\partial \nabla \cdot u^p}{\partial t} = \nabla \cdot \frac{\partial u^p}{\partial t}$$

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$$\tilde{r}^o = \nabla^2 \tilde{p}^n - \nabla \cdot u^{p,n+1} \approx \nabla \cdot u^{p,n} - \nabla \cdot u^{p,n+1} \approx \Delta t \frac{\partial \nabla \cdot u^p}{\partial t} = \Delta t \nabla \cdot \frac{\partial u^p}{\partial t}$$

Initial guess → $\tilde{p}^n = \Delta t \, p^n$

$$\nabla^2 \tilde{p}^{n+1} = \nabla \cdot \vec{u}^{p}$$

Residual of Poisson's equation

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^p$$

Initial guess → p^n

$$r^o \approx \frac{\partial \nabla \cdot u^p}{\partial t}$$

$$\tilde{r}^o \approx \Delta t \frac{\partial \nabla \cdot u^p}{\partial t}$$

Initial guess → $\tilde{p}^n = \Delta t \, p^n$

$$\nabla^2 \tilde{p}^{n+1} = \nabla \cdot \vec{u}^p$$

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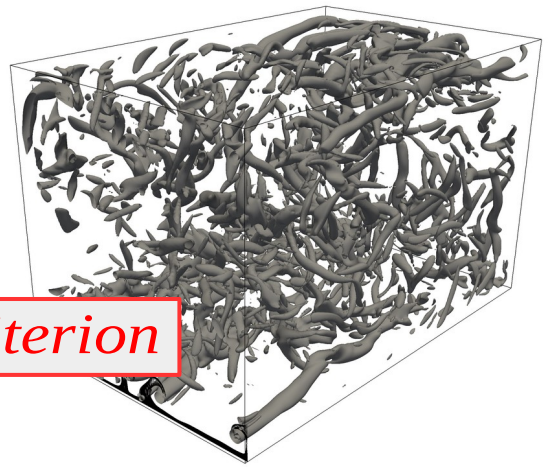


$Q_G - criterion$

Initial guess → p^n

What is $\nabla \cdot u^p$?

$$r^o \approx \frac{\partial \nabla \cdot u^p}{\partial t}$$

$$\nabla \cdot u^p = \cancel{\nabla \cdot u^n} - \Delta t \nabla \cdot (u^n \cdot \nabla u^n) \cancel{+ \nu \Delta t \nabla \cdot \nabla^2 u^n} = 2 \Delta t \, Q_G$$

$$\tilde{r}^o \approx \Delta t \frac{\partial \nabla \cdot u^p}{\partial t}$$

$$Q_G = -\frac{1}{2} tr(G^2) \quad \text{where} \quad G = \nabla u^n$$

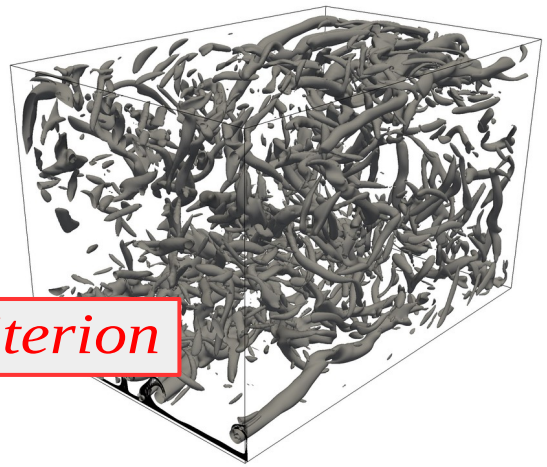
Initial guess → $\tilde{p}^n = \Delta t \, p^n$

$$\nabla^2 \tilde{p}^{n+1} = \nabla \cdot \vec{u}^p$$

Residual of Poisson's equation

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^p$$

Initial guess → p^n



$Q_G - criterion$

$$r^o \approx \frac{\partial \nabla \cdot u^p}{\partial t} = 2\,\Delta t \frac{\partial Q_G}{\partial t}$$

$$\tilde{r}^o \approx \Delta t \frac{\partial \nabla \cdot u^p}{\partial t} = 2\,\Delta t^2 \frac{\partial Q_G}{\partial t}$$

$$R_G = det(G) = \frac{1}{3} tr(G^3)$$

$$Q_G = -\frac{1}{2} tr(G^2) \quad \text{where} \quad G = \nabla u^n$$

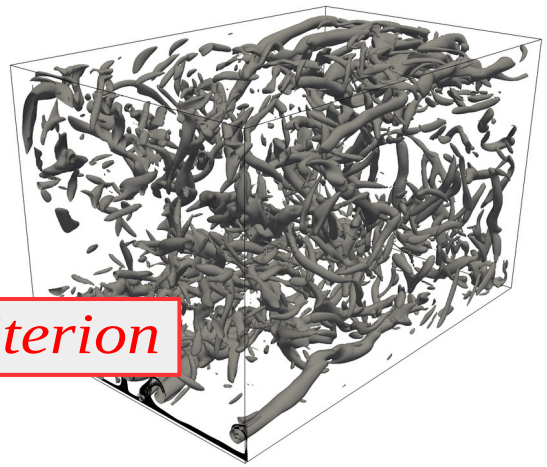
Exact equations for restricted Euler :

$$\frac{dQ_G}{dt} = -3 R_G \longrightarrow \frac{\partial Q_G}{\partial t} = -(u \cdot \nabla) Q_G - 3 R_G$$

Residual of Poisson's equation

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^p$$

Initial guess → p^n



$$r^o \approx \frac{\partial \nabla \cdot u^p}{\partial t} = 2\Delta t \frac{\partial Q_G}{\partial t} \approx -2\Delta t \{(u \cdot \nabla) Q_G + 3 R_G\}$$

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Exact equations for restricted Euler :

$$\frac{dQ_G}{dt} = -3 R_G \longrightarrow \frac{\partial Q_G}{\partial t} = -(u \cdot \nabla) Q_G - 3 R_G$$

Residual of Poisson's equation

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t} \nabla \cdot \vec{u}^p$$

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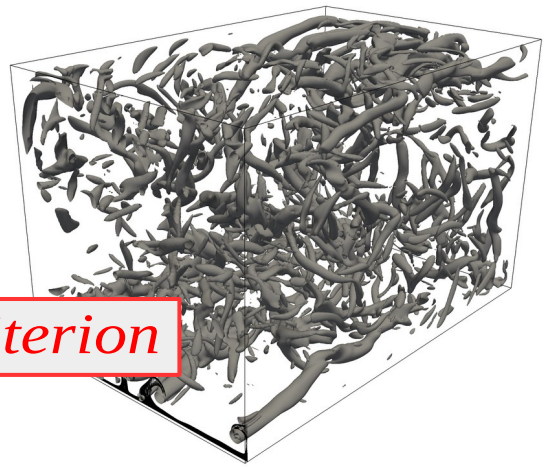

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Initial guess → $\tilde{p}^n = \Delta t \, p^n$

$$\nabla^2 \tilde{p}^{n+1} = \nabla \cdot \vec{u}^p$$

Residual of Poisson's equation in Fourier space

In summary:

$$r^o \approx \frac{\partial \nabla\cdot u^p}{\partial t} = 2\Delta t^q \frac{\partial Q_G}{\partial t} \approx -2\Delta t^q \{(u\cdot\nabla)Q_G + 3R_G\}$$

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t}\nabla\cdot\vec{u}^p$$

$$q = \{1, 2\}$$

$$\nabla^2 \tilde{p}^{n+1} = \nabla\cdot\vec{u}^p$$

$$\frac{\Delta t}{t_l} \sim \mathrm{Re}^{\alpha} \begin{cases} \alpha = -1/2 & (\text{K41 or diffusion dominated}) \\ \alpha = -3/4 & (\text{convection dominated}) \end{cases}$$

$$\frac{1}{N_x^{\mathrm{K41}}} = \frac{\Delta x}{L_x} \sim \frac{\eta}{l} \propto \mathrm{Re}^{-3/4}$$

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$$\|r\|^2 = \int_\Omega r^2 dV = \int_1^{k_{max}} \hat{r}_k^2 dk$$

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Solver convergence

$$\|r^n\|^2 = \int_1^{k_{max}} \left(\hat{\omega}_k^n \hat{r}_k^0\right)^2 dk \approx \int_1^{C_k \mathrm{Re}^{3/4}} \hat{\omega}_k^{2n} \mathrm{Re}^{2\tilde{\alpha}} k^{2\beta} dk$$

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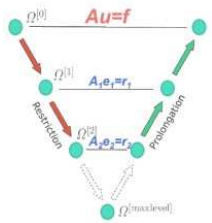

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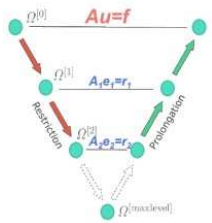

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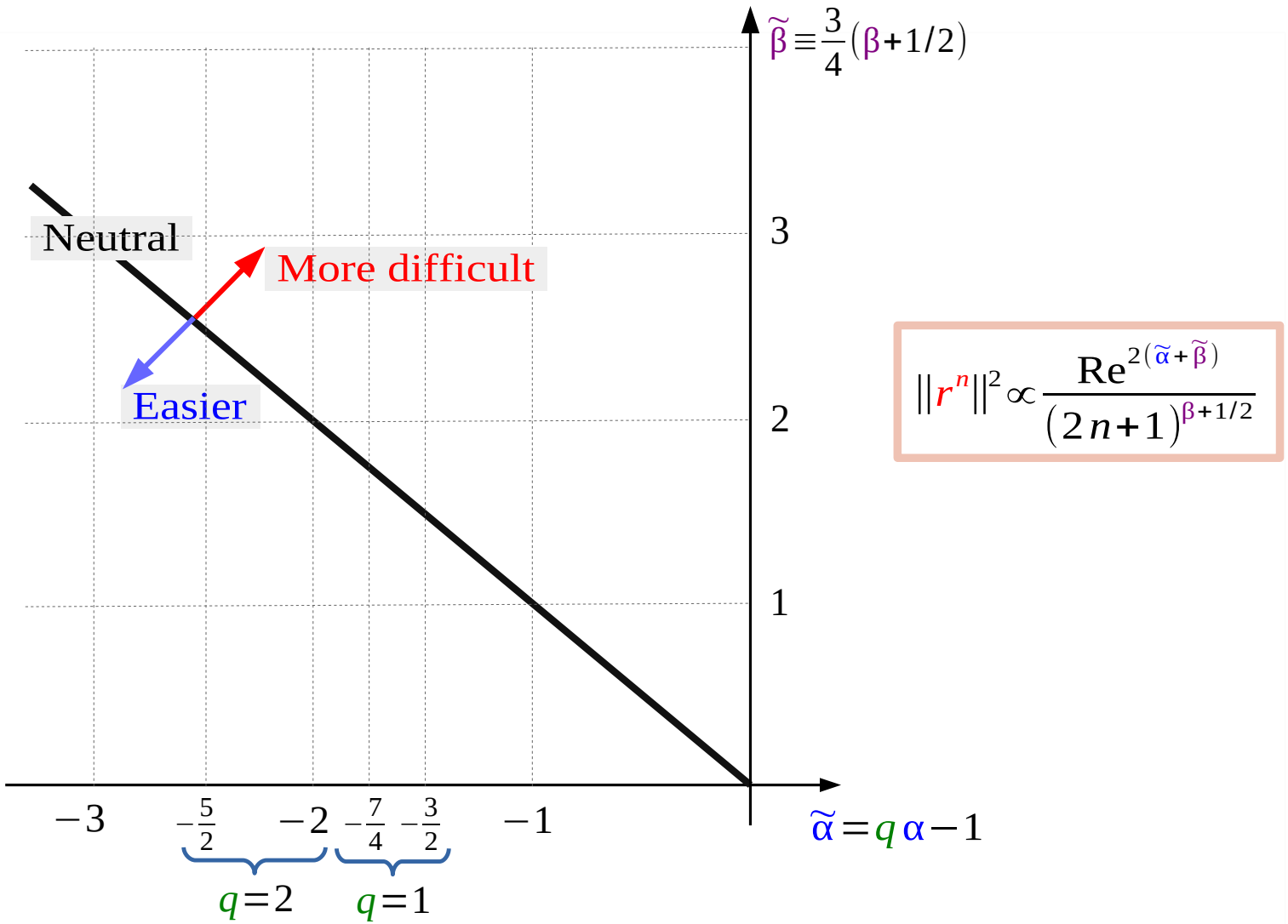
Solver convergence

