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Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

A stable regularization of the gradient model

F.Xavier Trias[1], Andrey Gorobets[2], Assensi Oliva[1]

[1]Heat and Mass Transfer Technological Center, Technical University of Catalonia
[2]Keldysh Institute of Applied Mathematics of RAS, Russia

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Direct & Large Eddy Simulation
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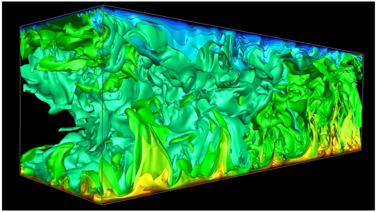
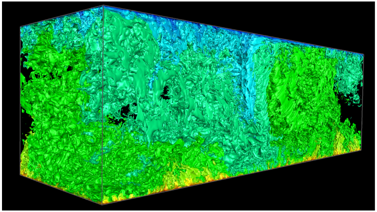


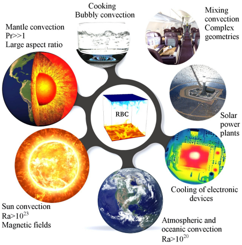


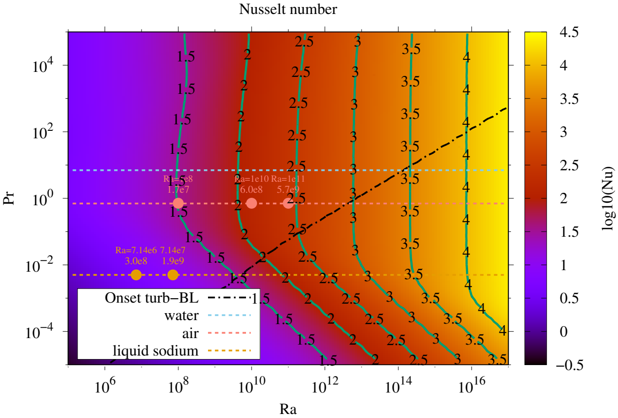
Contents

Motivation

General research question:

- Can we hit the ultimate regime of thermal turbulence ?

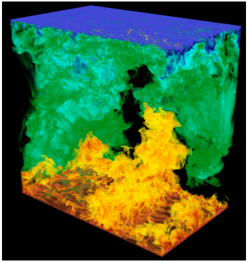


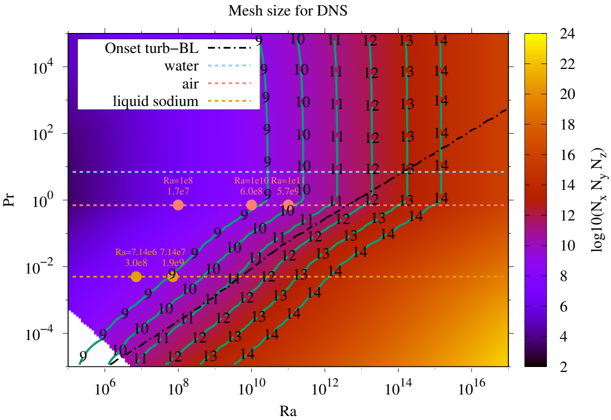


Motivation

General research question:

- Can we hit the ultimate regime of thermal turbulence with **DNS**?

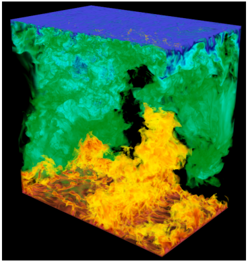


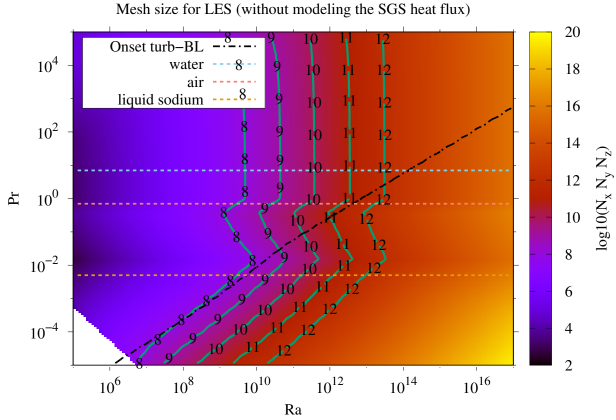


Motivation

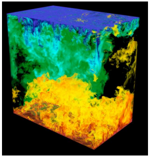
General research question:

- Can we hit the ultimate regime of thermal turbulence with **LES**?



