Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

UNIVERSITÀ DEGLI STUDI DI PADOVA

Roadmap for extreme-scale simulations

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ParCFD 2024
35th Parallel CFD International Conference 2024
02. - 04. Sep. 2024, University Club Bonn, Germany

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Roadmap for extreme-scale simulations: on the evolution of Poisson solvers

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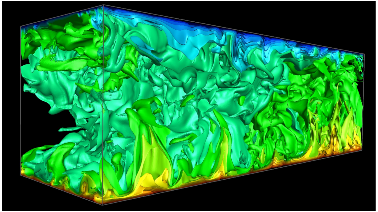
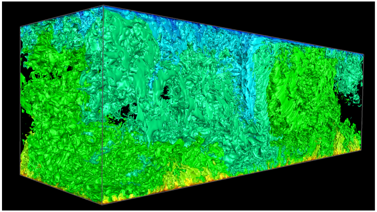




Contents

1. Motivation
2. Two competing effects
3. Residual of Poisson's equation
4. Solver convergence
5. Results
6. Conclusions

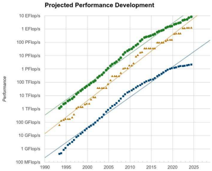
Tera, Peta, Exa,..., Zetta, Yotta

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		



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

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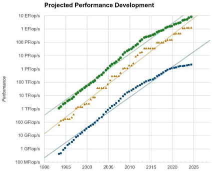

Tera, Peta, Exa,..., Zetta, Yotta

~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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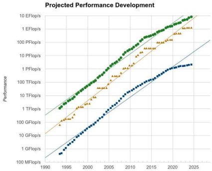
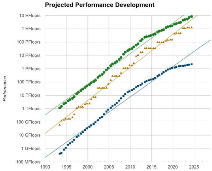


Tera, Peta, Exa,..., Zetta, Yotta

~10 years ~5 years ~10 years

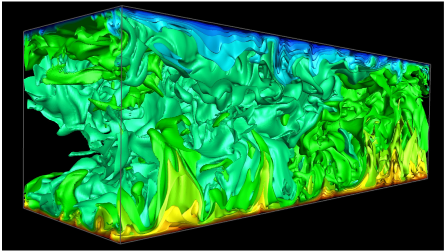
	PetaFLOPS		#1 in LINPACK	#1 in HPCG	Cutting-edge CFD simulation	'Routine' CFD simulation
Zetta	10^6		2037	2047	2052	2062
Exa	10^3	14 years	**2022** (Frontier)	2032	2037	2047
Peta	1		**2008** (Roadrunner)	**2018** (Summit)	2023	2033
Tera	10^{-3}	11 years	**1997** (ASCI Red)	No data		

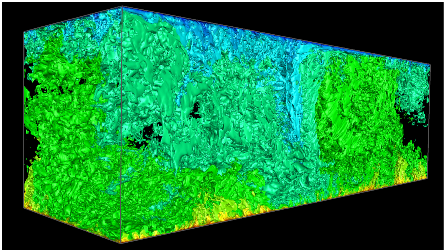


Motivation

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?

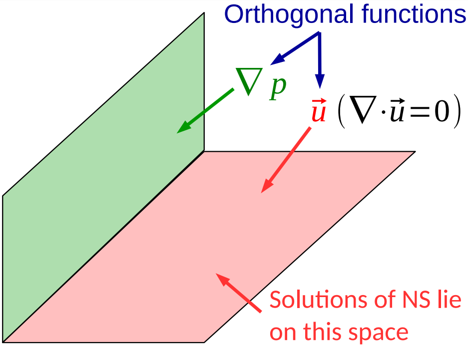




DNS[1] of air-filled Rayleigh–Bénard convection at $Ra = 10^8$ and 10^{10}

[1] B.Sanderse, F.X.Trias. *Energy-consistent discretization of viscous dissipation with application to natural convection flow.* (https://arxiv.org/abs/2307.10874)

