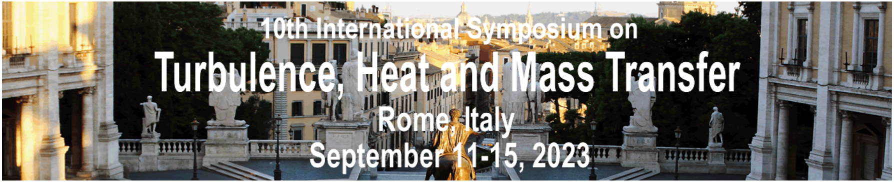
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

termofluids

Exa, zetta, yotta and beyond

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

[1]Heat and Mass Transfer Technological Center, Technical University of Catalonia
[2]Termo Fluids S.L. Carrer de Magí Colet 8, 08204 Sabadell (Barcelona), Spain



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Exa, zetta, yotta and beyond: On the evolution of Poisson solvers for extreme-scale simulations

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

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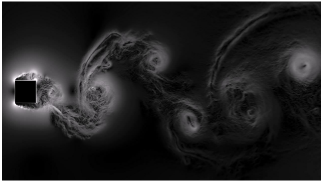
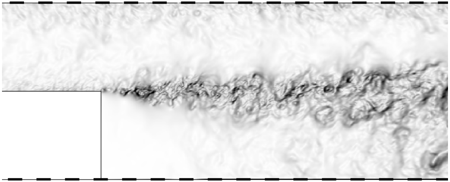


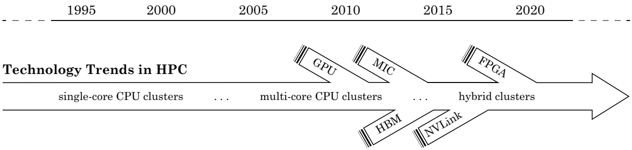


Contents

Motivation

Research question #1:

- How can we develop **portable** and **efficient** CFD codes for large-scale simulations on modern supercomputers?



[1] X.Álvarez, A.Gorobets, F.X.Trias. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers*. **Computers & Fluids**, 214:104768, 2021.

[2] À.Alsalti-Baldellou, X.Álvarez-Farré, F.X.Trias, A.Oliva. *Exploiting spatial symmetries for solving Poisson's equation*. **Journal of Computational Physics**, 486:112133, 2023.

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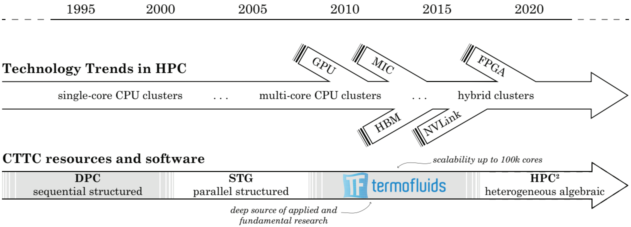
- How can we develop **portable** and **efficient** CFD codes for large-scale simulations on modern supercomputers?



HPC^2: portable, algebra-based framework for heterogeneous computing is being developed[1]. Traditional stencil-based data and sweeps are replaced by algebraic structures (sparse matrices and vectors) and kernels. SpMM-based strategies to increase the arithmetic intensity are being considered[2].

[1] X.Álvarez, A.Gorobets, F.X.Trias. *A hierarchical parallel implementation for heterogeneous computing. Application to algebra-based CFD simulations on hybrid supercomputers*. **Computers & Fluids**, 214:104768, 2021.

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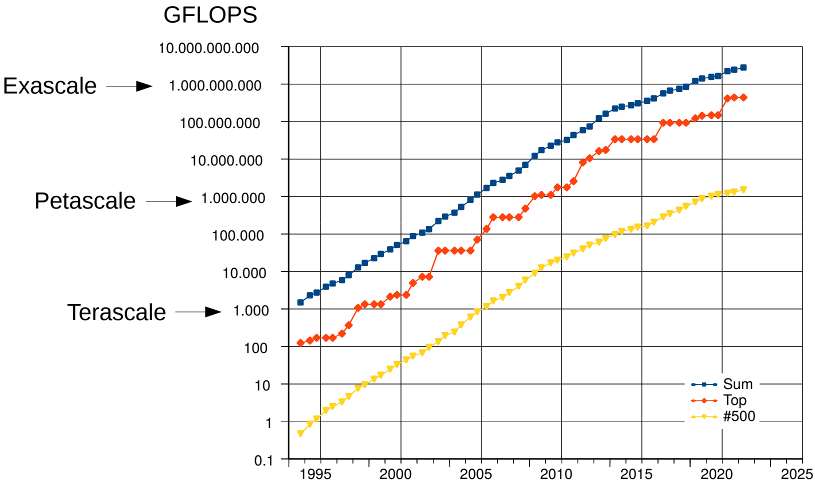
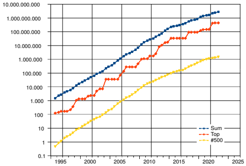
Tera, Peta, Exa,..., Zetta, Yotta