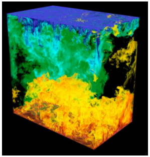


Motivation



DNS {

Motivation



HAWK	MareNostrum 4	Marconi100
		
Rank #27 5,632 nodes with: 2 AMD EPYC 7742 (64 cores each)	Rank #82 3456 nodes with: 2x Intel Xeon 8160 1x Intel Omni-Path	Rank #21 980 nodes with: 2 IBM Power9 4 NVIDIA Volta V100

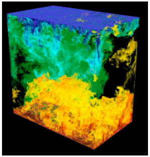
PRACE

intel XEON PLATINUM inside

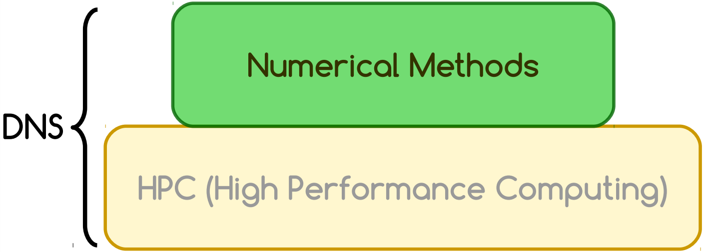
DNS {

HPC (High Performance Computing)

Motivation

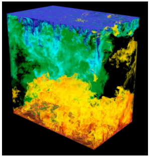


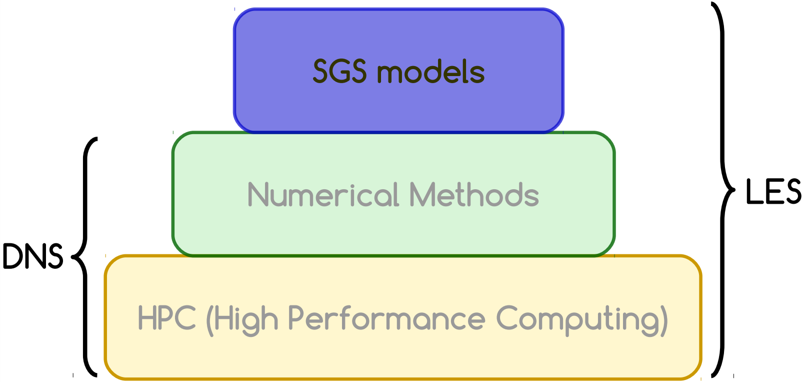
How to properly discretize NS?



Motivation

How to properly model SGS?





How to model the subgrid heat flux in LES?

$$\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} = \nu \nabla^2 \overline{\boldsymbol{u}} - \nabla \overline{p} \qquad - \nabla \cdot \tau(\overline{\boldsymbol{u}}) \; ; \qquad \nabla \cdot \overline{\boldsymbol{u}} = 0$$

$$\text{eddy-viscosity} \;\longrightarrow\; \tau\,(\overline{u}) = -2\nu_t S(\overline{u})$$

$$\boxed{\nu_t \approx (C_m \delta)^2 D_m(\overline{\boldsymbol{u}})} \;\longrightarrow\; \{\text{WALE, Vreman, QR, Sigma, S3PQR,...}\}$$

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$$G \equiv \nabla \overline{\boldsymbol{u}} \qquad\qquad \boldsymbol{q} = -\frac{\delta^2}{12} G \nabla \overline{T} + \mathcal{O}(\delta^4)$$

A priori alignment trends[1]

$$\text{eddy-diffusivity} \longrightarrow \boldsymbol{q} \approx -\alpha_t \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{eddy})$$

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[1] F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 29:105103, 2017.