Poisson's equation: a quick reminder

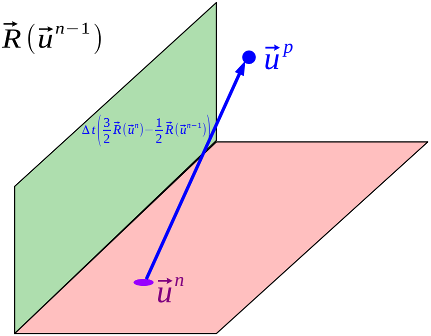


Semi-discrete (just in time) NS equations

$$\begin{cases} \dfrac{\vec{u}^{\,n+1} - \vec{u}^{\,n}}{\Delta t} = \dfrac{3}{2}\vec{R}(\vec{u}^{\,n}) - \dfrac{1}{2}\vec{R}(\vec{u}^{\,n-1}) - \nabla p^{n+1} \\ \nabla \cdot \vec{u}^{\,n+1} = 0 \end{cases}$$

Poisson's equation: a quick reminder

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



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$$\begin{cases} \dfrac{\vec{u}^{n+1}-\vec{u}^{n}}{\Delta t}=\dfrac{3}{2}\vec{R}(\vec{u}^{n})-\dfrac{1}{2}\vec{R}(\vec{u}^{n-1})-\nabla p^{n+1} \\ \nabla\cdot\vec{u}^{n+1}=0 \end{cases}$$

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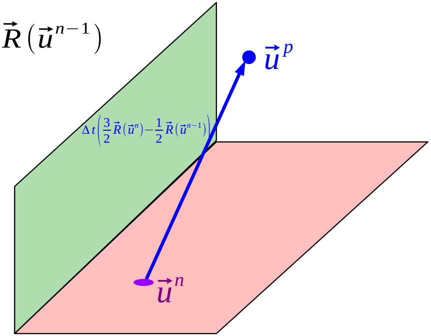
Step 1: $\dfrac{\vec{u}^{p}-\vec{u}^{n}}{\Delta t}=\dfrac{3}{2}\vec{R}(\vec{u}^{n})-\dfrac{1}{2}\vec{R}(\vec{u}^{n-1})$

Step 2: $\boxed{\nabla^2 p^{n+1}=\dfrac{1}{\Delta t}\nabla\cdot\vec{u}^{p}}$



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$$\begin{cases}\dfrac{\vec{u}^{n+1}-\vec{u}^{n}}{\Delta t}=\dfrac{3}{2}\vec{R}(\vec{u}^{n})-\dfrac{1}{2}\vec{R}(\vec{u}^{n-1})-\nabla p^{n+1}\\ \nabla\cdot\vec{u}^{n+1}=0\end{cases}$$

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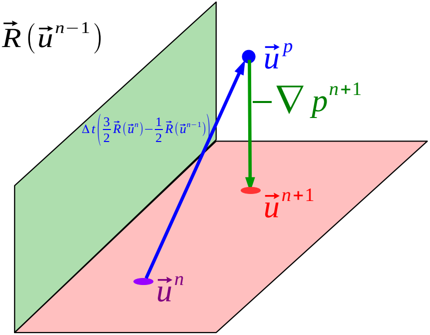
Step 1: $\dfrac{\vec{u}^{p}-\vec{u}^{n}}{\Delta t}=\dfrac{3}{2}\vec{R}(\vec{u}^{n})-\dfrac{1}{2}\vec{R}(\vec{u}^{n-1})$

Step 2: $\boxed{\nabla^{2}p^{n+1}=\dfrac{1}{\Delta t}\nabla\cdot\vec{u}^{p}}$

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



Semi-discrete (just in time) NS equations

$$\left\{\begin{array}{l}\dfrac{\vec{u}^{n+1}-\vec{u}^{n}}{\Delta t}=\dfrac{3}{2}\vec{R}(\vec{u}^{n})-\dfrac{1}{2}\vec{R}(\vec{u}^{n-1})-\nabla p^{n+1}\\ \nabla\cdot\vec{u}^{n+1}=0\end{array}\right.$$

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?