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

~10 years

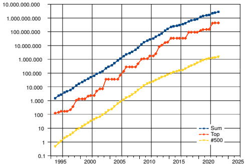
	PetaFLOPS		#1 in LINPACK	#1 in HPCG	Cutting-edge CFD simulation	'Routine' CFD simulation
Zetta	10^6					
Exa	10^3	14 years	**2022** (Frontier)			
Peta	1		**2008** (Roadrunner)	**2018** (Summit)		
Tera	10^{-3}	11 years	**1997** (ASCI Red)	No data		



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

~10 years →

	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**		
Peta	1		**2008** (Roadrunner)	**2018** (Summit)		
Tera	10^{-3}	11 years ↑	**1997** (ASCI Red)	No data		



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**	
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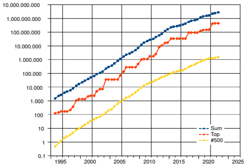
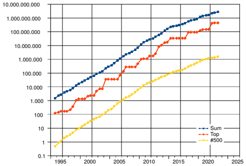
Peta	1	↑ 11 years	**2008** (Roadrunner)	**2018** (Summit)	**2023**	
Tera	10^{-3}		**1997** (ASCI Red)	No data		



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

~10 years → ~5 years → ~10 years

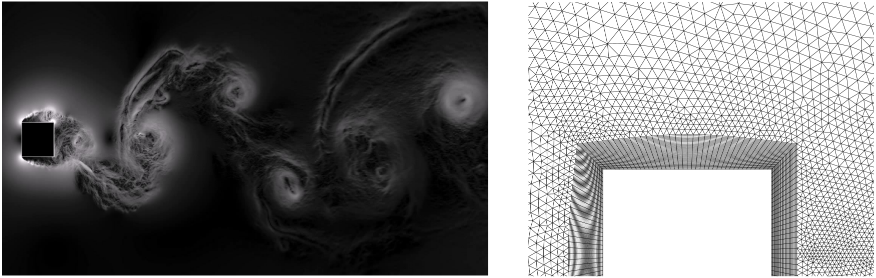
	PetaFLOPS		#1 in LINPACK	#1 in HPCG	Cutting-edge CFD simulation	'Routine' CFD simulation
Zetta	10^6		**2037**	**2047**	**2052**	**2062**
Exa	10^3	**14 years** ↑	**2022** (Frontier)	**2032**	**2037**	**2047**
Peta	1		**2008** (Roadrunner)	**2018** (Summit)	**2023**	**2033**
Tera	10^{-3}	**11 years** ↑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



Motivation

Research question #2:

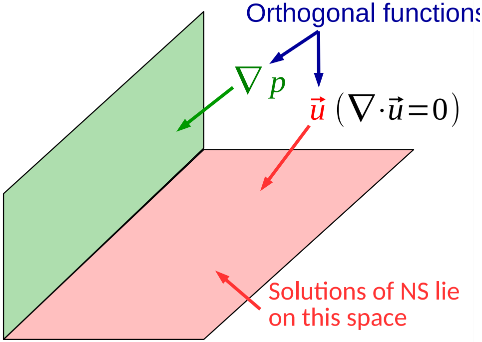
- Will the **complexity** of numerically solving **Poisson's equation** increase or decrease for **very large scale DNS/LES** simulations of incompressible turbulent flows?



DNS[3] of the turbulent flow around a square cylinder at $Re = 22000$

[3] F.X.Trias, A.Gorobets, A.Oliva. *Turbulent flow around a square cylinder at Reynolds number 22000: a DNS study*, **Computers&Fluids**, 123:87-98, 2015.