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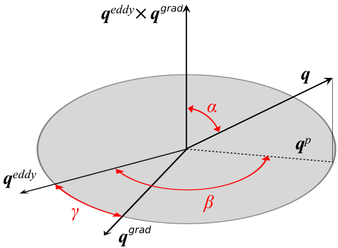

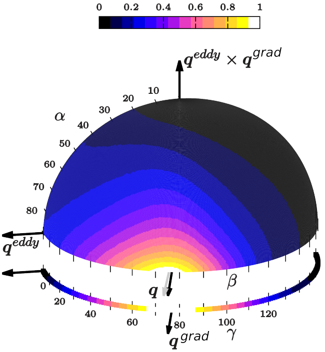

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[2] S.Peng and L.Davidson. **Int.J.Heat Mass Transfer**, 45:1393-1405, 2002.

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Peng&Davidson[2] $\longrightarrow$ $\boldsymbol{q} \approx -\frac{\delta^2}{12} S \nabla \overline{T} \quad (\equiv \boldsymbol{q}^{PD})$

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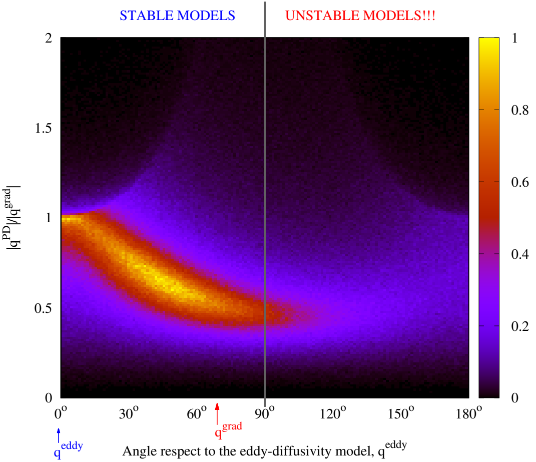
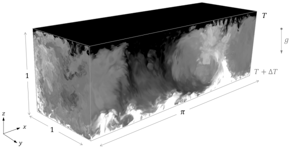
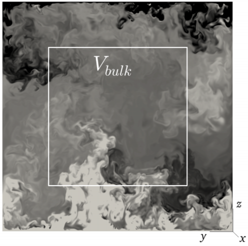
A priori alignment trends

$$\boldsymbol{q}^{grad} \equiv -\frac{\delta^2}{12} G \nabla \overline{T} \qquad \boxed{\boldsymbol{q}^{PD} \equiv -\frac{\delta^2}{12} S \nabla \overline{T}}$$







How to model the subgrid heat flux in LES?

$$\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}} \cdot \nabla)\overline{\boldsymbol{u}} = \nu \nabla^2 \overline{\boldsymbol{u}} - \nabla \overline{p} + \overline{\boldsymbol{f}} - \nabla \cdot \tau(\overline{\boldsymbol{u}}) \quad ; \quad \nabla \cdot \overline{\boldsymbol{u}} = 0$$

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Deconstructing the gradient model

Research question #1:

- Can we implement the gradient model **re-using discrete operators** in such a way that we **avoid unnecessary interpolations**?

$$\text{gradient model} \quad \longrightarrow \quad \boldsymbol{q} \approx -\frac{\delta^2}{12} \nabla \overline{\boldsymbol{u}} \nabla \overline{T} \qquad (\equiv \boldsymbol{q}^{grad})$$

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Continuous	Discrete
$\dfrac{\partial \boldsymbol{u}}{\partial t} + C(\boldsymbol{u}, \boldsymbol{u}) = \nu \nabla^2 \boldsymbol{u} - \nabla p$	$\Omega \dfrac{d\boldsymbol{u}_h}{dt} + \mathsf{C}(\boldsymbol{u}_h)\boldsymbol{u}_h = \mathsf{D}\boldsymbol{u}_h - \mathsf{G}\boldsymbol{p}_h$
$\nabla \cdot \boldsymbol{u} = 0$	$\mathsf{M}\boldsymbol{u}_h = \boldsymbol{0}_h$

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Continuous	Discrete
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$\nabla\cdot\boldsymbol{u} = 0$	$\mathsf{M}\boldsymbol{u}_h = \boldsymbol{0}_h$
$\langle C(\boldsymbol{u},\varphi_1),\varphi_2\rangle = -\langle C(\boldsymbol{u},\varphi_2),\varphi_1\rangle$	$\mathsf{C}(\boldsymbol{u}_h) = -\mathsf{C}^T(\boldsymbol{u}_h)$

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Deconstructing the gradient model

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$\left\langle\nabla^2\boldsymbol{a},\boldsymbol{b}\right\rangle = \left\langle\boldsymbol{a},\nabla^2\boldsymbol{b}\right\rangle$	$\mathsf{D} = \mathsf{D}^T \quad def -$

Deconstructing the gradient model

Continuous

$$\boldsymbol{q}^{grad} = -\frac{\delta^2}{12}\nabla \boldsymbol{u} \nabla T$$

Discrete

????