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

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

$\mathrm{Re}\uparrow \;\to\; \Delta x \downarrow \;\longrightarrow\; N_x \uparrow \;\longrightarrow\;$ Larger system $\downarrow$

$\mathrm{Re}\uparrow \;\to\; \Delta t \downarrow \;\longrightarrow\;$ Better initial guess $\uparrow$

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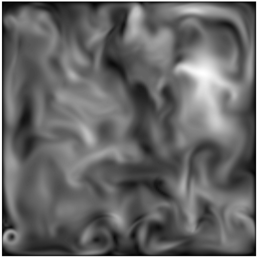
$Ra = 10^8$



[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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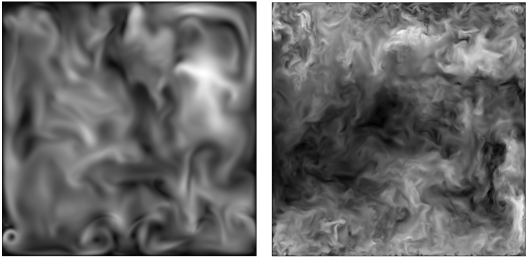
$Ra = 10^8$ $\qquad$ $Ra = 10^{10}$



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Poisson's equation: getting more tough or not?

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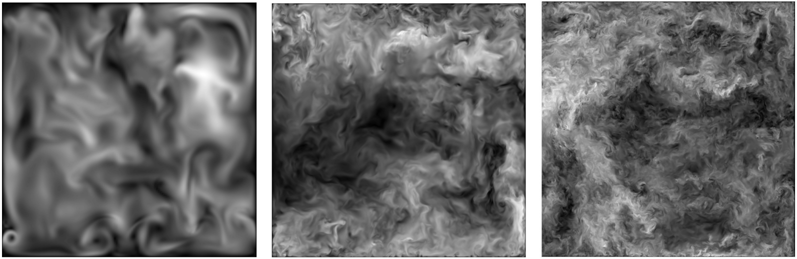
$Ra = 10^8$ $\qquad$ $Ra = 10^{10}$ $\qquad$ $Ra = 10^{11}$



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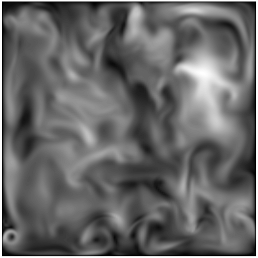
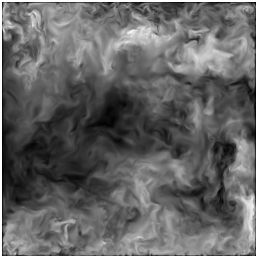
$Ra = 10^8$



$208 \times 208 \times 400$

17.5M

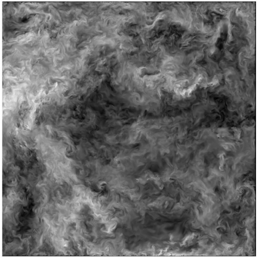
$Ra = 10^{10}$



$768 \times 768 \times 1024$

607M

$Ra = 10^{11}$



$1662 \times 1662 \times 2048$

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?

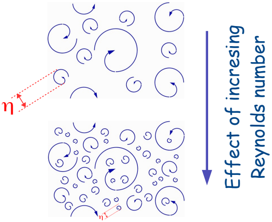
Two competing effects: who (if any) will eventually win?

$$\mathrm{Re}\uparrow \;\rightarrow\; \Delta x \downarrow \;\rightarrow\; N_x \uparrow \;\rightarrow\; \text{Larger system } \downarrow$$

$$\mathrm{Re}\uparrow \;\rightarrow\; \Delta t \downarrow \;\rightarrow\; \text{Better initial guess } \uparrow$$

l: biggest eddies (driving scale)

η: smallest eddies (Kolmogorov length scale)



Question: ?

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

From classical K41 theory:

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

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

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

Smaller and smaller, but how much?