$\{\tilde{\alpha}, \tilde{\beta}\}$ phase space



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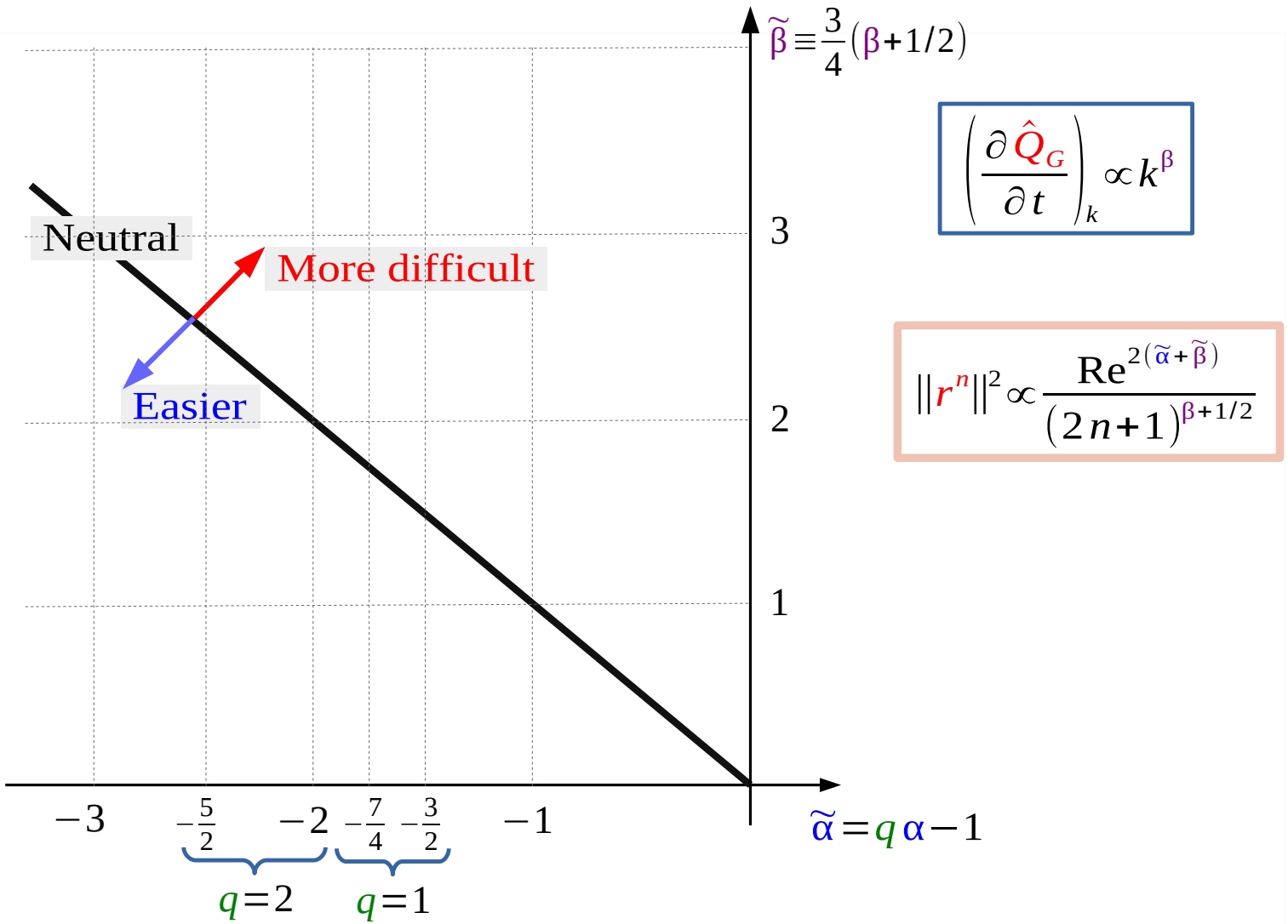

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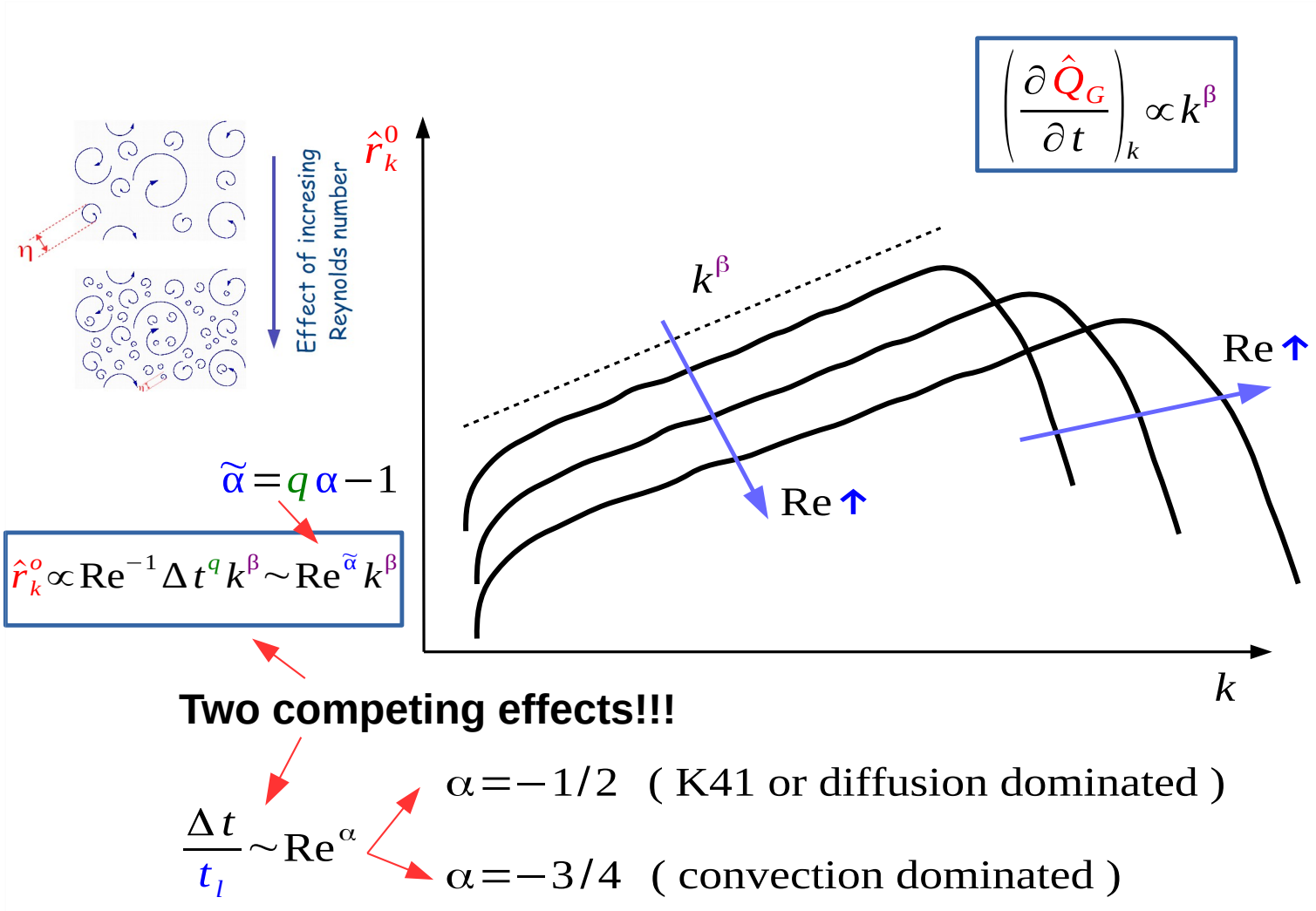

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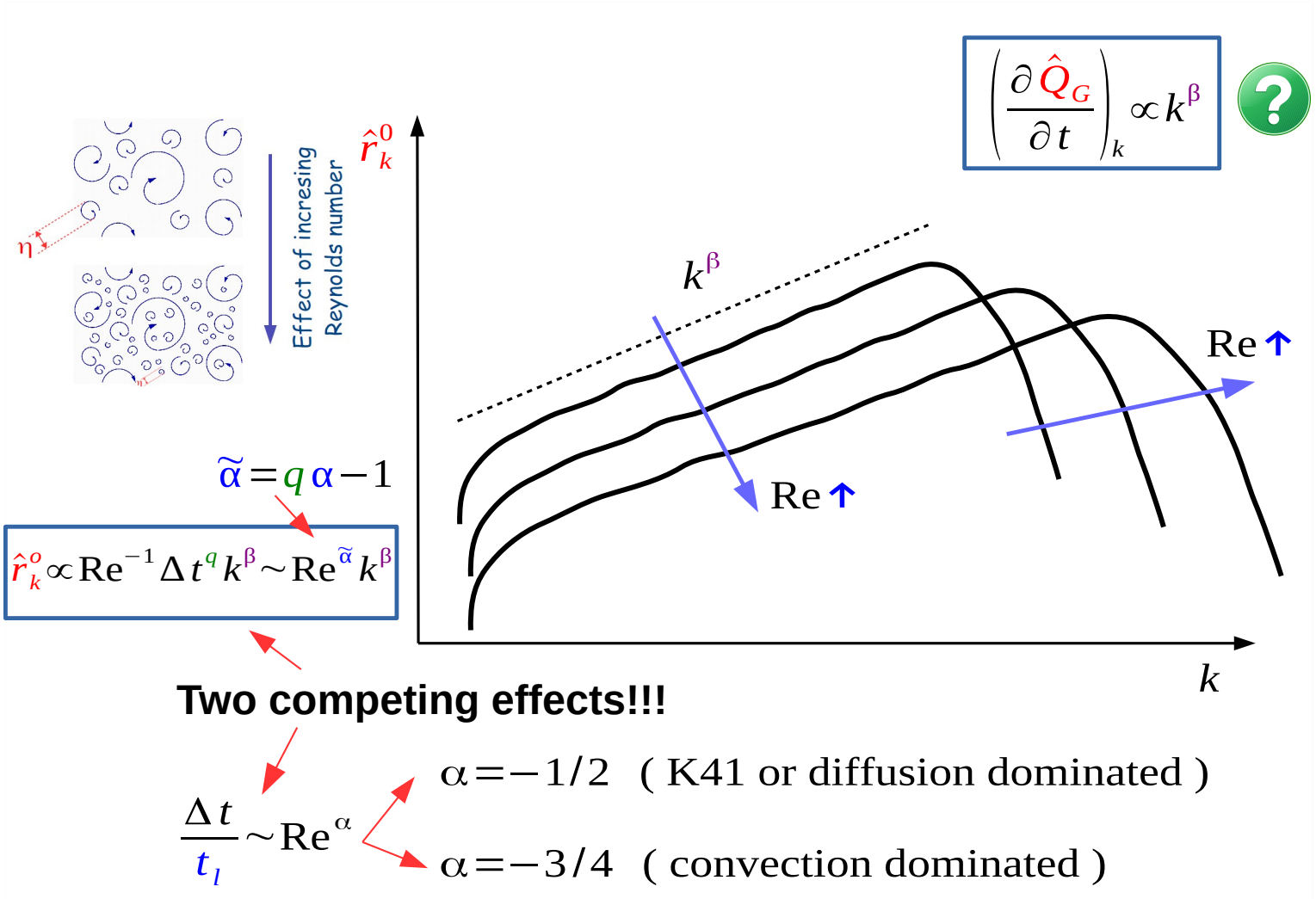

Homogeneous isotropic turbulence

Kolmogorov theory predictions

$$E_k = C_k \varepsilon^{2/3} k^{-5/3}$$

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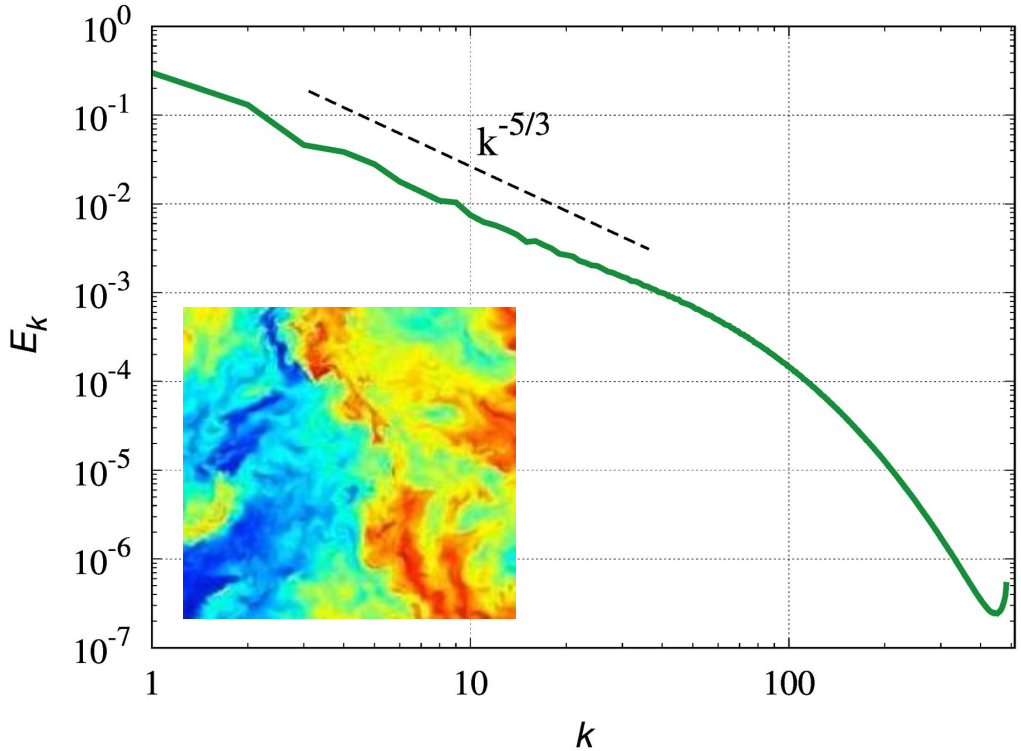

