



Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA



Symmetry-preserving approximate deconvolutions

F.Xavier Trias¹, Andrey Gorobets², Assensi Oliva¹

¹Heat and Mass Transfer Technological Center, Technical University of Catalonia

²Keldysh Institute of Applied Mathematics of RAS, Russia





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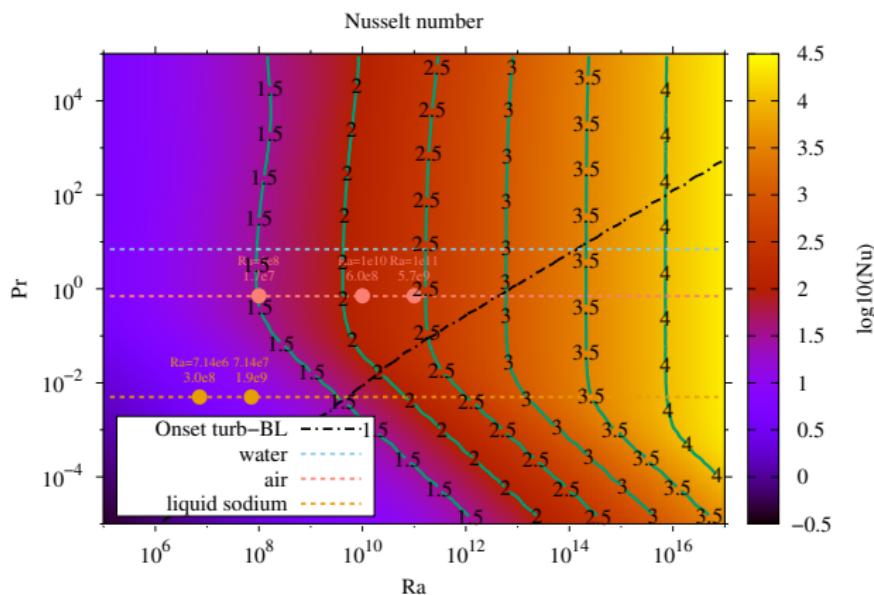
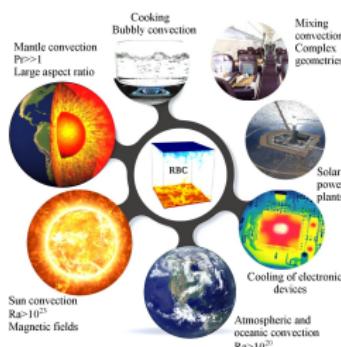
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- 2 Modeling the subgrid heat flux
- 3 Deconstructing the gradient model
- 4 Stabilizing the gradient model
- 5 Conclusions

Motivation

General research question:

- Can we hit the ultimate regime of thermal turbulence

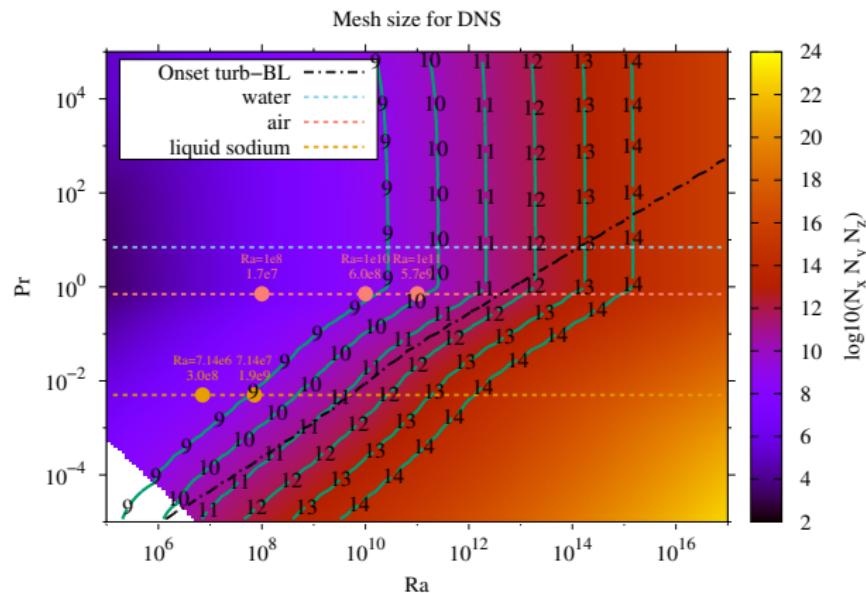
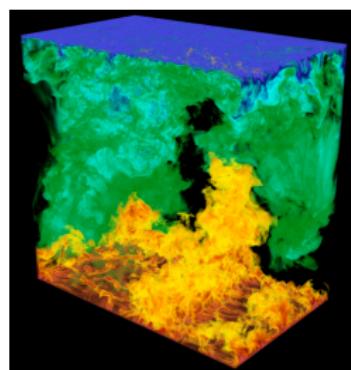
?