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

$$\mathrm{Re}\uparrow \;\to\; \Delta x \downarrow \;\to\; N_x \uparrow \;\to\; \text{Larger system } \downarrow$$

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From CFL condition:

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

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

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

Smaller and smaller, but how much?

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

$$\mathrm{Re}\uparrow \;\to\; \Delta x\downarrow \;\to\; N_x\uparrow \;\to\; \text{Larger system } \downarrow$$

$$\mathrm{Re}\uparrow \;\to\; \Delta t\downarrow \;\to\; \text{Better initial guess } \uparrow$$

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

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

$$\Big\downarrow \text{ Initial guess } \rightarrow \; p^{n}$$

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

Residual of Poisson's equation

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

$\big\downarrow$ Initial guess $\rightarrow$ p^n

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

Residual of Poisson's equation

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

$\downarrow$ Initial guess $\rightarrow$ p^n

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

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

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

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

Residual of Poisson's equation

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

Initial guess → p^n

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

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

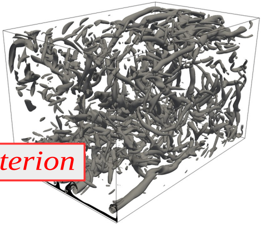
Initial guess → $\tilde{p}^n = \Delta t\, p^n$

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

Residual of Poisson's equation

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

Initial guess → p^n



$Q_G - criterion$

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

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

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

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

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

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

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

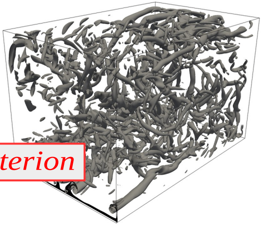
Residual of Poisson's equation

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

Initial guess → p^n

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

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



$Q_G - criterion$

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

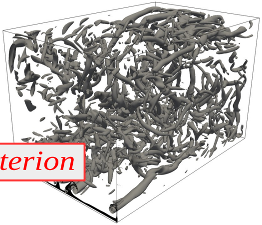
$$Q_G = -\frac{1}{2} tr(G^2) \quad \text{where} \quad G = \nabla u^n$$

Exact equations for restricted Euler:

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

Residual of Poisson's equation

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



$Q_G - criterion$

Initial guess → p^n

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

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

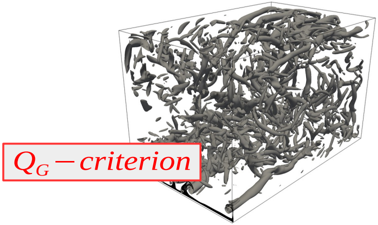
Exact equations for restricted Euler:

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

Residual of Poisson's equation

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

Initial guess → p^n



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

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

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

$$\boxed{\nabla^2 \widetilde{p}^{n+1} = \nabla \cdot \vec{u}^{\,p}}$$

Residual of Poisson's equation in Fourier space

In summary:

$$r^o \approx \frac{\partial \nabla \cdot u^p}{\partial t} = 2\Delta t^p \frac{\partial Q_G}{\partial t} \approx -2\Delta t^p \{(u\cdot\nabla) Q_G + 3 R_G\} \qquad p=\{1,2\}$$

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

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

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

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

Residual of Poisson's equation in Fourier space

In summary:

$$r^o \approx \frac{\partial \nabla \cdot u^p}{\partial t} = 2\Delta t^p \frac{\partial Q_G}{\partial t} \approx -2\Delta t^p \{ (u\cdot\nabla) Q_G + 3 R_G \} \qquad p = \{1, 2\}$$

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Hypothesis:
(inertial range)

$$\left(\frac{\partial \hat{Q}_G}{\partial t} \right)_k \propto k^\beta \longrightarrow \hat{r}^o_k \propto \Delta t^p k^\beta \sim \mathrm{Re}^{p\alpha} k^\beta = \mathrm{Re}^{\tilde{\alpha}} k^\beta$$

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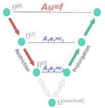

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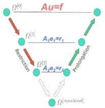