Poisson's equation: a quick reminder

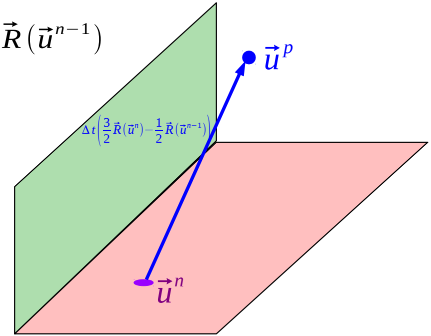


Semi-discrete (just in time) NS equations

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

Poisson's equation: a quick reminder

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



Semi-discrete (just in time) NS equations

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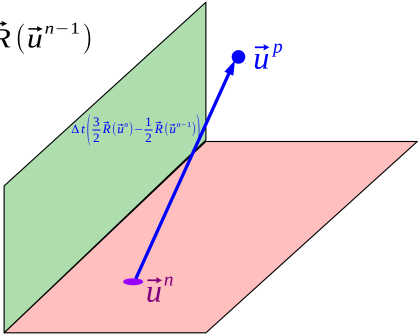
Step 2: $\nabla^{2}p^{n+1}=\dfrac{1}{\Delta t}\nabla\cdot\vec{u}^{p}$



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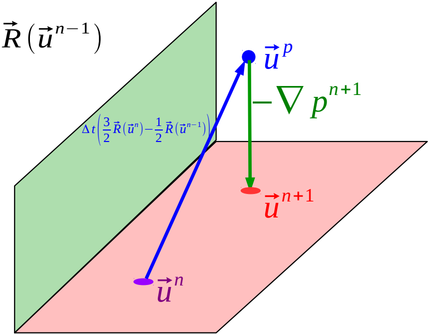
Step 3: $\vec{u}^{n+1}=\vec{u}^{p}-\Delta t\,\nabla p^{n+1}$



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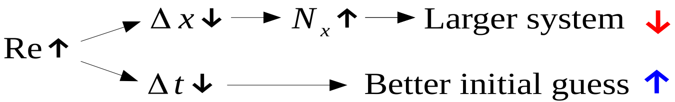
Poisson's equation: getting more tough or not?

Research question #2:

- 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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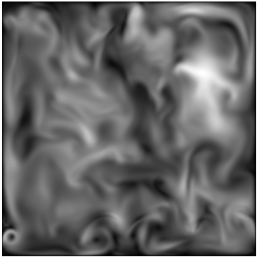
$Ra = 10^8$



[4] 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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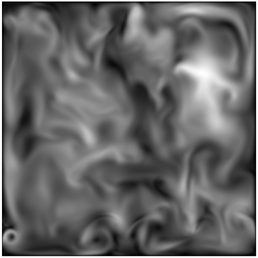
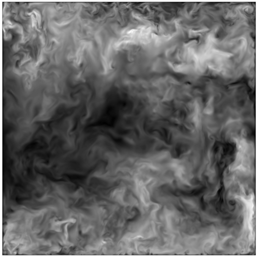


$Ra = 10^{10}$



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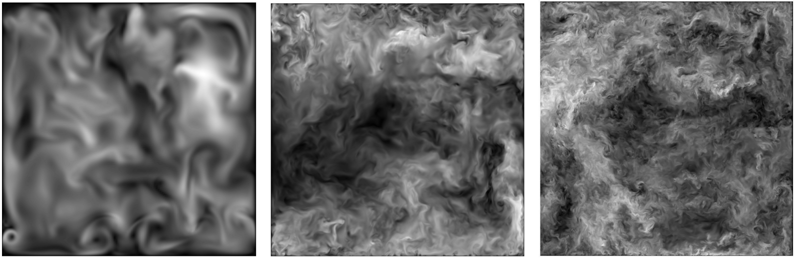
PRACE

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



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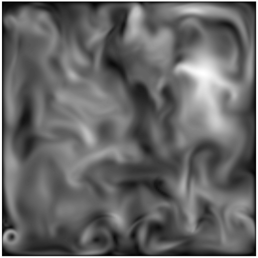
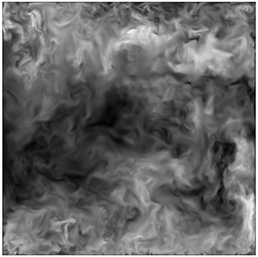