Deconstructing the gradient model

Continuous	Discrete
$\boldsymbol{q}^{grad} = -\frac{\delta^2}{12}\nabla \boldsymbol{u} \nabla T$	????
$-\nabla \cdot \boldsymbol{q}^{grad} =$	

Deconstructing the gradient model

Continuous	Discrete
$\boldsymbol{q}^{grad} = -\frac{\delta^2}{12}\nabla \boldsymbol{u} \nabla T$	????
$-\nabla \cdot \boldsymbol{q}^{grad} =$	

$$C(\boldsymbol{u}, T) - \widetilde{C(\boldsymbol{u}, T)} = \frac{\tilde{\delta}^2}{24}\nabla^2 \nabla \cdot (\boldsymbol{u} T) = \frac{\tilde{\delta}^2}{24}\nabla \cdot \nabla^2 (\boldsymbol{u} T)$$

$$C(\boldsymbol{u}, T) - C(\tilde{\boldsymbol{u}}, T) = \frac{\tilde{\delta}^2}{24}\nabla \cdot ((\nabla^2 \boldsymbol{u}) T)$$

$$C(\boldsymbol{u}, T) - C(\boldsymbol{u}, \widetilde{T}) = \frac{\tilde{\delta}^2}{24}\nabla \cdot (\boldsymbol{u} \nabla^2 T)$$

Deconstructing the gradient model

Continuous	Discrete

$$\boldsymbol{q}^{grad} = -\frac{\delta^2}{12}\nabla\boldsymbol{u}\nabla T$$

????

$$-\nabla\cdot\boldsymbol{q}^{grad} = C(\boldsymbol{u},T) + \widetilde{C(\boldsymbol{u},T)} - C(\tilde{\boldsymbol{u}},T) - C(\boldsymbol{u},\tilde{T})$$

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Deconstructing the gradient model

Continuous

$$\boldsymbol{q}^{grad} = -\frac{\delta^2}{12}\nabla\boldsymbol{u}\nabla T$$

$$-\nabla\cdot\boldsymbol{q}^{grad} = C(\boldsymbol{u},T) + \widetilde{C(\boldsymbol{u},T)} - C(\tilde{\boldsymbol{u}},T) - C(\boldsymbol{u},\tilde{T})$$

Discrete

????

$$-\mathrm{M}\boldsymbol{q}_h^{grad} = \mathrm{C}(\boldsymbol{u}_h)T_h + \mathrm{F}\mathrm{C}(\boldsymbol{u}_h)T_h - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h)T_h - \mathrm{C}(\boldsymbol{u}_h)\mathrm{F}T_h$$

$$C(\boldsymbol{u},T) - \widetilde{C(\boldsymbol{u},T)} = \frac{\tilde{\delta}^2}{24}\nabla^2\nabla\cdot(\boldsymbol{u}T) = \frac{\tilde{\delta}^2}{24}\nabla\cdot\nabla^2(\boldsymbol{u}T)$$