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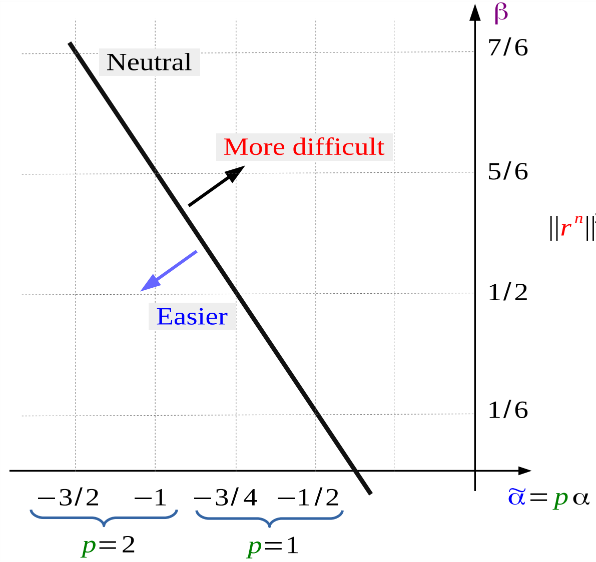
Solver convergence

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



$$\|r^n\|^2 \propto \boxed{\frac{\mathrm{Re}^{2(\tilde{\alpha}+3/4(\beta+1/2))}}{2(2n+1)}}$$

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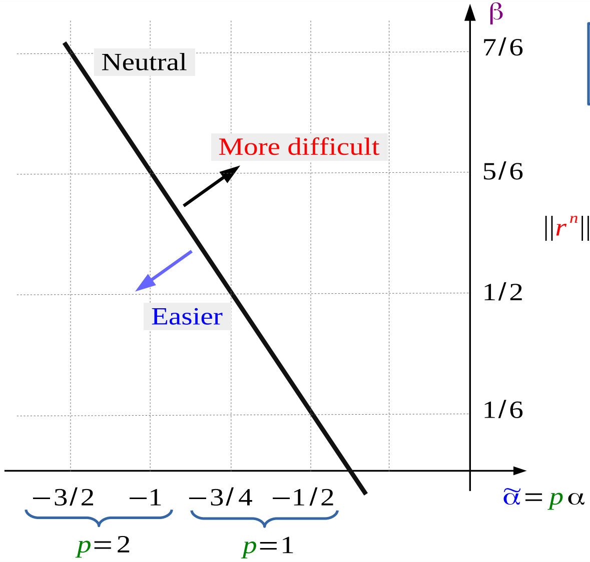

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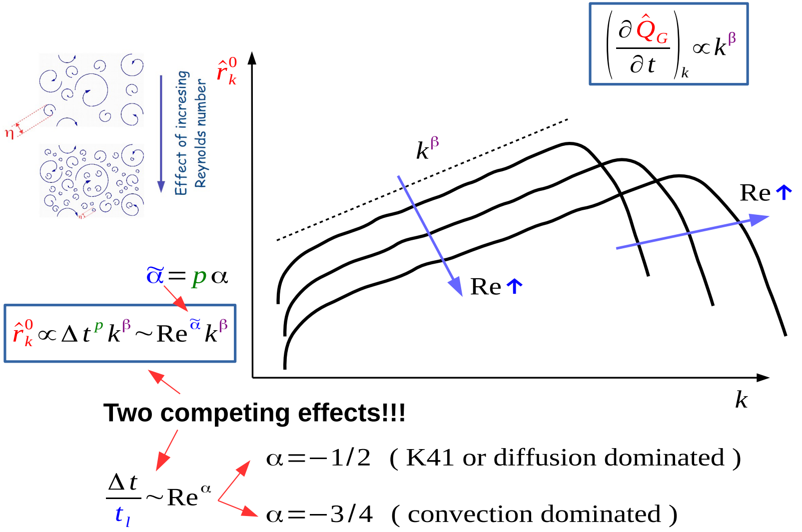

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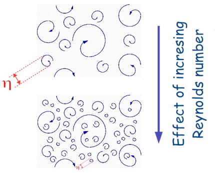