$208 \times 208 \times 400$

17.5M

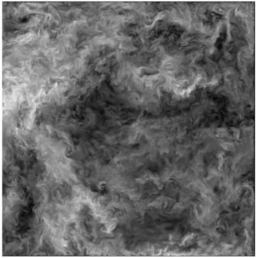
$Ra = 10^{10}$



$768 \times 768 \times 1024$

607M

$Ra = 10^{11}$



$1662 \times 1662 \times 2048$

5600M

[4] 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?

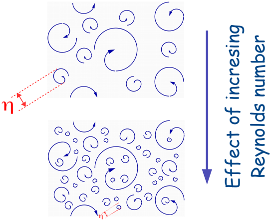
Two competing effects: who (if any) will eventually win?

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

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

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?

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

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

From classical K41 theory:

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

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?

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

$\mathrm{Re}\uparrow \rightarrow \Delta t \downarrow \rightarrow$ 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

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

Initial guess → p^n

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

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

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

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

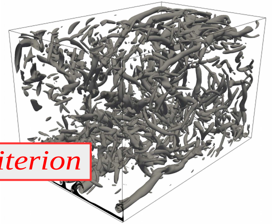
Initial guess → $\tilde{p}^n = \Delta t \, p^n$

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

Residual of Poisson's equation

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

Initial guess → p^n



$Q_G - criterion$

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

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

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

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

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

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

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

S.B.Pope, 2000.

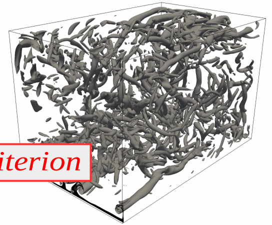
Residual of Poisson's equation

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

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:

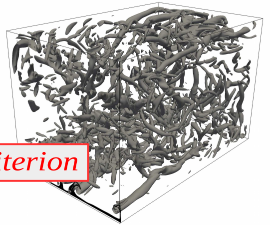
$$\frac{dQ_G}{dt} = -3R_G \longrightarrow \frac{\partial Q_G}{\partial t} = -(u \cdot \nabla) Q_G - 3R_G$$

S.B.Pope, 2000.

Residual of Poisson's equation

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

Initial guess → p^n



$Q_G - criterion$

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

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

Exact equations for restricted Euler:

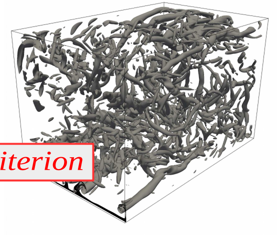
$$\frac{d Q_G}{dt} = -3 R_G \longrightarrow \frac{\partial Q_G}{\partial t} = -(u \cdot \nabla) Q_G - 3 R_G$$

S.B.Pope, 2000.

Residual of Poisson's equation

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

Initial guess → p^n



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Residual of Poisson's equation in Fourier space

In summary:

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

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

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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

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

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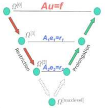

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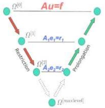

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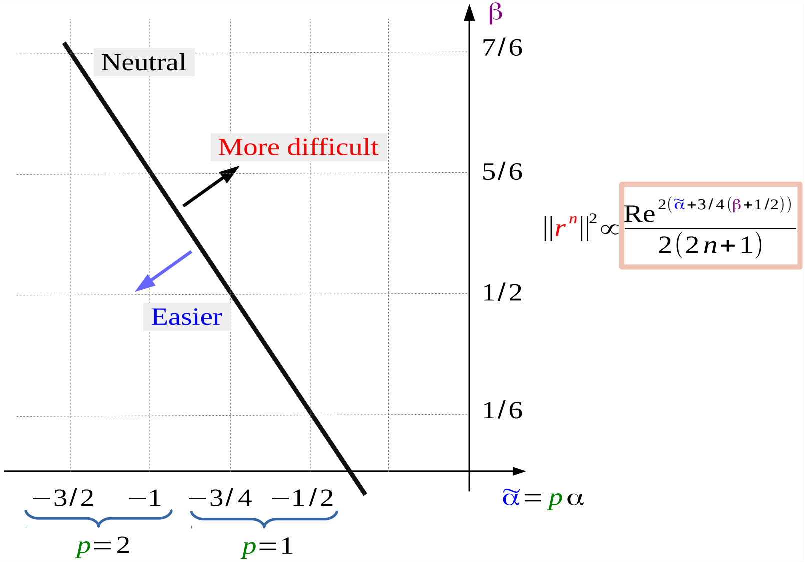
$\{\tilde{\alpha}, \beta\}$ phase space