Motivation

General research question:

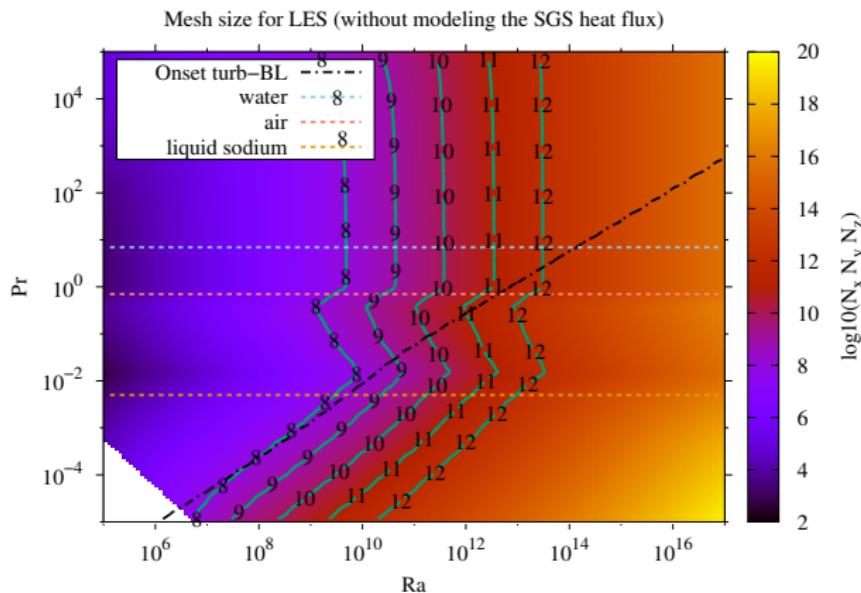
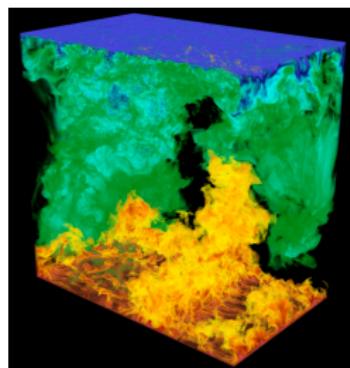
- Can we hit the ultimate regime of thermal turbulence with **DNS**?



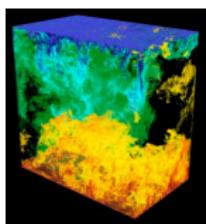
Motivation

General research question:

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

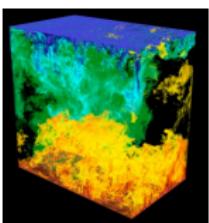


Motivation



DNS {

Motivation



HAWK



Rank #27
5,632 nodes with:
2 AMD EPYC 7742
(64 cores each)

MareNostrum 4



Rank #82
3456 nodes with:
2x Intel Xeon 8160
1x Intel Omni-Path

Marconi100



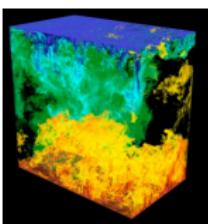
Rank #21
980 nodes with:
2 IBM Power9
4 NVIDIA Volta V100