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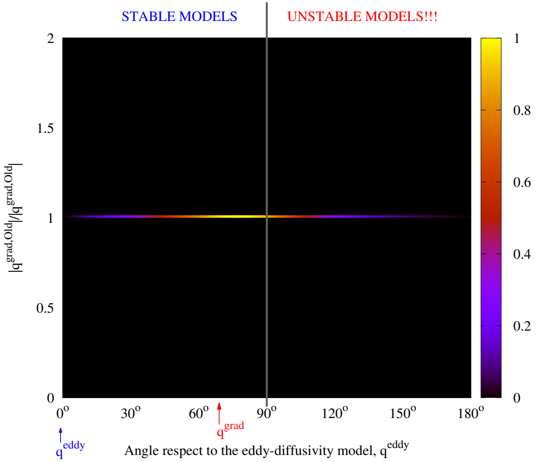
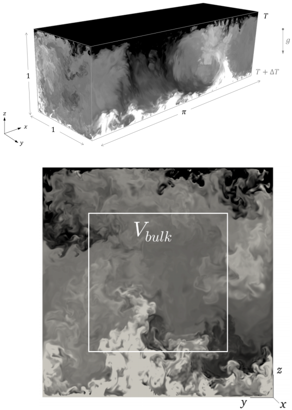
Deconstructing the gradient model

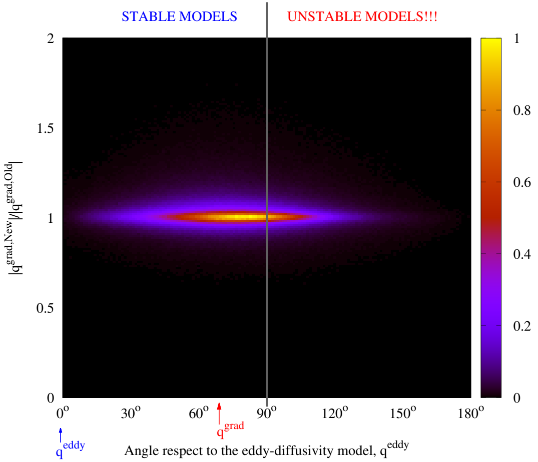
$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h + \mathsf{F}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h - \mathsf{C}(\boldsymbol{u}_h)\mathsf{F}T_h$$

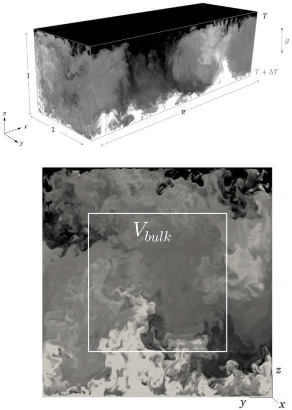




Deconstructing the gradient model

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h + \mathsf{F}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h - \mathsf{C}(\boldsymbol{u}_h)\mathsf{F}T_h$$





Deconstructing the gradient model

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h + \mathsf{F}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h - \mathsf{C}(\boldsymbol{u}_h)\mathsf{F}T_h$$

Deconstructing the gradient model

$$\boxed{-\mathrm{M}\boldsymbol{q}_h^{grad} = \mathrm{C}(\boldsymbol{u}_h)T_h + \mathrm{F}\mathrm{C}(\boldsymbol{u}_h)T_h - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h)T_h - \mathrm{C}(\boldsymbol{u}_h)\mathrm{F}T_h}$$

$$-\mathrm{M}\boldsymbol{q}_h^{grad} = \begin{pmatrix} \mathrm{I} \\ \mathrm{F} \end{pmatrix}^T \begin{pmatrix} \mathrm{C}(\boldsymbol{u}_h) - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h) & \boxed{-\mathrm{C}(\boldsymbol{u}_h)} \\ \boxed{\mathrm{C}(\boldsymbol{u}_h)} & 0 \end{pmatrix} \begin{pmatrix} \mathrm{I} \\ \mathrm{F} \end{pmatrix} T_h$$

Deconstructing the gradient model

$$\boxed{-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}(\boldsymbol{u}_h)\mathsf{R}T_h}$$

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}(\boldsymbol{u}_h) - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h) & \boxed{-\mathsf{C}(\boldsymbol{u}_h)} \\ \boxed{\mathsf{C}(\boldsymbol{u}_h)} & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix} T_h$$

Alternatively, it can expressed as follows

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{R} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}(\boldsymbol{u}_h) - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h) & \boxed{\mathsf{C}(\boldsymbol{u}_h)} \\ \boxed{-\mathsf{C}(\boldsymbol{u}_h)} & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{R} \end{pmatrix} T_h$$

where $\mathsf{F} = \mathsf{I} - \mathsf{R}$.