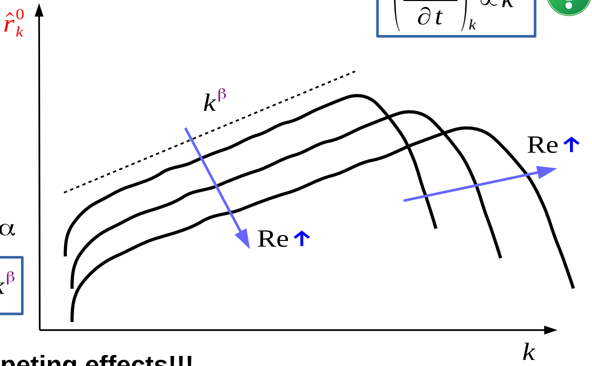

$\tilde{\alpha} = p\,\alpha$

$$\boxed{\hat{r}_k^0 \propto \Delta t^{p} k^{\beta} \sim \mathrm{Re}^{\tilde{\alpha}} k^{\beta}}$$

Two competing effects!!!

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

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

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Homogeneous isotropic turbulence

Kolmogorov theory predictions

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

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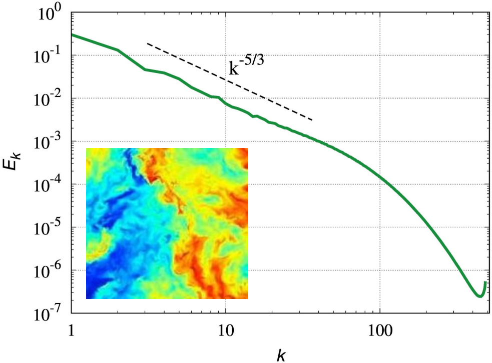

$\mathrm{Re}_\lambda \approx 433 \ (1024^3)$ from https://turbulence.pha.jhu.edu/

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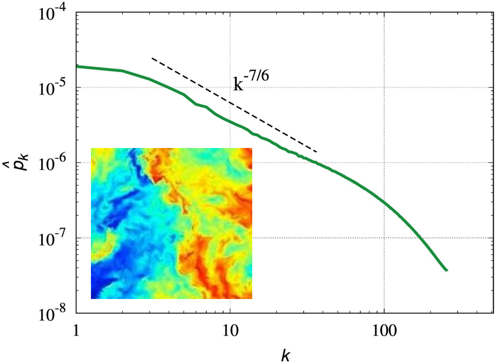

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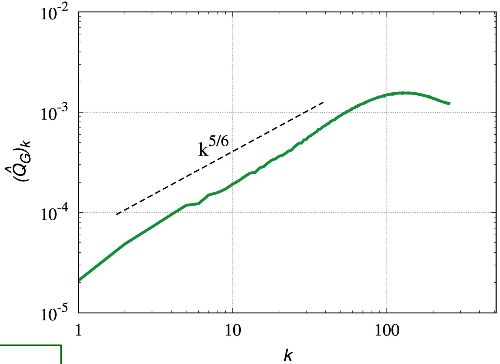

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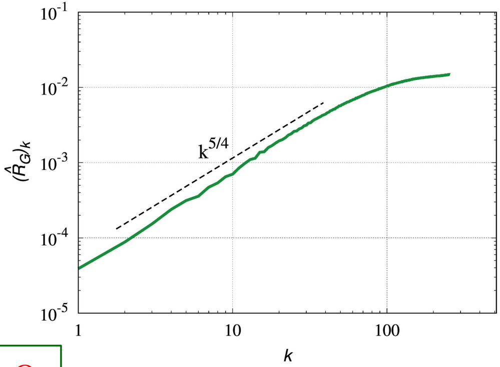