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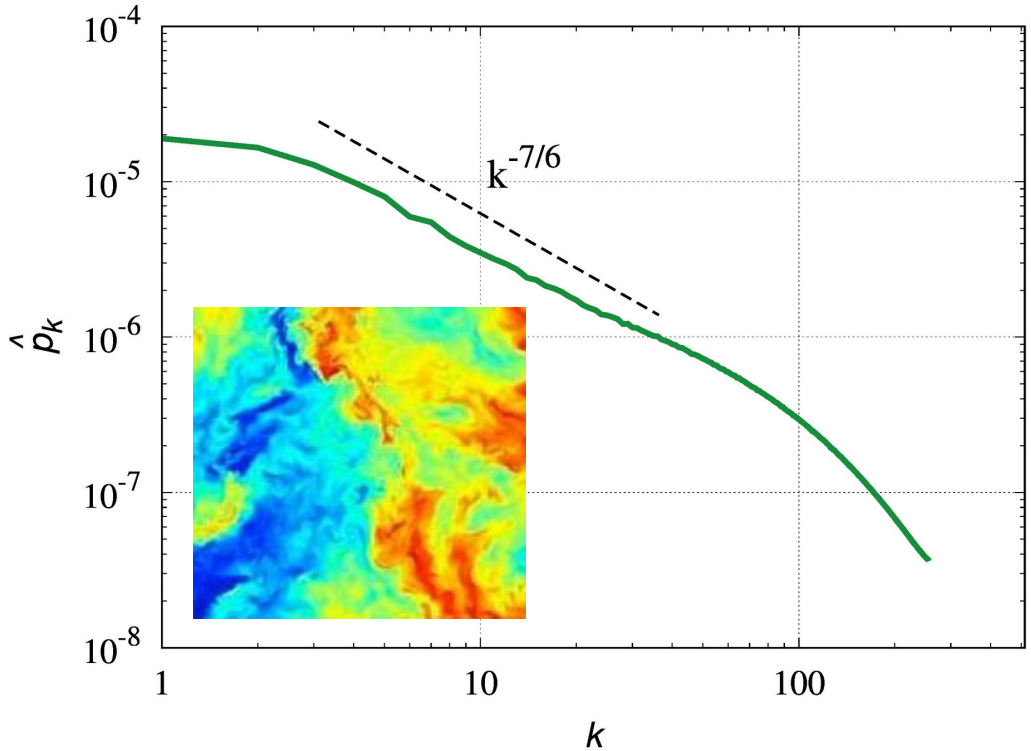

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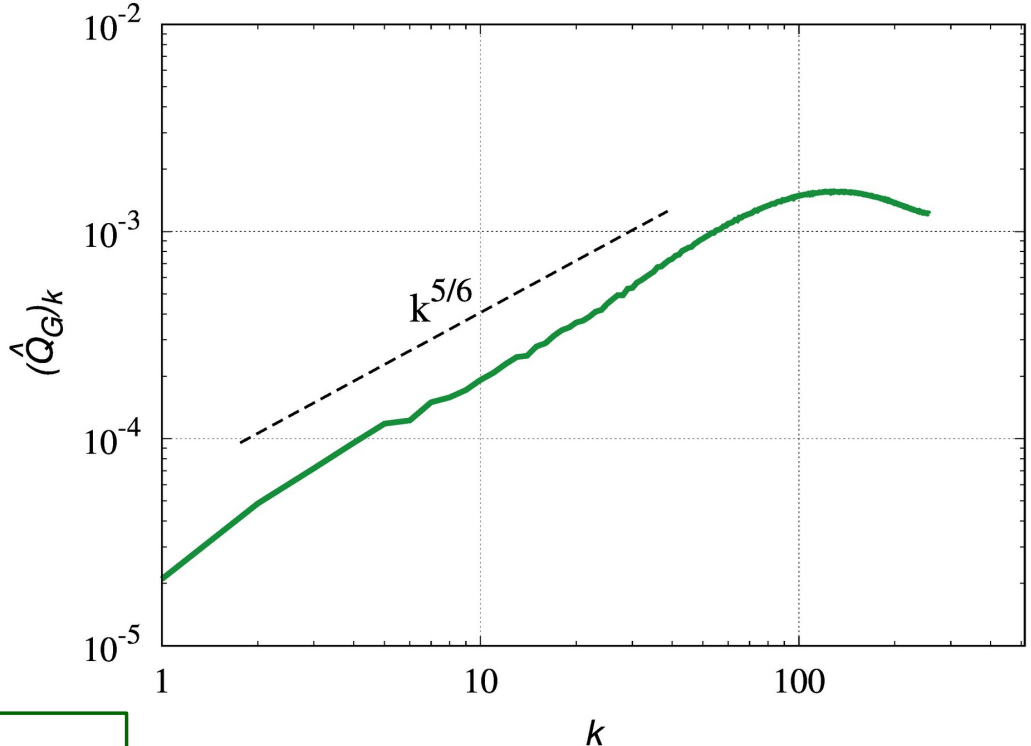

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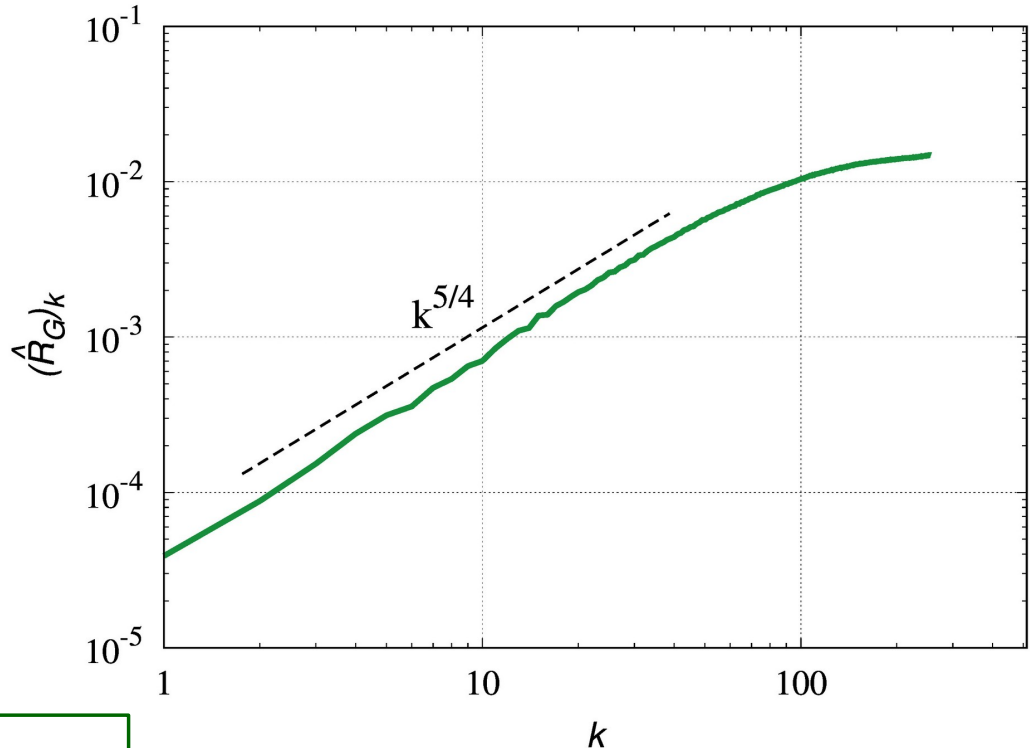

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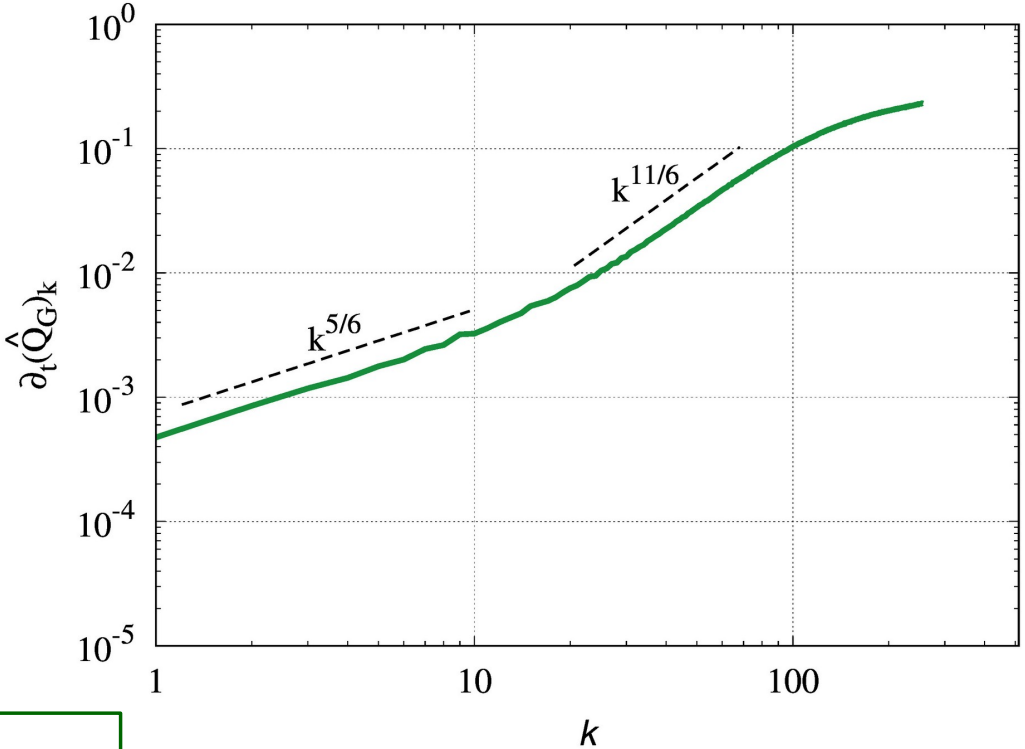

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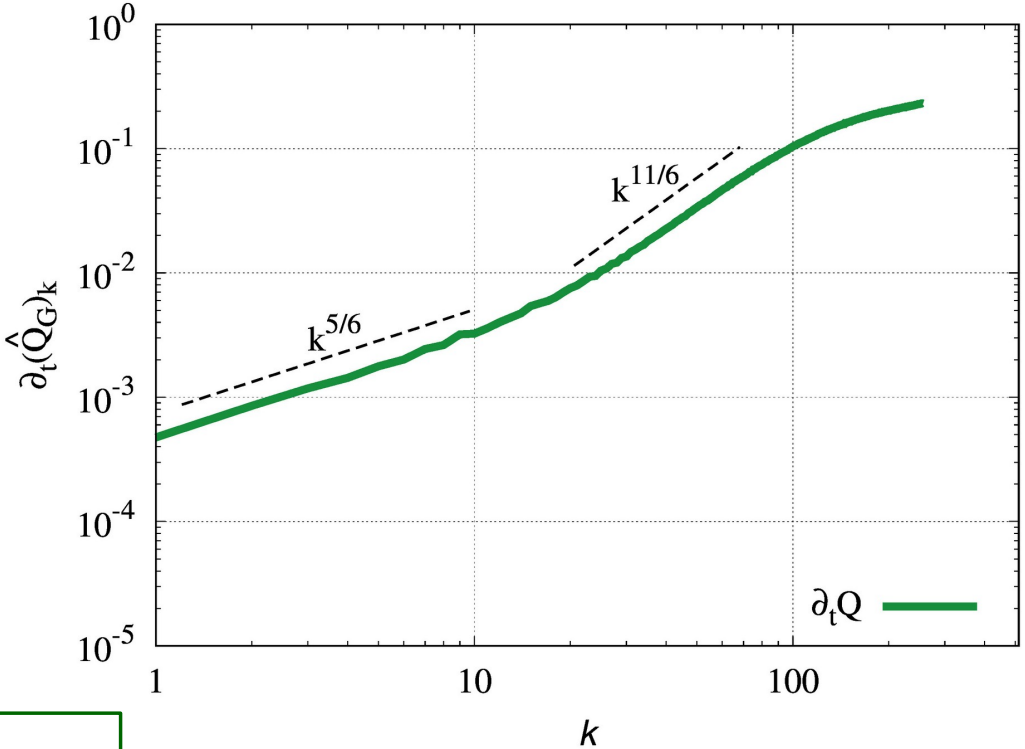

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$$(\hat{Q}_G)_k \propto k^{-7/6+2} = k^{5/6}$$