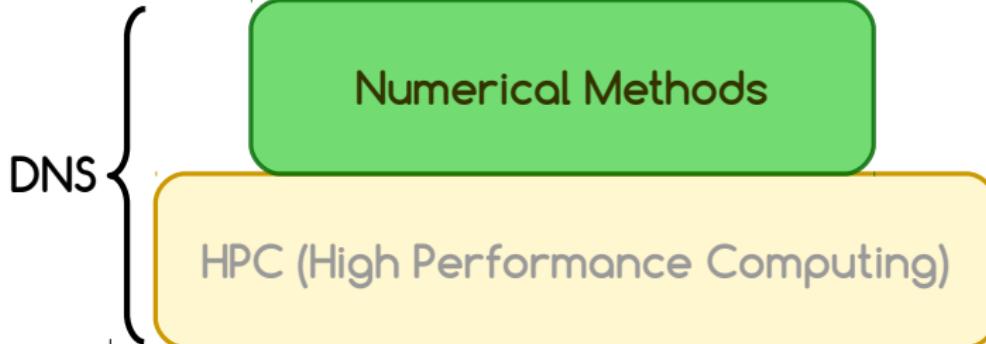
DNS

HPC (High Performance Computing)

Motivation

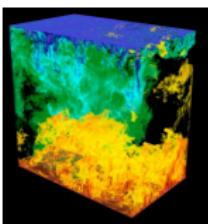


How to properly discretize NS?



Motivation

How to
properly
model SGS?



How to model the subgrid heat flux in LES?

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

eddy-viscosity $\longrightarrow \tau(\bar{\mathbf{u}}) = -2\nu_t S(\bar{\mathbf{u}})$

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

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$$G \equiv \nabla \bar{\mathbf{u}} \quad \mathbf{q} = -\frac{\delta^2}{12} G \nabla \bar{T} + \mathcal{O}(\delta^4)$$

A priori alignment trends¹

$$\text{eddy-diffusivity} \longrightarrow \mathbf{q} \approx -\alpha_t \nabla \bar{T} \quad (\equiv \mathbf{q}^{\text{eddy}})$$

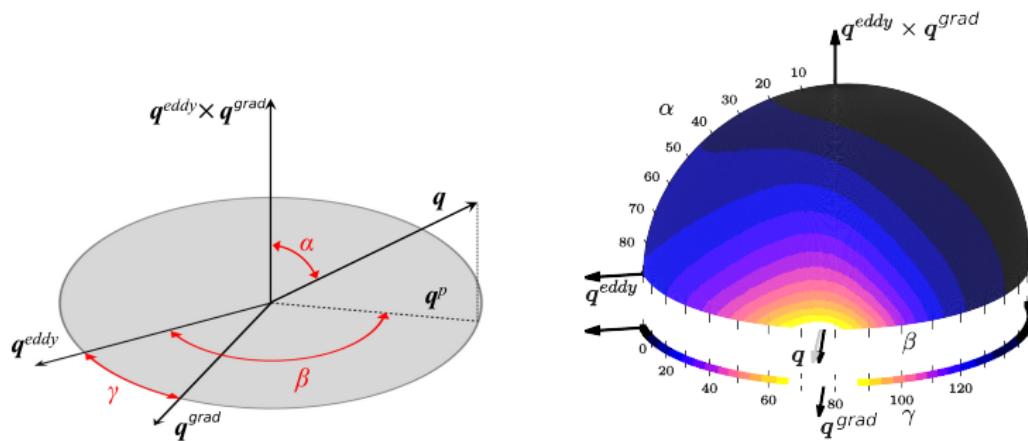
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¹F.Dabbagh, F.X.Trias, A.Gorobets, A.Oliva. *A priori study of subgrid-scale features in turbulent Rayleigh-Bénard convection*, **Physics of Fluids**, 29:105103, 2017.