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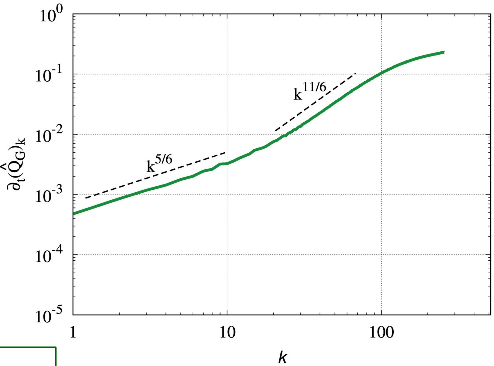

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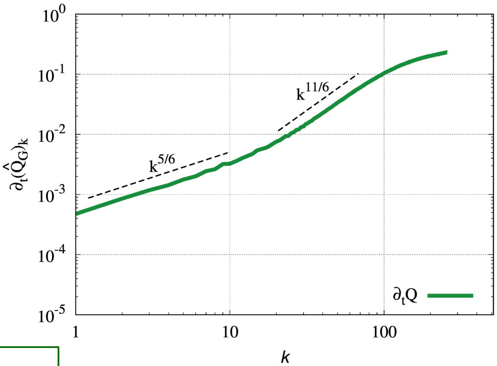

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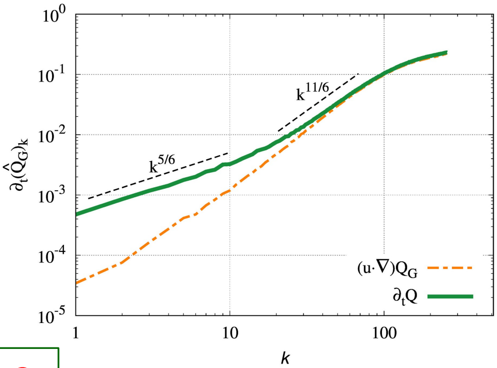

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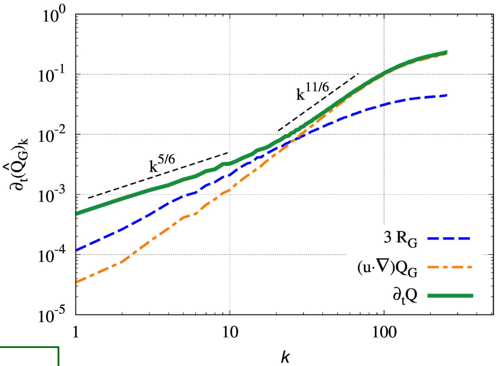

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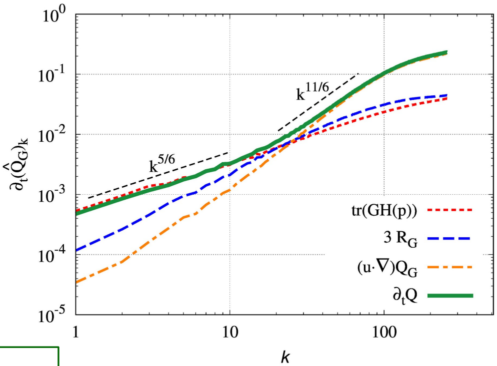

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- **Two competing effects** on the convergence of Poisson's equation have been identified.

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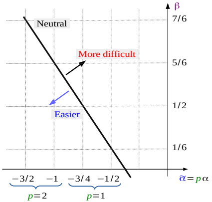

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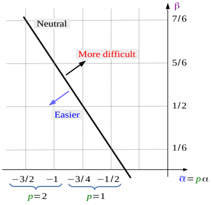

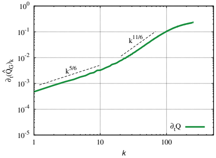

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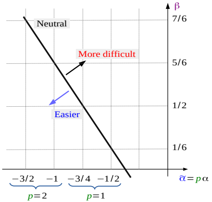

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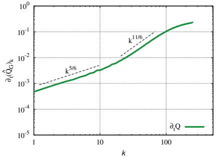

On-going research:

- Extend the analysis up to $Re_\lambda \approx 1200$ using 8192^3 nodes
- Analysis of more complex flows

Thank you for your attendance