Deconstructing the gradient model

$$\boxed{-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}(\boldsymbol{u}_h)\mathsf{R}\,T_h}$$

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}(\boldsymbol{u}_h) - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h) & \boxed{-\mathsf{C}(\boldsymbol{u}_h)} \\ \boxed{\mathsf{C}(\boldsymbol{u}_h)} & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix} T_h$$

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where $\mathsf{F} = \mathsf{I} - \mathsf{R}$. Recalling that $\mathsf{C} = -\mathsf{C}^T$ and $\mathsf{F} = \mathsf{F}^T$, leads to

$$-T_h \cdot \mathsf{M}\boldsymbol{q}_h^{grad} = T_h \cdot (\mathsf{R}\mathsf{C} - \mathsf{C}\mathsf{R})\,T_h$$

Deconstructing the gradient model

$$\boxed{-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}(\boldsymbol{u}_h)\mathsf{R}T_h}$$

Stability is determined by the sign of the Rayleigh quotient of $\mathsf{RC} - \mathsf{CR}$

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix}^T \begin{pmatrix} \mathsf{C}(\boldsymbol{u}_h) - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h) & \boxed{-\mathsf{C}(\boldsymbol{u}_h)} \\ \boxed{\mathsf{C}(\boldsymbol{u}_h)} & 0 \end{pmatrix} \begin{pmatrix} \mathsf{I} \\ \mathsf{F} \end{pmatrix} T_h$$

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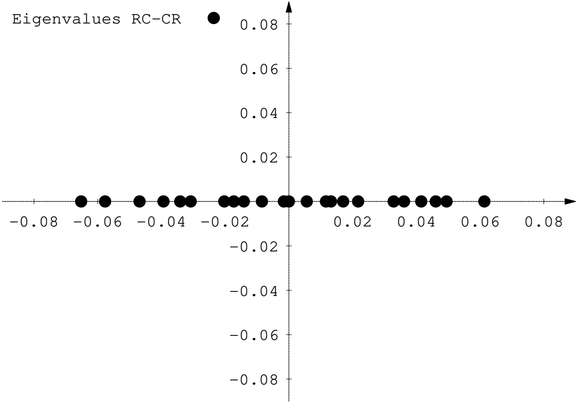
$$-T_h \cdot \mathsf{M}\boldsymbol{q}_h^{grad} = T_h \cdot (\mathsf{RC} - \mathsf{CR})T_h$$

Stabilizing the gradient model

$$-\mathrm{M}\boldsymbol{q}_h^{grad} = \mathrm{C}(\boldsymbol{u}_h)T_h - \mathrm{RC}\quad(\boldsymbol{u}_h)T_h - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h)T_h + \mathrm{C}\quad(\boldsymbol{u}_h)\mathrm{R}T_h$$

Stability is determined by the sign of the Rayleigh quotient of RC − CR

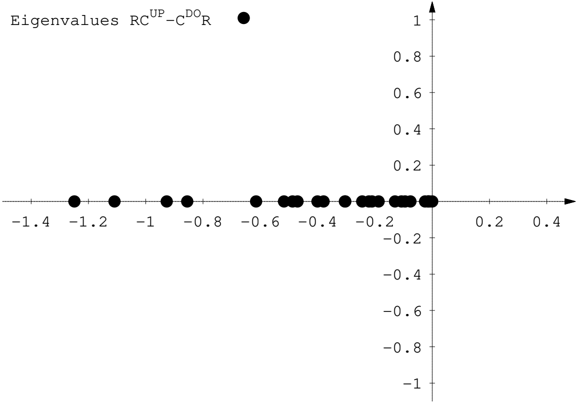


RC − CR

Stabilizing the gradient model

$$-\mathrm{M}\boldsymbol{q}_h^{grad} = \mathrm{C}(\boldsymbol{u}_h)\,T_h - \mathrm{R}\mathrm{C}^{\mathrm{UP}}(\boldsymbol{u}_h)\,T_h - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h)\,T_h + \mathrm{C}^{DO}(\boldsymbol{u}_h)\mathrm{R}\,T_h$$

Stability is determined by the sign of the Rayleigh quotient of $\mathrm{RC} - \mathrm{CR}$