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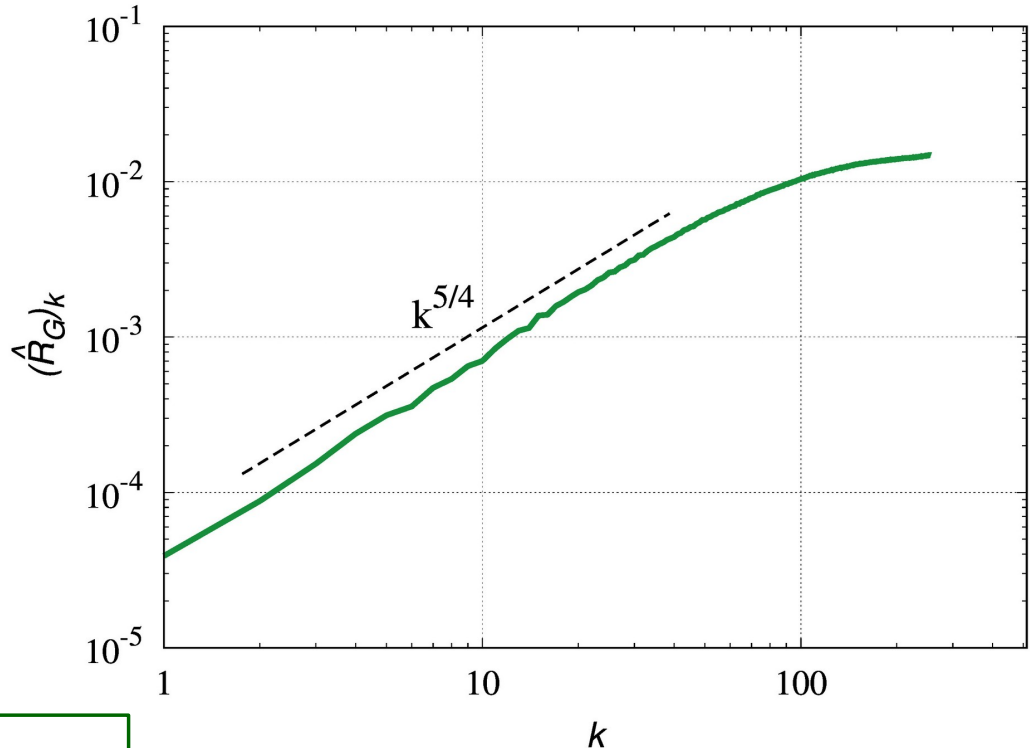
$$\hat{r}_k^o \propto \mathrm{Re}^{-1} \Delta t^q k^{\beta} \sim \mathrm{Re}^{\tilde{\alpha}} k^{\beta}$$



$$\nabla^2 \tilde{p}^{n+1} = \nabla \cdot \vec{u}^p = 2 \Delta t \, Q_G$$

$\mathrm{Re}_\lambda \approx 433$ (1024^3) from https://turbulence.pha.jhu.edu/

Homogeneous isotropic turbulence

New derivations

$$E_k = C_k \varepsilon^{2/3} k^{-5/3}$$

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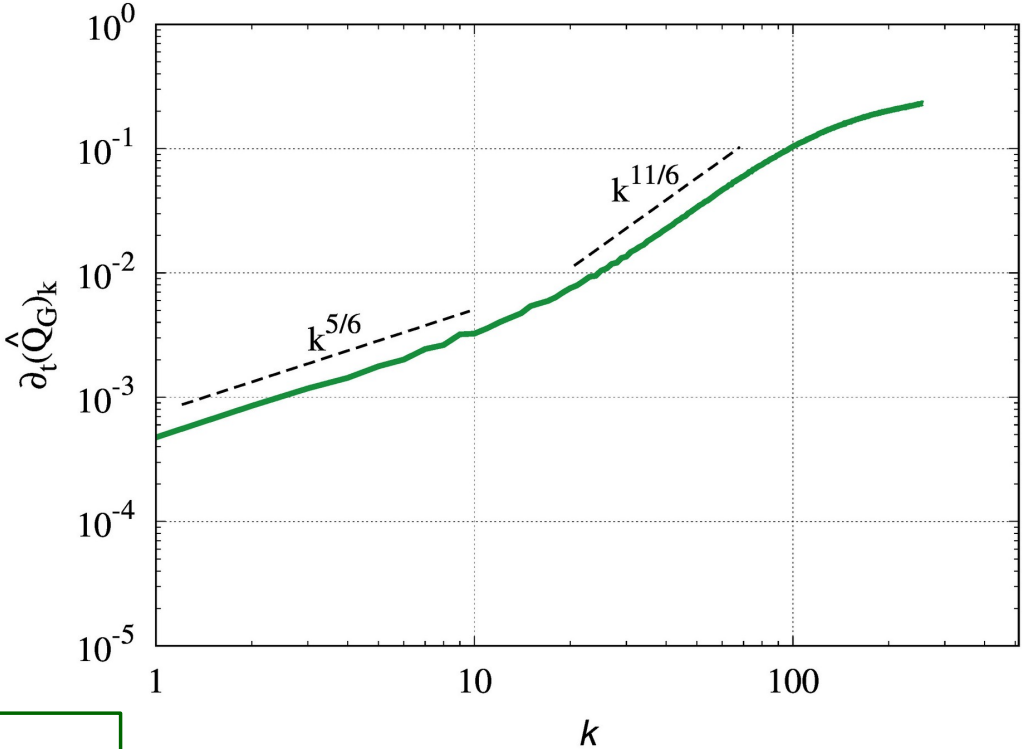

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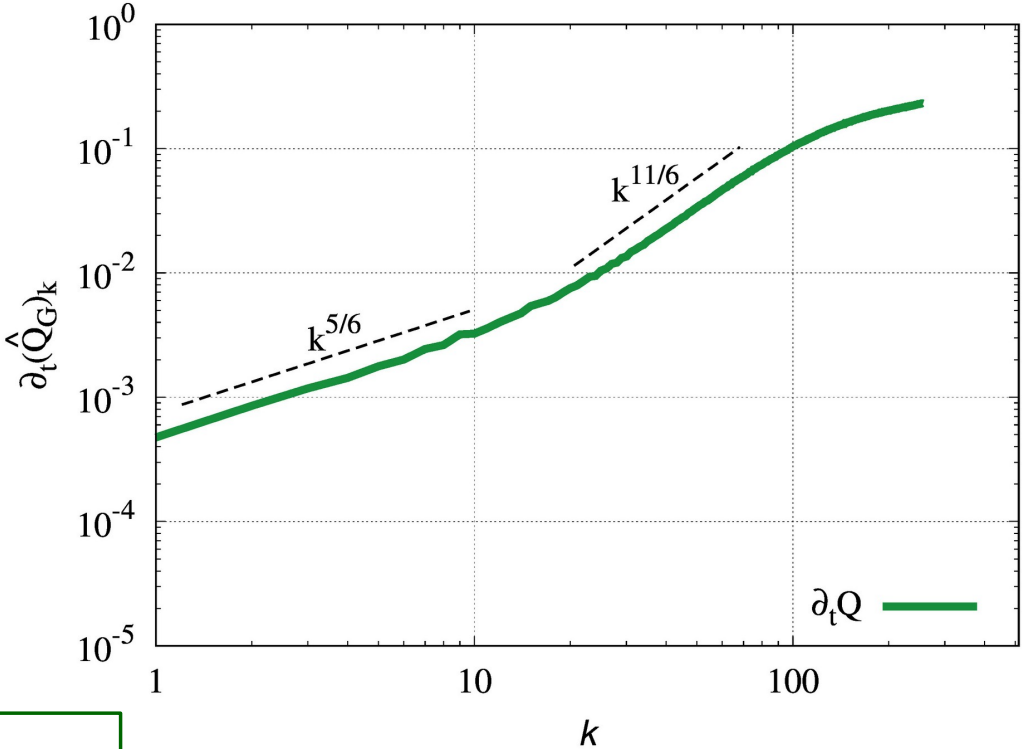

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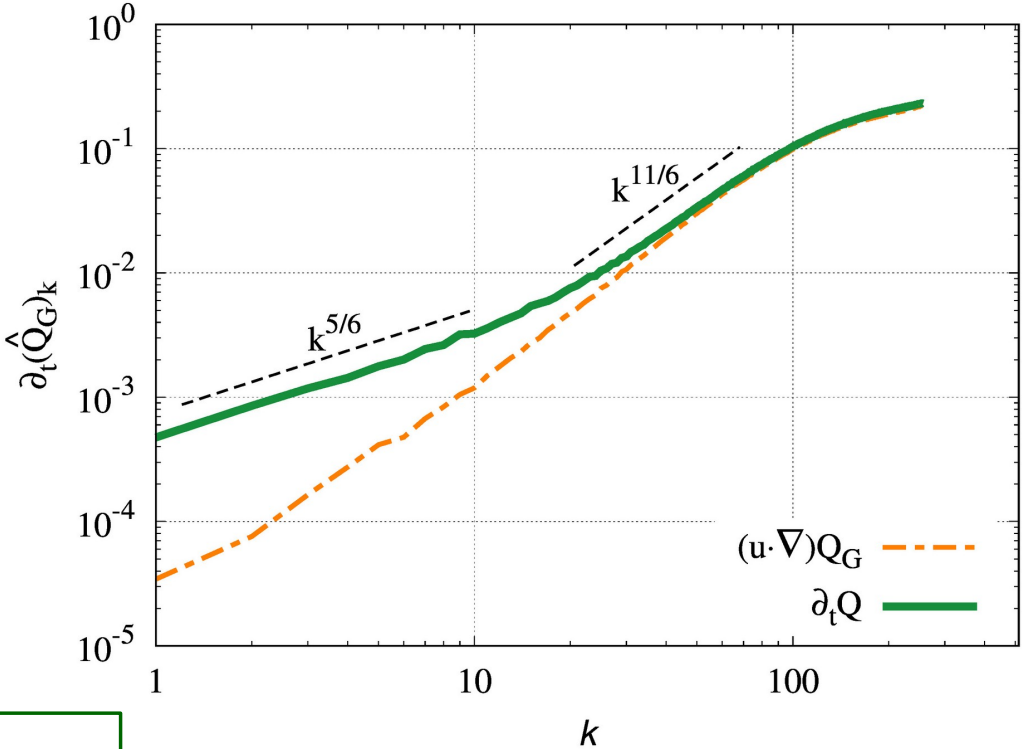

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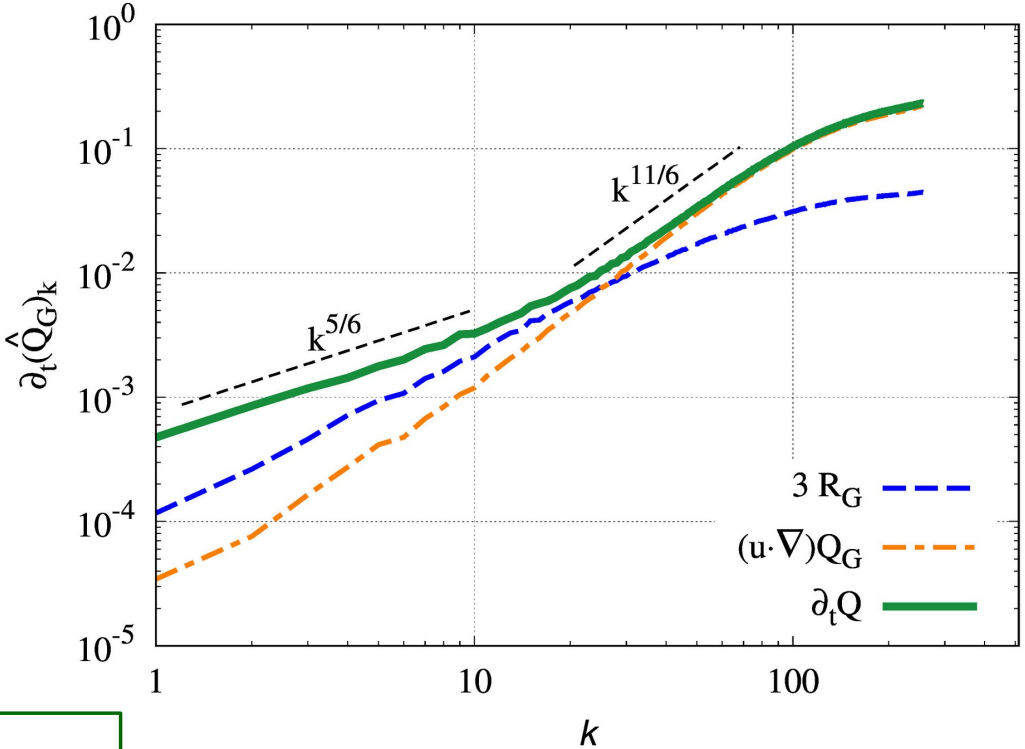

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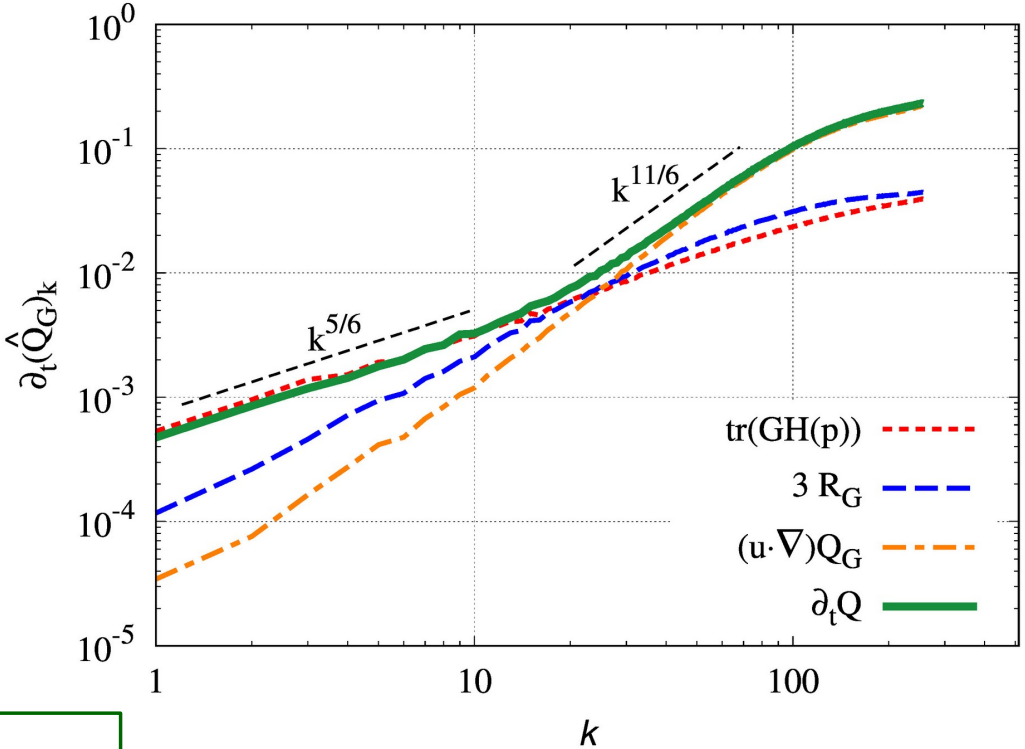