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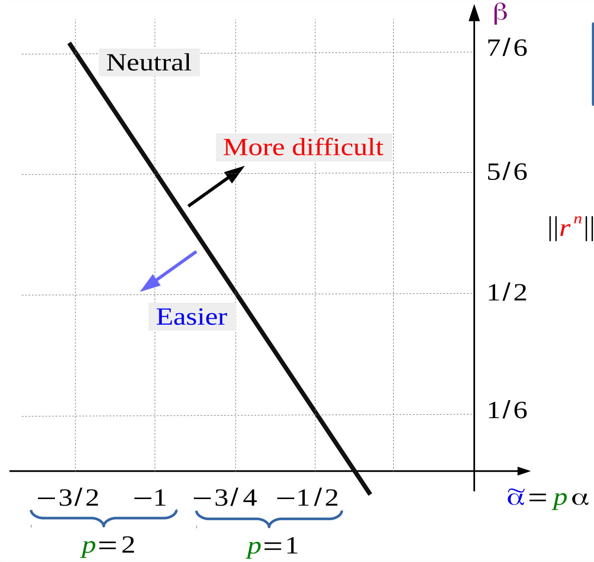

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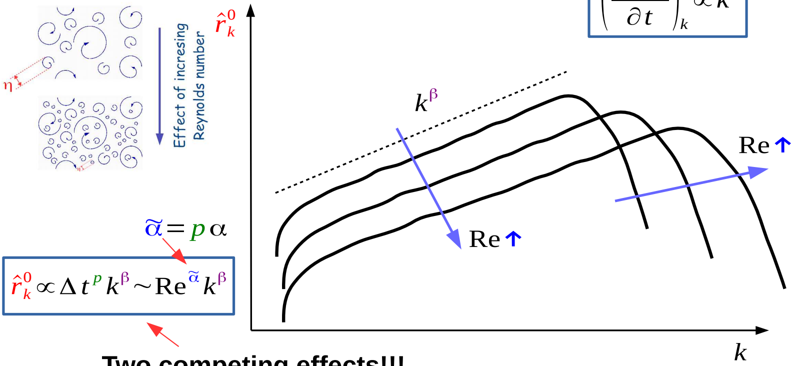

$$\tilde{\alpha} = p\,\alpha$$

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

Two competing effects!!!

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

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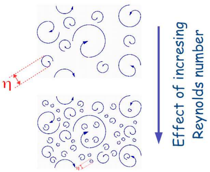

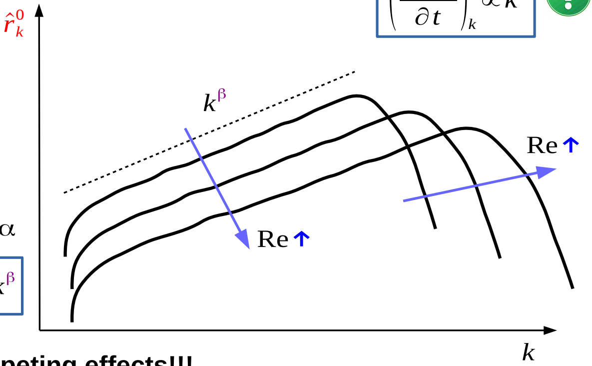

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Kolmogorov theory predictions

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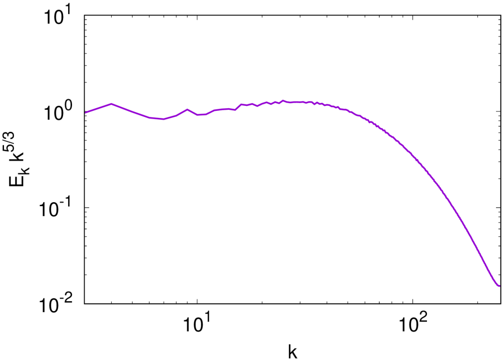

SpNS: pseudo-spectral CFD code publicly available at `https://github.com/adalbal/SpNS`.