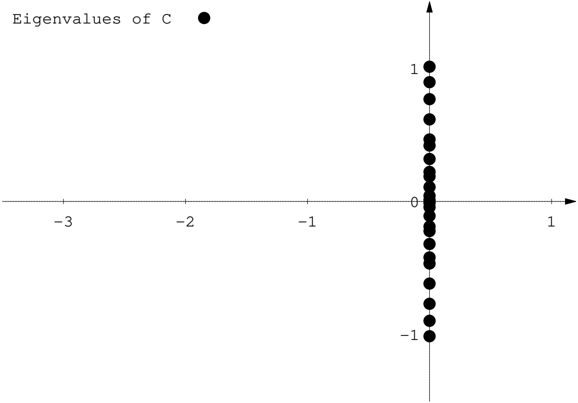


Idea: $\mathrm{RC}^{\mathrm{UP}} - \mathrm{C}^{\mathrm{DO}}\mathrm{R}$ instead of $\mathrm{RC} - \mathrm{CR}$ guarantees stability

Stabilizing the gradient model

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}^{\mathsf{UP}}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}^{DO}(\boldsymbol{u}_h)\mathsf{R}T_h$$

Stability is determined by the sign of the Rayleigh quotient of $\mathsf{RC} - \mathsf{CR}$



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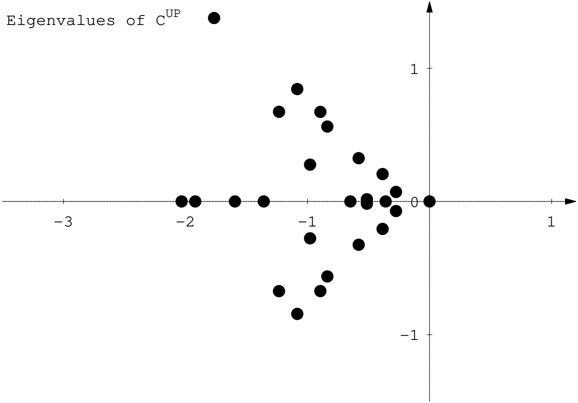
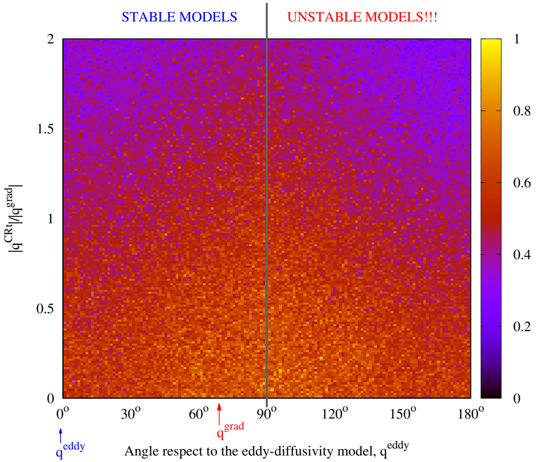
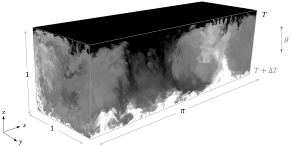


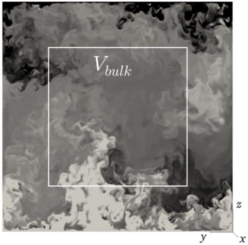
Idea: $\mathsf{RC}^{\mathsf{UP}} - \mathsf{C}^{\mathsf{DO}}\mathsf{R}$ instead of $\mathsf{RC} - \mathsf{CR}$ guarantees stability

Stabilizing the gradient model

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h \boxed{-\mathsf{R}\mathsf{C}\quad(\boldsymbol{u}_h)T_h} - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h \boxed{+\mathsf{C}\quad(\boldsymbol{u}_h)\mathsf{R}T_h}$$