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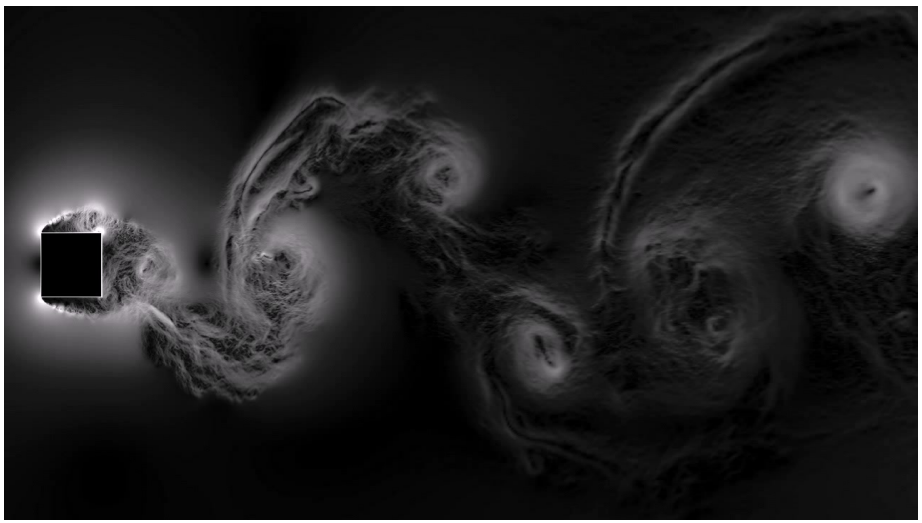
Non-homogeneous turbulent flows

Flow around a square cylinder

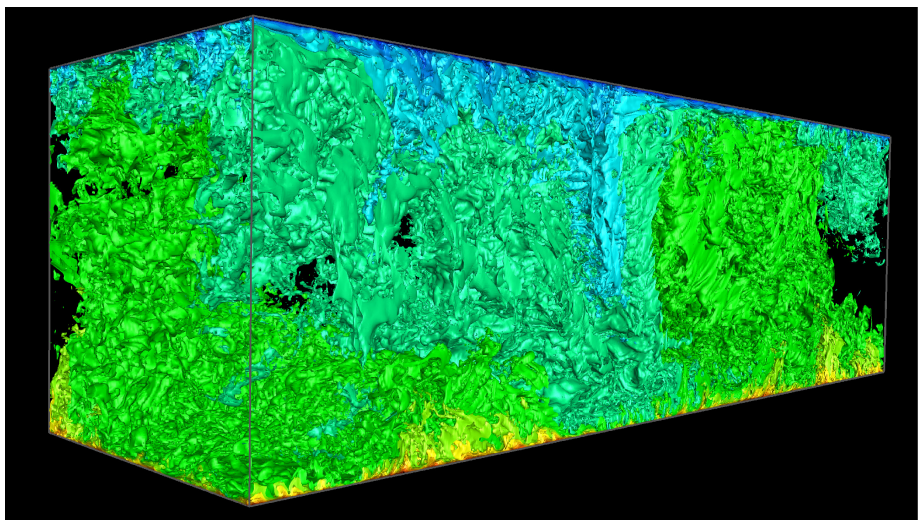


$Re = 22000$ (330M grid points)

$Re = 55000$ (2.6B grid points)

$Re = 100000$ (10B grid points) on-going

Air-filled Rayleigh–Bénard



$Ra = 10^{10}$ (604M grid points)

$Ra = 10^{11}$ (5.7B grid points)

Non-homogeneous turbulent flows

Flow around a square cylinder at $Re = 22000$

$$\widetilde{r}^{o} = \nabla^2 \widetilde{p}^{n} - \nabla \cdot u^{p,n+1} \approx \Delta t \, \nabla \cdot \frac{\partial u^{p}}{\partial t} \approx 2 \Delta t \frac{\partial Q_G}{\partial t}$$

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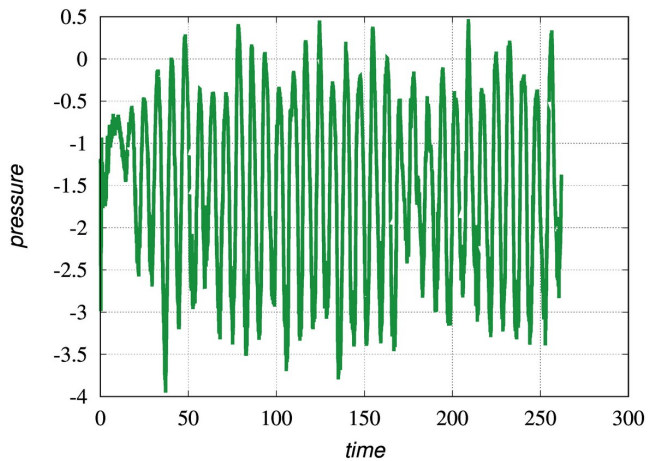

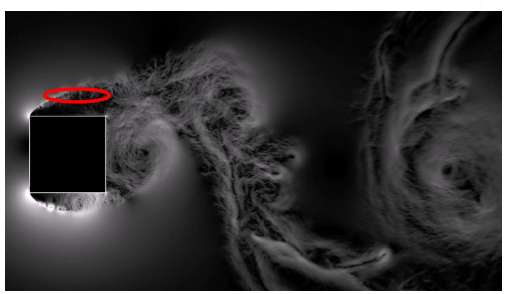

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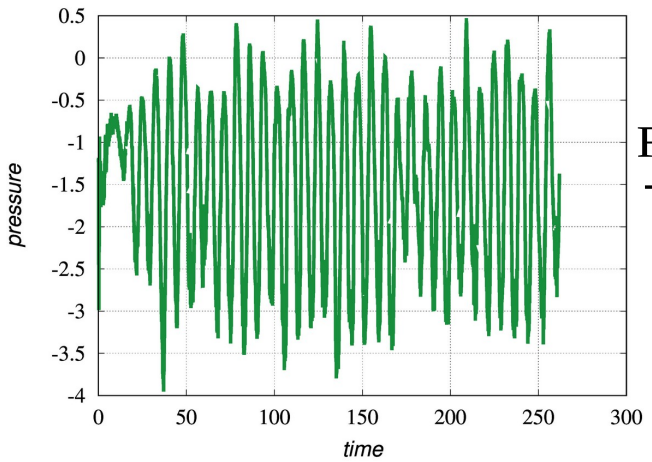
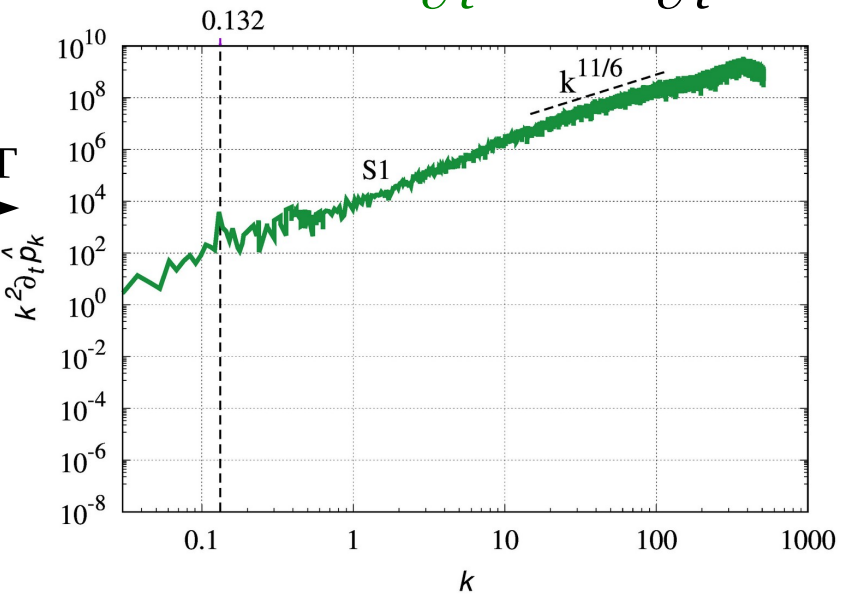
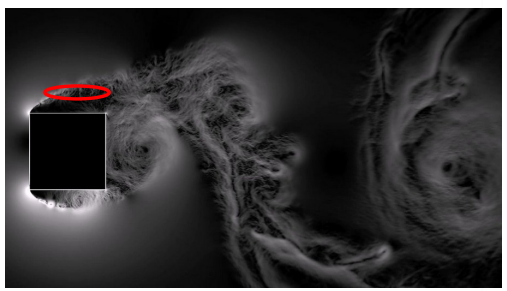


FFT



$$k^2 \frac{\partial \hat{p}_k}{\partial t} \approx -2 \frac{\partial \hat{Q}_G}{\partial t}$$

$$k^2 \frac{\partial \hat{p}_k}{\partial t} \propto k^{\beta} \quad \text{with} \quad \beta = 11/6$$



Non-homogeneous turbulent flows

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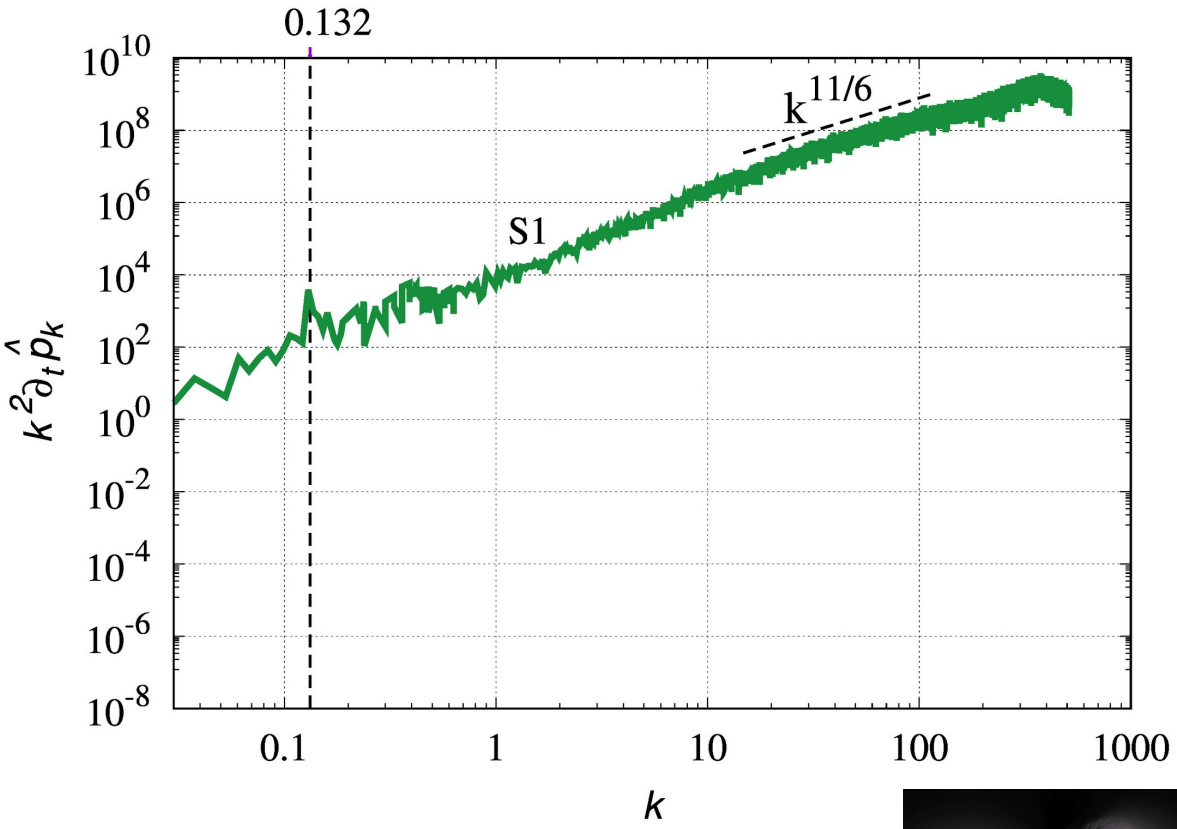

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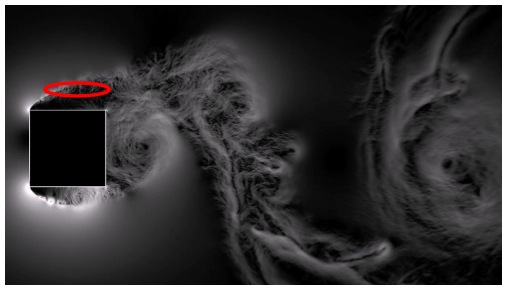