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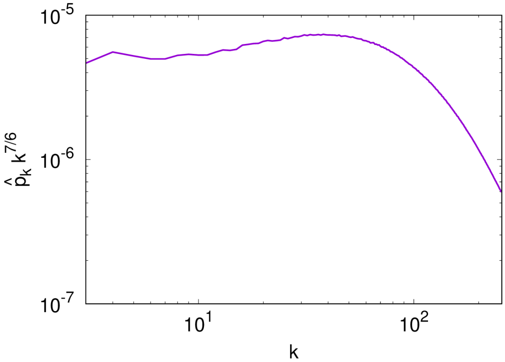

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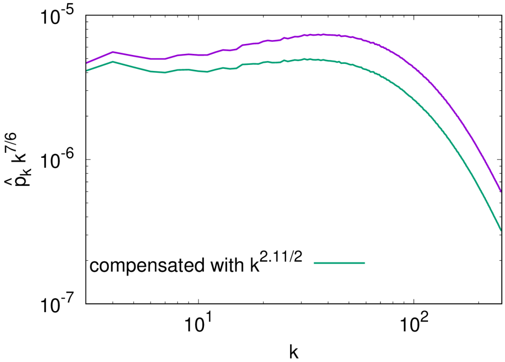

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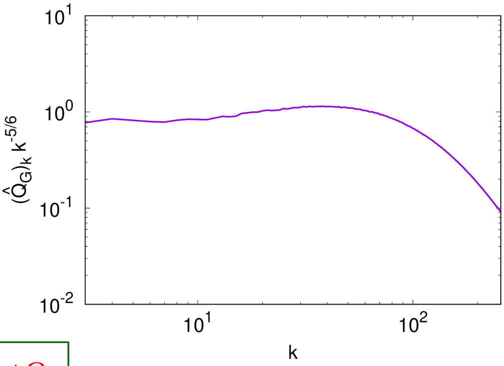

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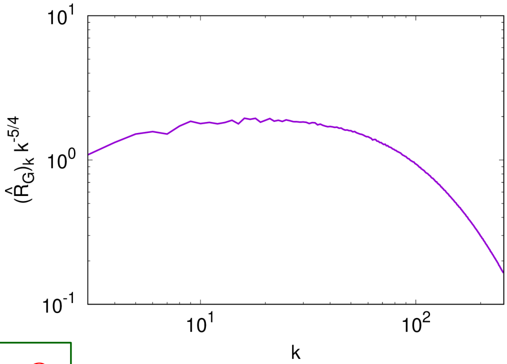

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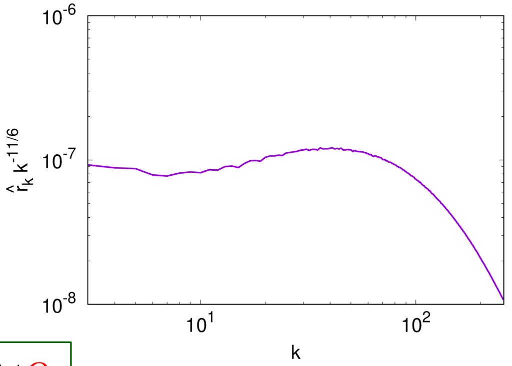

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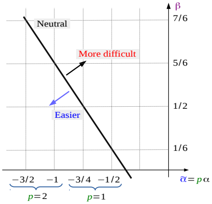

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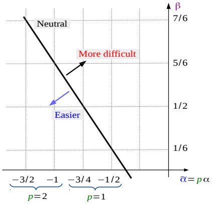

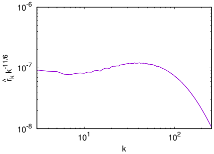

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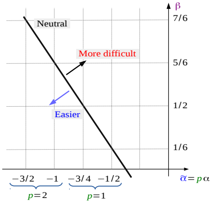

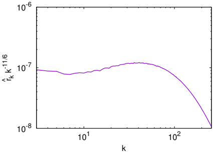

On-going and near future research:

- Carrying out simulations at higher Re_λ
- Extending the analysis to more complex flows

Thank you for your attendance