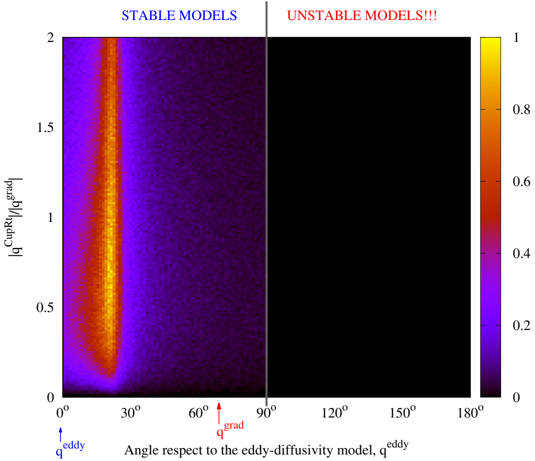


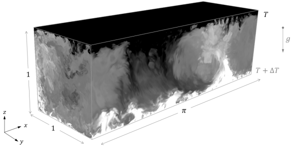


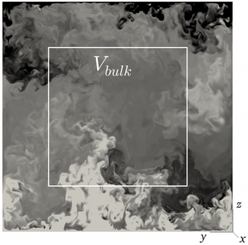


Stabilizing the gradient model

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h \boxed{-\mathsf{R}\mathsf{C}^{UP}(\boldsymbol{u}_h)T_h} - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h \boxed{+\mathsf{C}^{DO}(\boldsymbol{u}_h)\mathsf{R}T_h}$$







Concluding remarks

- A new way to implement the gradient model has been proposed ✓

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}(\boldsymbol{u}_h)\mathsf{R}T_h$$

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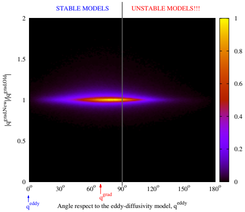
- Good *a priori* alignment trends ✓



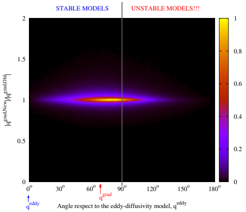
Concluding remarks

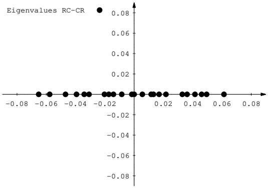
- A new way to implement the gradient model has been proposed ✓

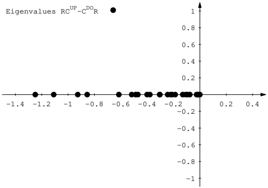
$$-\mathrm{M}\boldsymbol{q}_h^{grad} = \mathrm{C}(\boldsymbol{u}_h)T_h - \mathrm{RC}(\boldsymbol{u}_h)T_h - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h)T_h + \mathrm{C}(\boldsymbol{u}_h)\mathrm{R}T_h$$

- Good *a priori* alignment trends ✓
- Stabilization has been proposed and tested ✓

$$-\mathrm{M}\boldsymbol{q}_h^{grad} = \mathrm{C}(\boldsymbol{u}_h)T_h - \mathrm{RC}^{\mathrm{UP}}(\boldsymbol{u}_h)T_h - \mathrm{C}(\mathrm{F}\boldsymbol{u}_h)T_h + \mathrm{C}^{DO}(\boldsymbol{u}_h)\mathrm{R}T_h$$







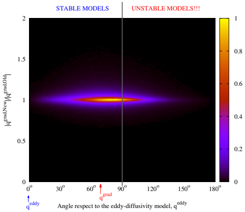
Concluding remarks

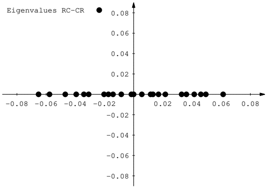
- A new way to implement the gradient model has been proposed ✓

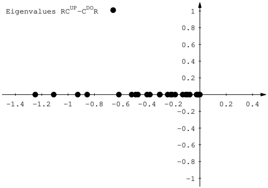
$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}(\boldsymbol{u}_h)\mathsf{R}T_h$$

- Good *a priori* alignment trends ✓
- Stabilization has been proposed and tested ✓

$$-\mathsf{M}\boldsymbol{q}_h^{grad} = \mathsf{C}(\boldsymbol{u}_h)T_h - \mathsf{R}\mathsf{C}^{\mathsf{UP}}(\boldsymbol{u}_h)T_h - \mathsf{C}(\mathsf{F}\boldsymbol{u}_h)T_h + \mathsf{C}^{DO}(\boldsymbol{u}_h)\mathsf{R}T_h$$







On-going research:

- *A posteriori* tests must be carried out

Thank you for your attendance