Non-homogeneous turbulent flows

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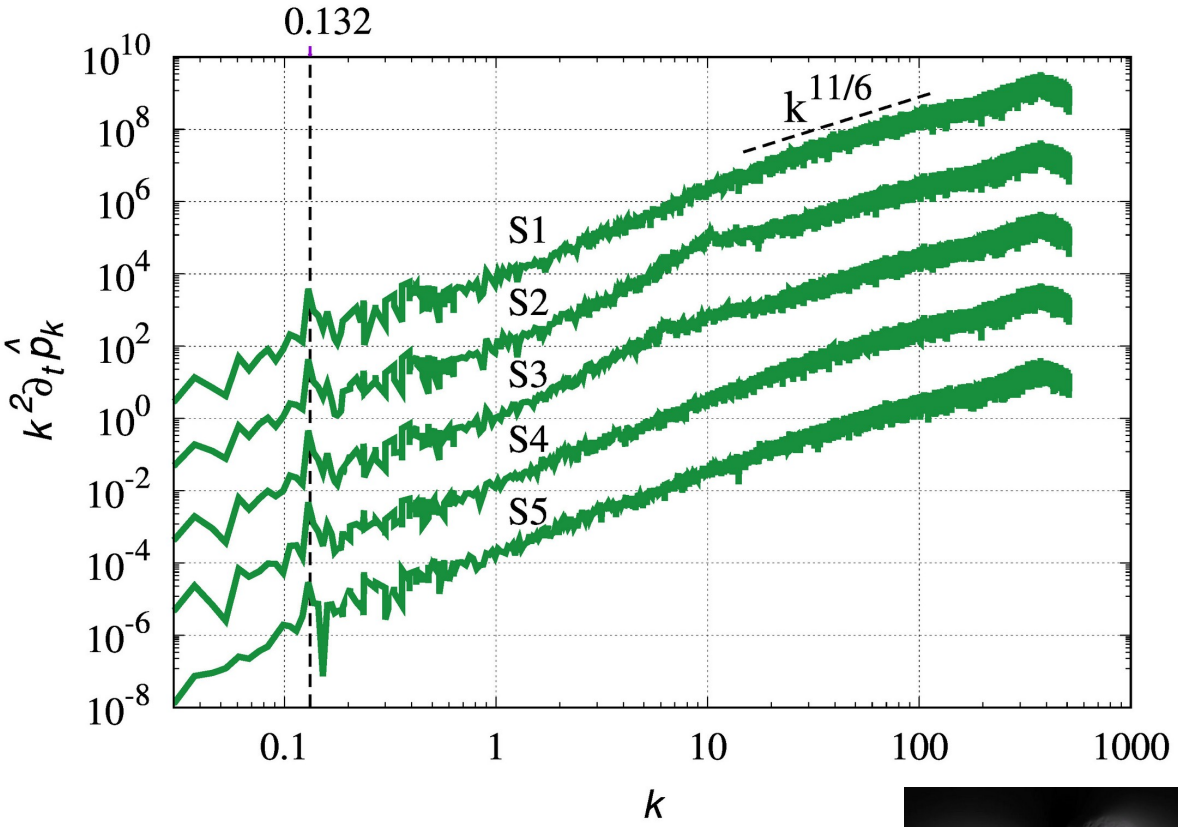

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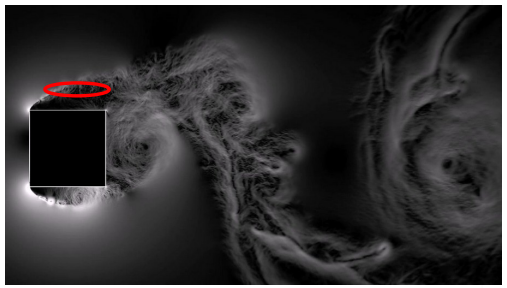
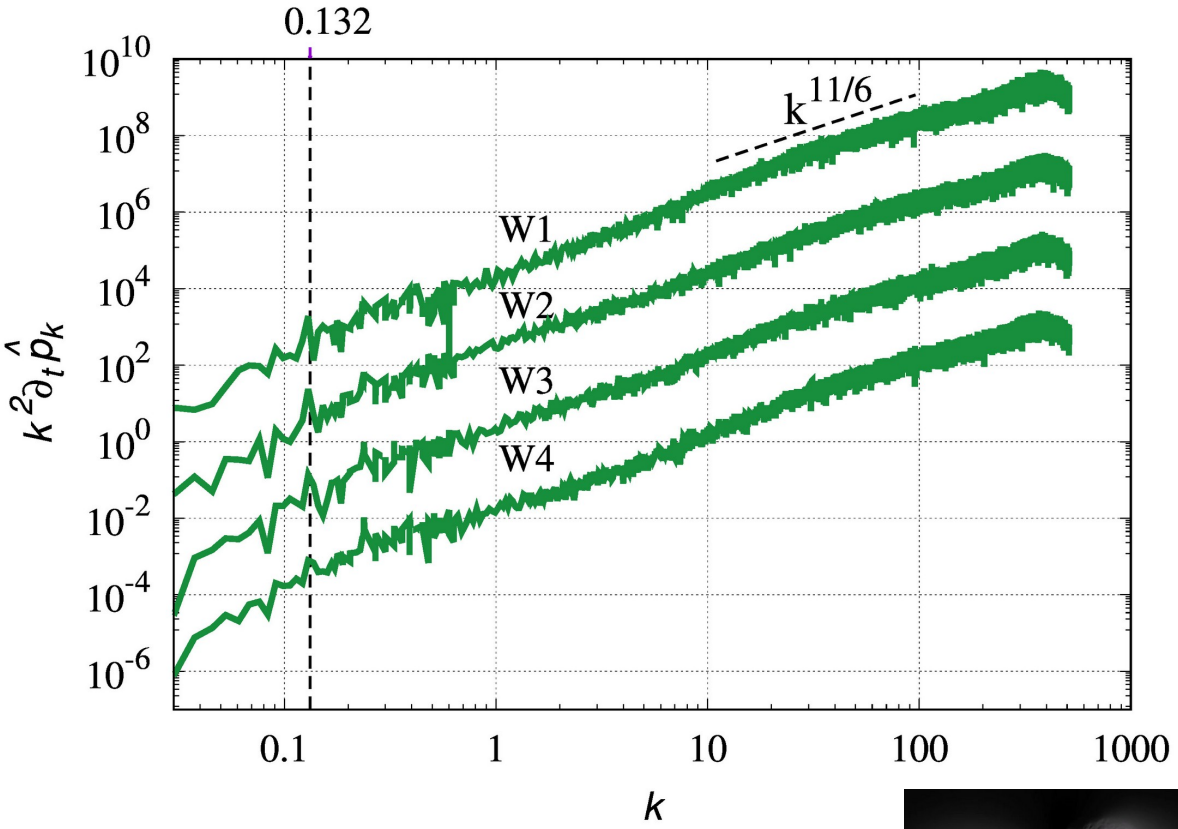


Non-homogeneous turbulent flows

Flow around a square cylinder at $Re = 22000$

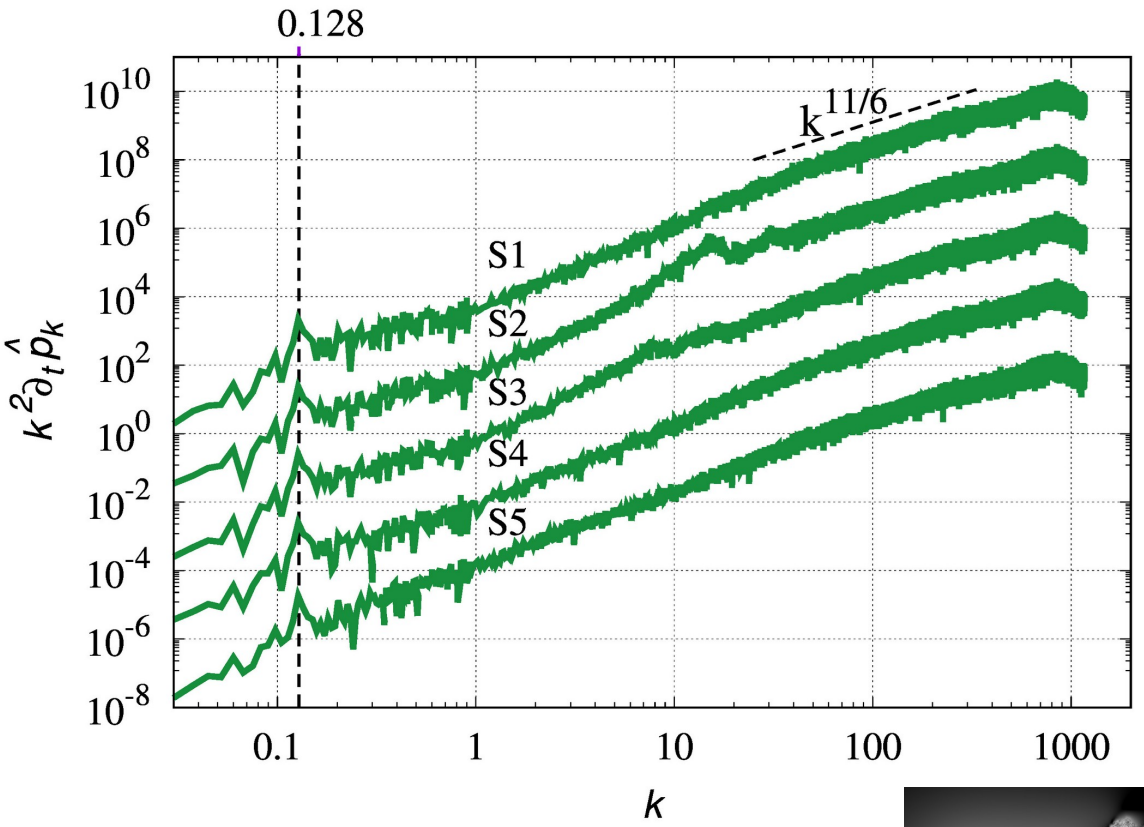


$$k^2 \frac{\partial \hat{p}_k}{\partial t} \propto k^{\beta} \quad \text{with} \quad \beta = 11/6$$



Non-homogeneous turbulent flows

Flow around a square cylinder at $Re = 55000$



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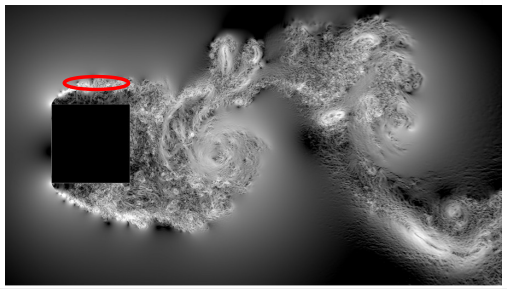
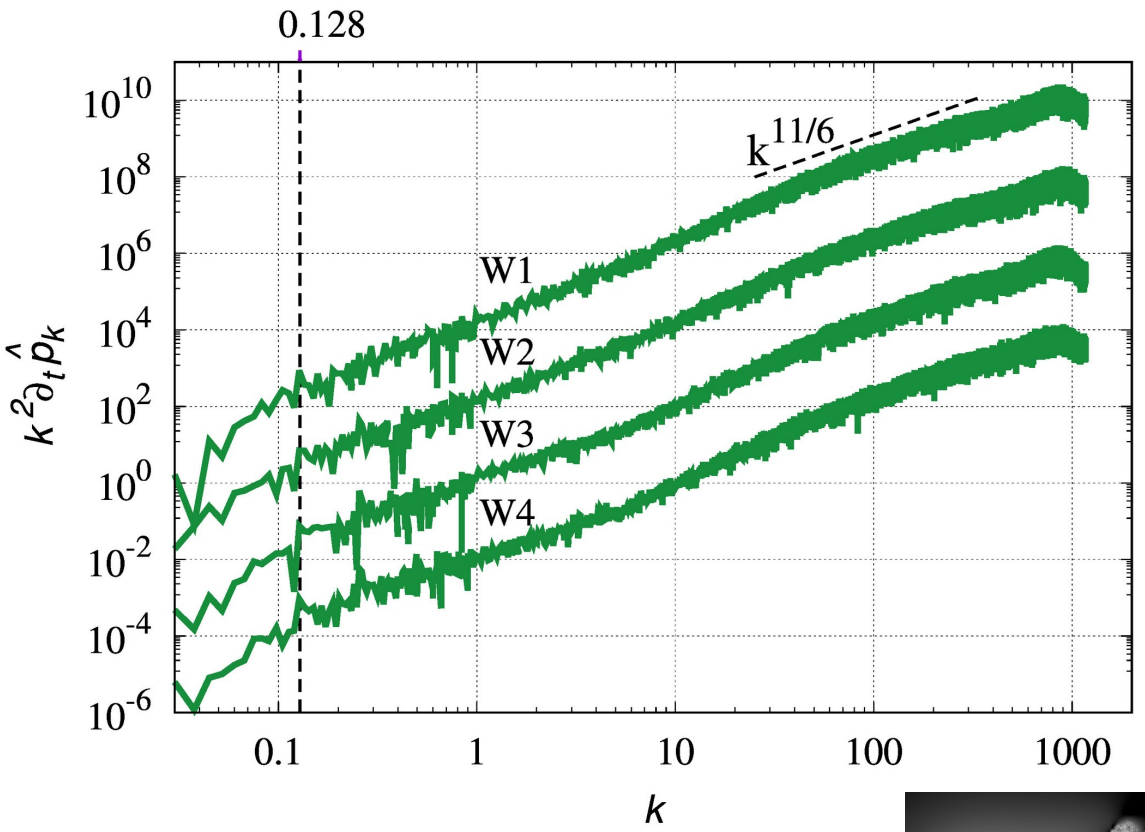


Non-homogeneous turbulent flows

Flow around a square cylinder at $Re = 55000$



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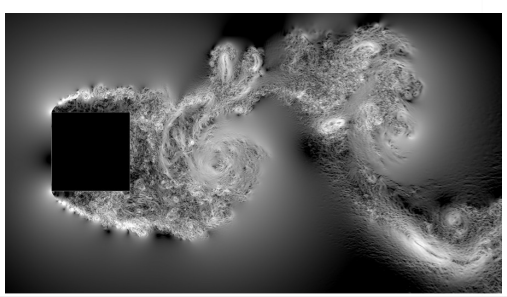
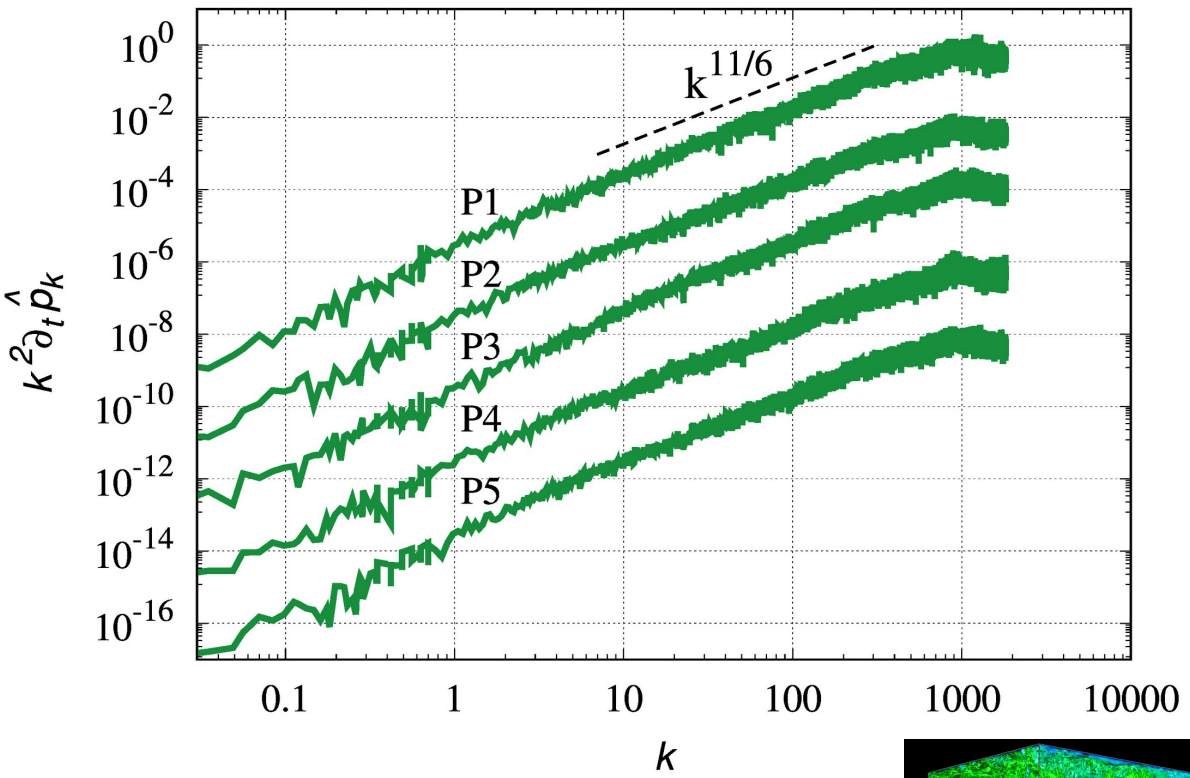


Non-homogeneous turbulent flows

Air-filled Rayleigh–Bénard at $Ra = 10^{10}$



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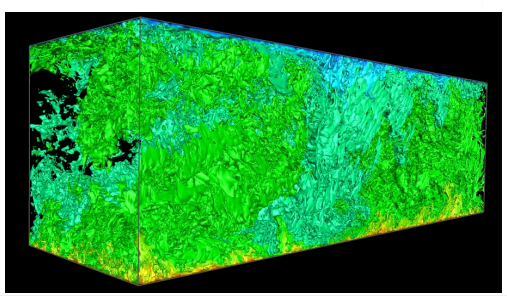
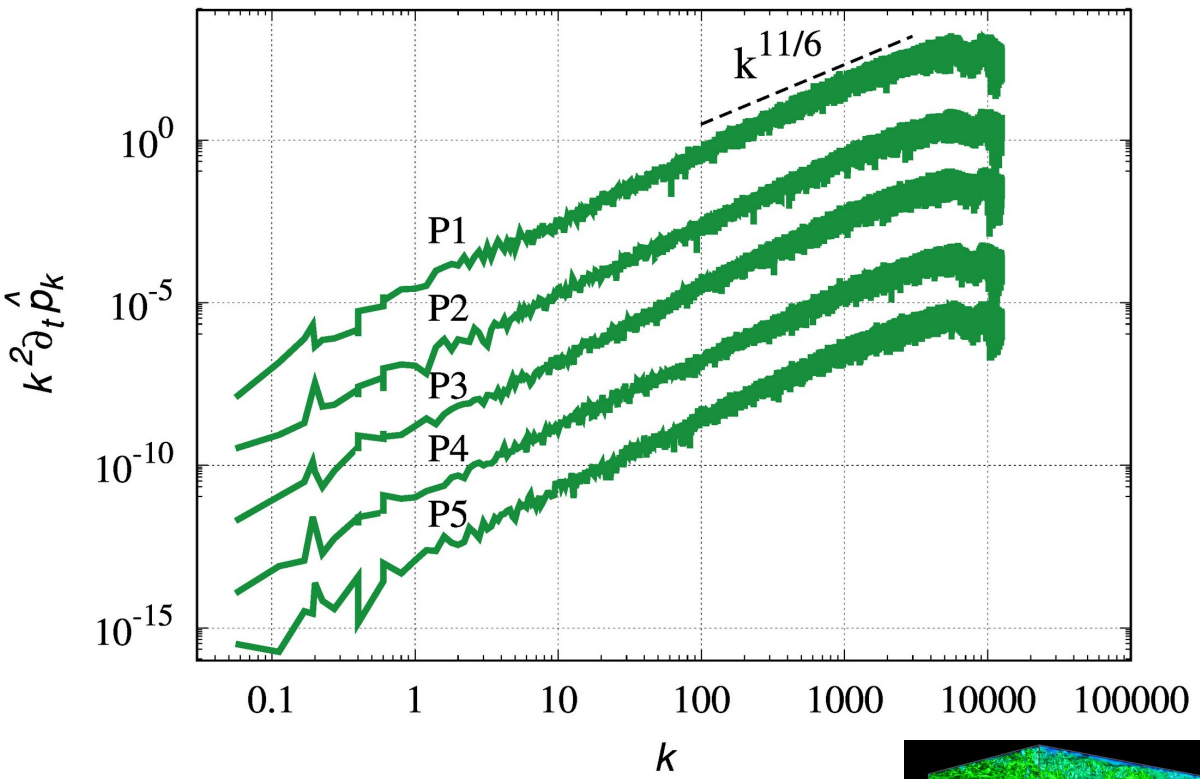


Non-homogeneous turbulent flows

Air-filled Rayleigh–Bénard at $Ra = 10^{11}$



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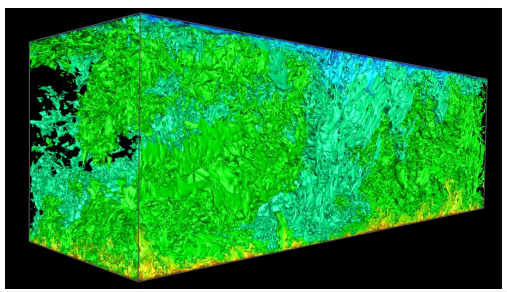
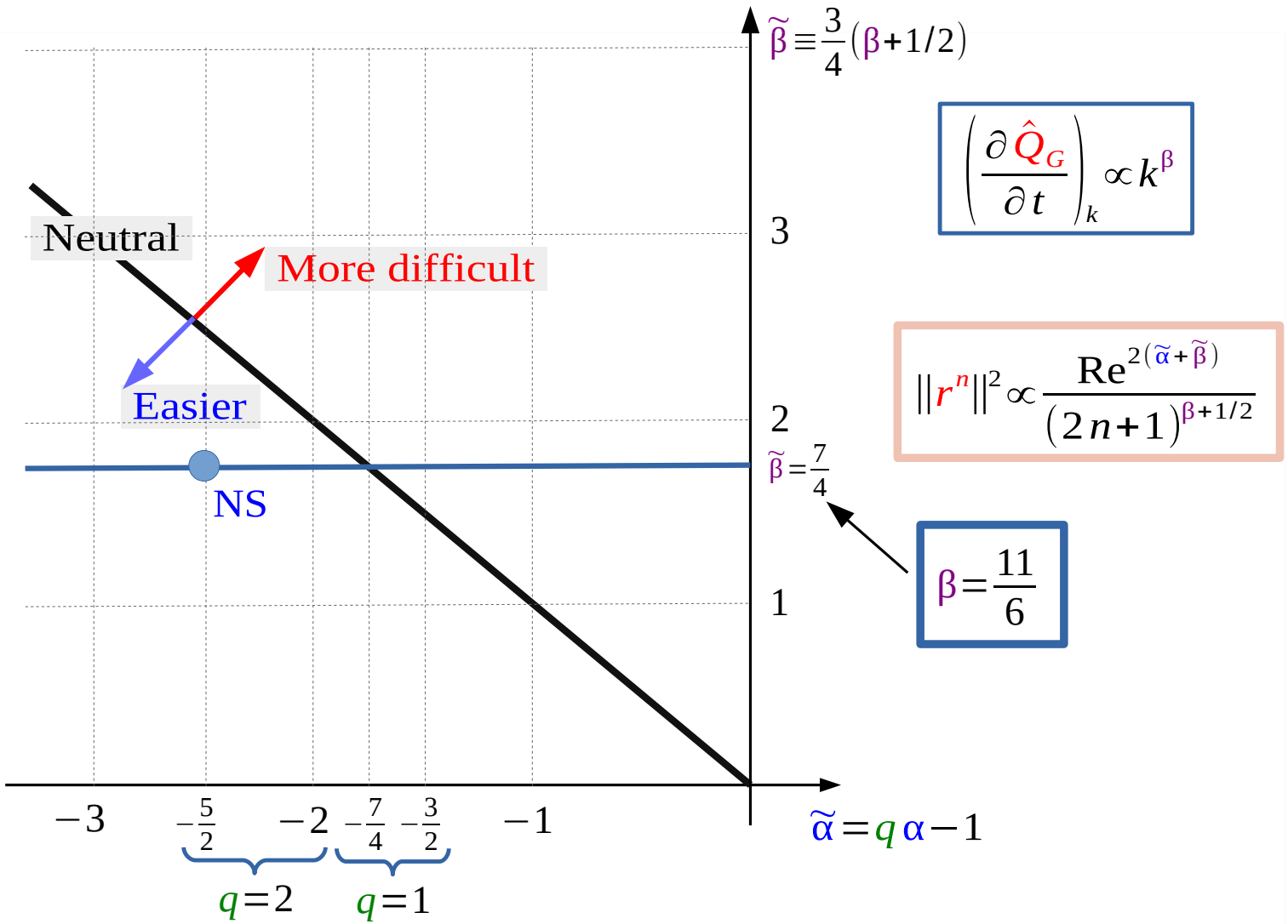


Solver convergence

$\{\tilde{\alpha}, \tilde{\beta}\}$ phase space



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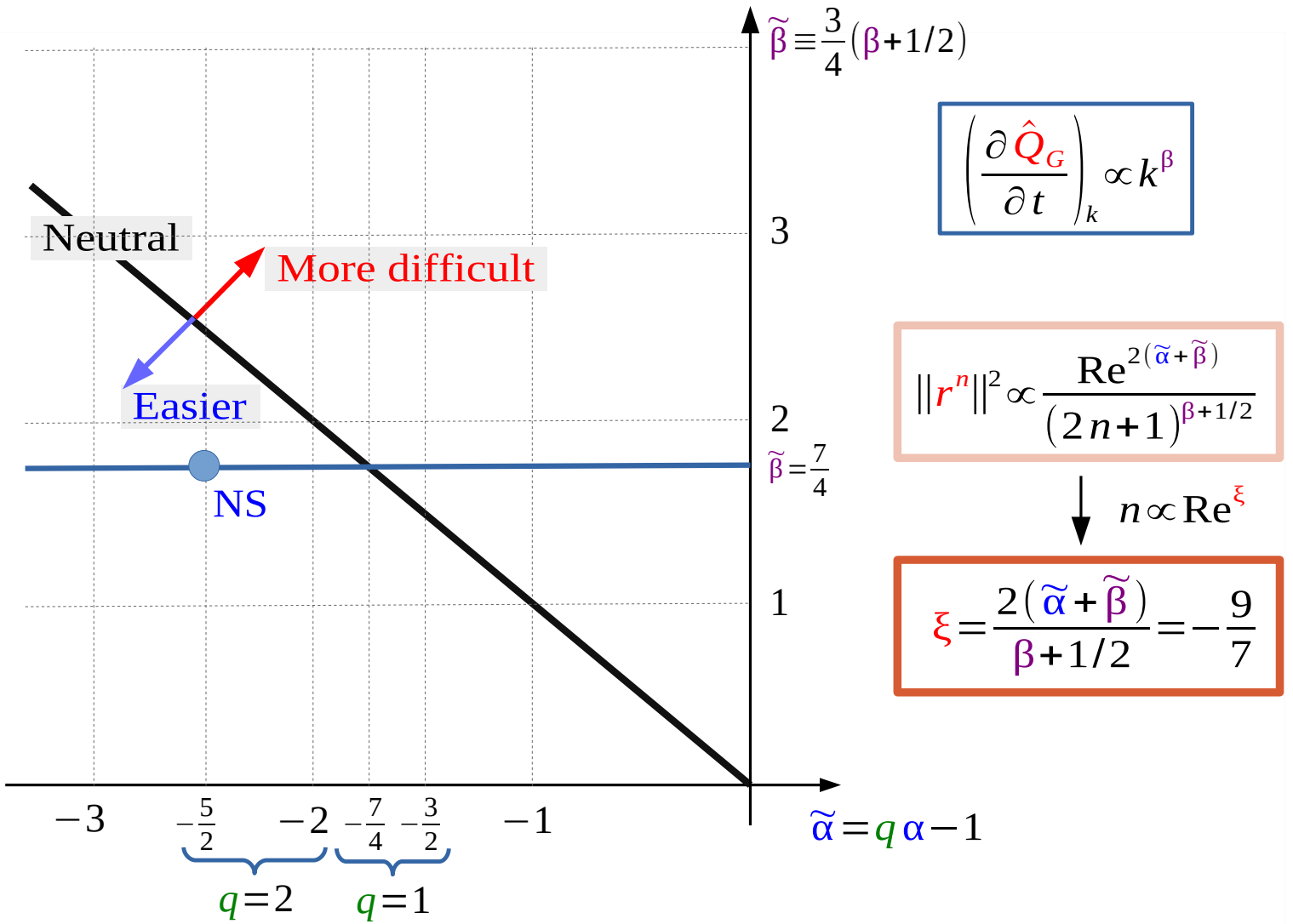

Solver convergence for Burgers' equation

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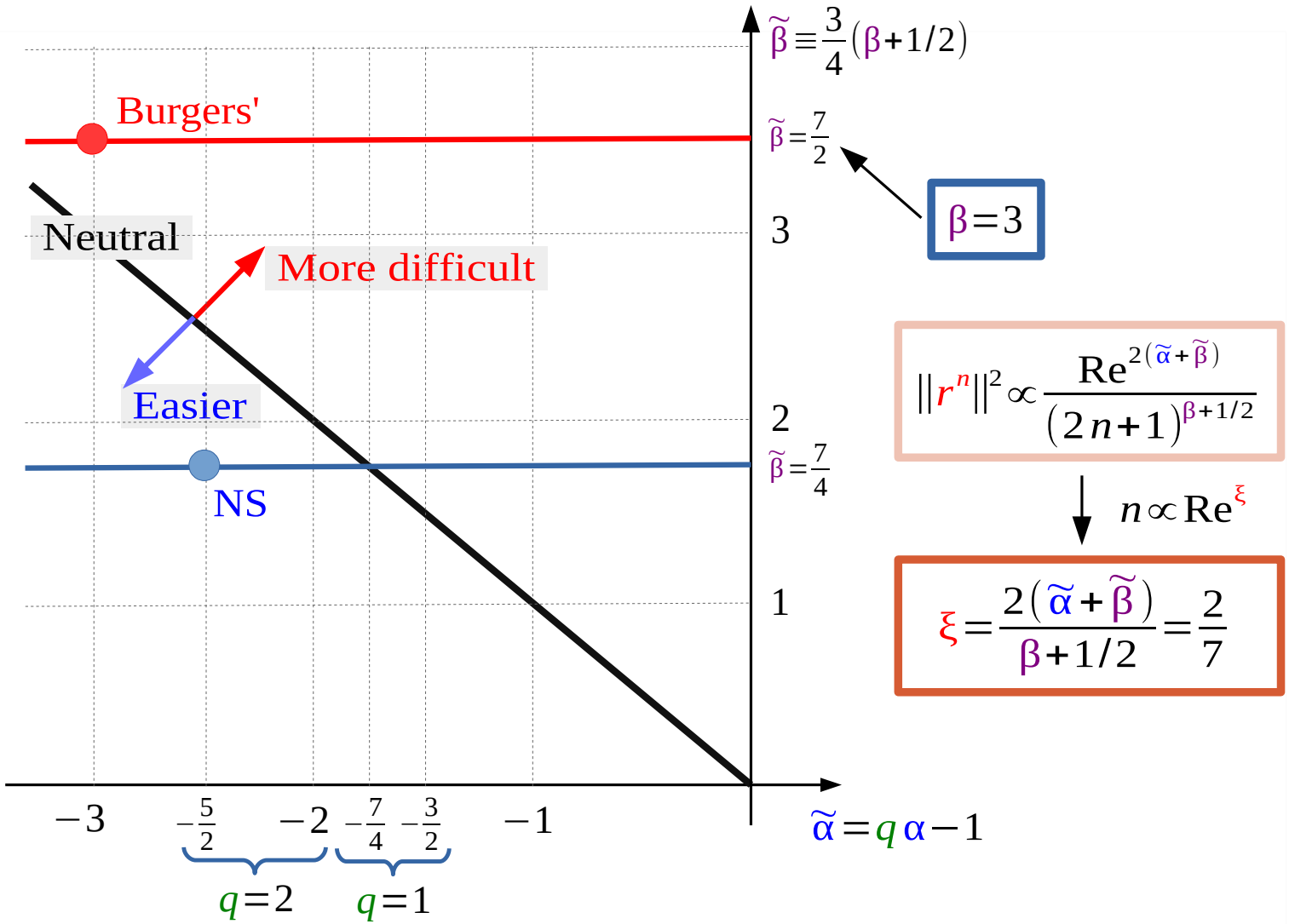

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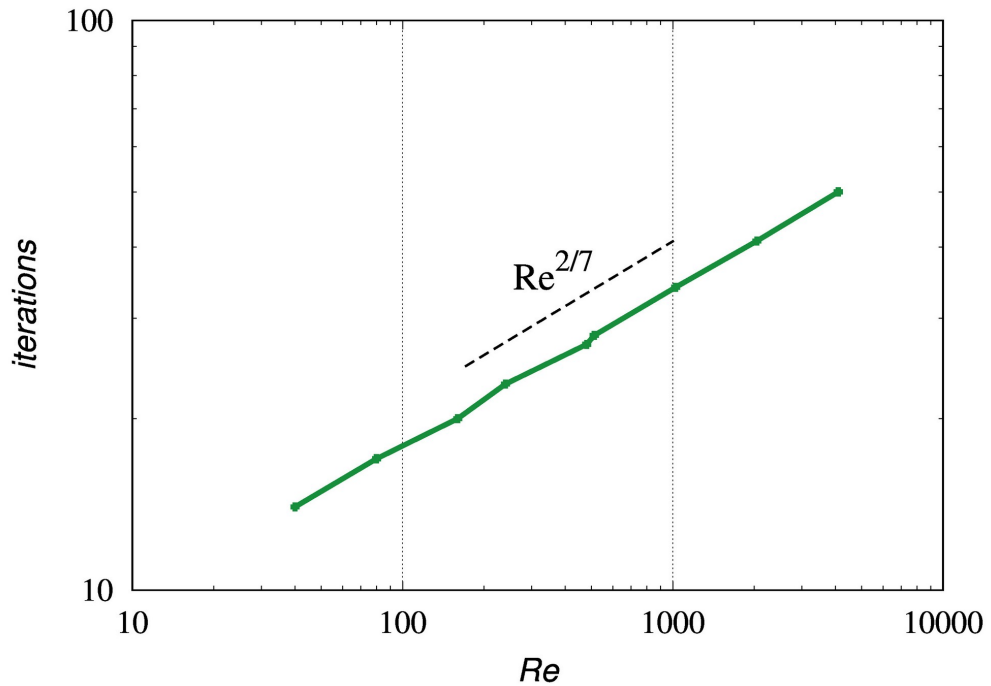

$$\|r^n\|^2 \propto \frac{\mathrm{Re}^{2(\tilde{\alpha}+\tilde{\beta})}}{(2n+1)^{\beta+1/2}}$$

$$\downarrow \quad n \propto \mathrm{Re}^{\xi}$$

$$\xi = \frac{2(\tilde{\alpha}+\tilde{\beta})}{\beta+1/2} = \frac{2}{7}$$

Concluding remarks

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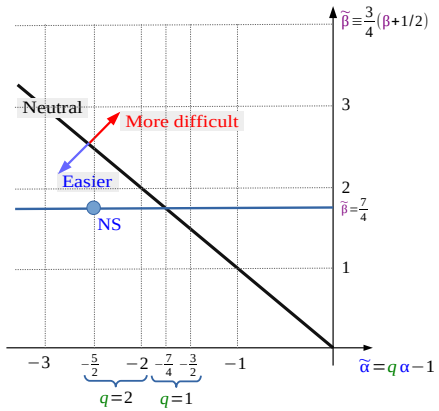

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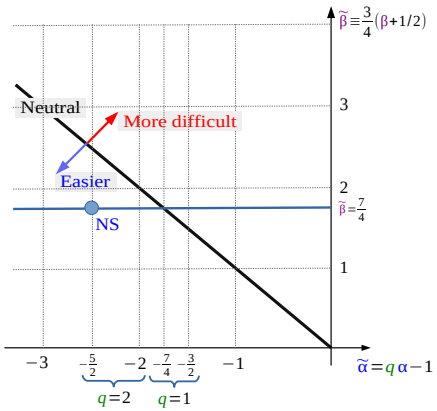
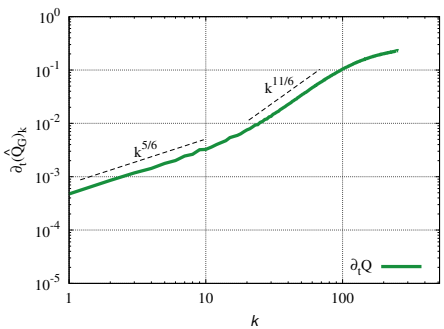
  - For HIT ✓





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- The $\{\tilde{\alpha}, \tilde{\beta}\}$ **phase space** is divided in two regions depending on the solver convergence.
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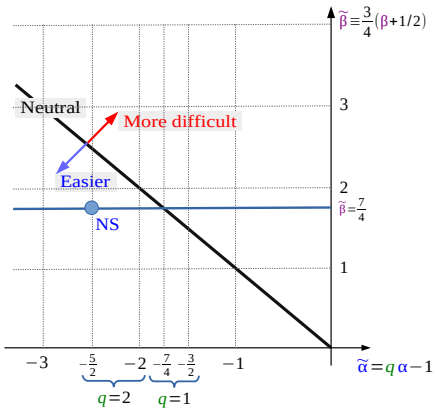
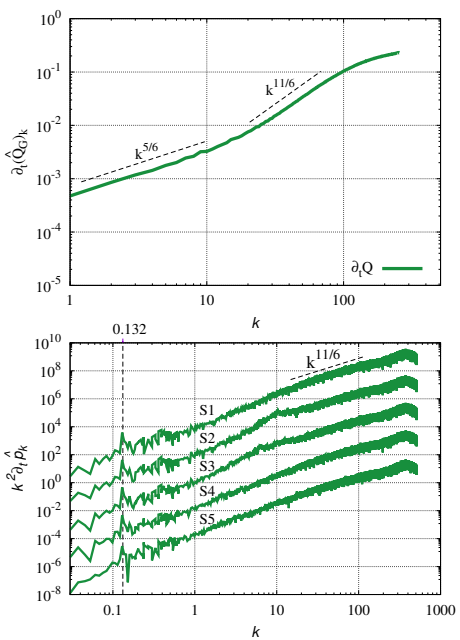
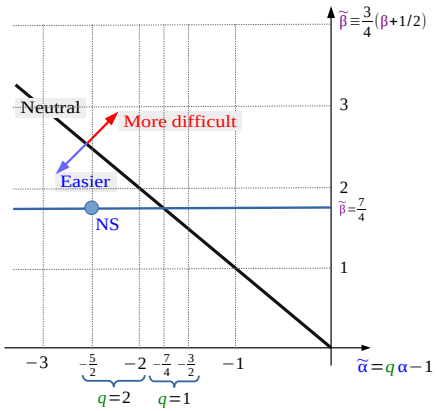
  - For HIT ✓
  - But also for non-homogeneous flows ✓

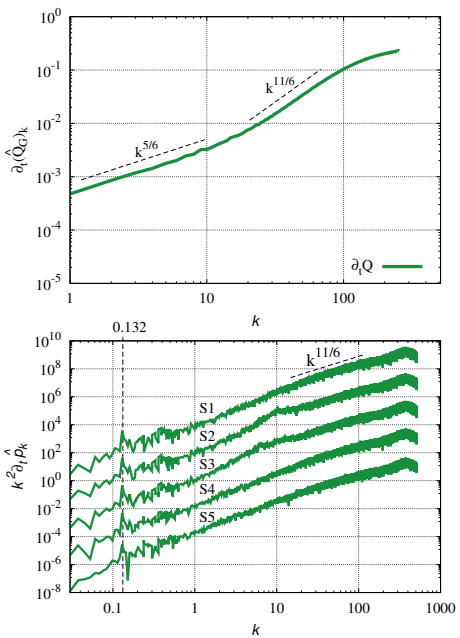




Concluding remarks

- **Two competing effects** on the convergence of Poisson's equation have been identified.
- The $\{\tilde{\alpha}, \tilde{\beta}\}$ **phase space** is divided in two regions depending on the solver convergence.
- Numerical **results** match well with the **developed theory** prediction $\beta \approx 11/6$
  - For HIT ✓
  - But also for non-homogeneous flows ✓





On-going research:

- Numerical analysis of the scaling of number of solver iterations with Re

Thank you for your attendance