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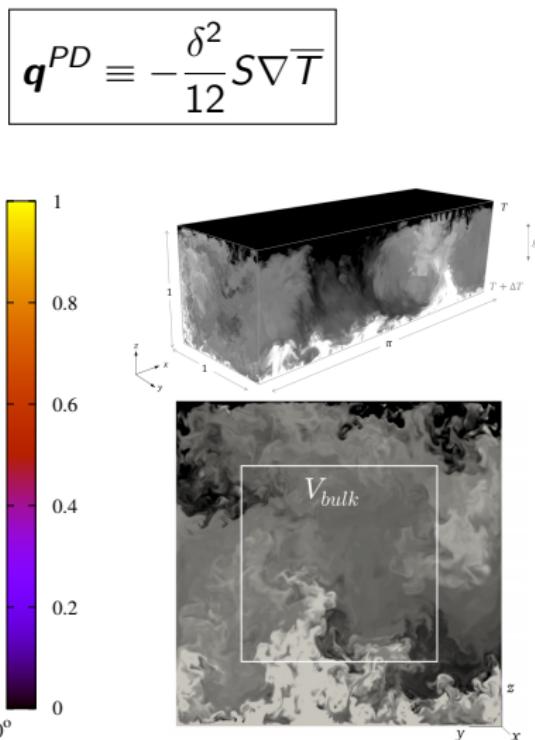
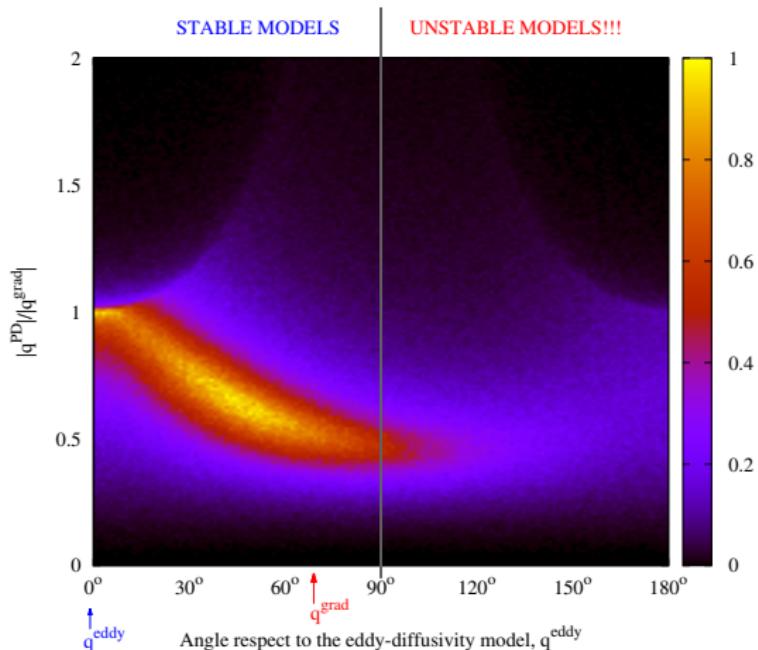
Peng&Davidson² $\rightarrow \mathbf{q} \approx -\frac{\delta^2}{12} S \nabla \bar{T} \quad (\equiv \mathbf{q}^{\text{PD}})$

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

A priori alignment trends

$$\mathbf{q}^{grad} \equiv -\frac{\delta^2}{12} G \nabla \bar{T}$$

$$\mathbf{q}^{PD} \equiv -\frac{\delta^2}{12} S \nabla \bar{T}$$



How to model the subgrid heat flux in LES?

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³S.Peng and L.Davidson. **Int.J.Heat Mass Transfer**, 45:1393-1405, 2002.

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**?

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

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Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + \mathcal{C}(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$

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

Discrete

$$\Omega \frac{d \mathbf{u}_h}{dt} + \mathcal{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D} \mathbf{u}_h - \mathbf{G} \mathbf{p}_h$$

$$\mathbf{M} \mathbf{u}_h = \mathbf{0}_h$$

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$$\mathbf{M} \mathbf{u}_h = \mathbf{0}_h$$

$$\langle \mathcal{C}(\mathbf{u}, \varphi_1), \varphi_2 \rangle = - \langle \mathcal{C}(\mathbf{u}, \varphi_2), \varphi_1 \rangle$$

$$\mathcal{C}(\mathbf{u}_h) = -\mathcal{C}^T(\mathbf{u}_h)$$

Deconstructing the gradient model

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$$\langle \nabla \cdot \mathbf{a}, \varphi \rangle = - \langle \mathbf{a}, \nabla \varphi \rangle$$

Discrete

$$\Omega \frac{d \mathbf{u}_h}{dt} + \mathcal{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D} \mathbf{u}_h - \mathbf{G} \mathbf{p}_h$$

$$\mathbf{M} \mathbf{u}_h = \mathbf{0}_h$$

$$\mathcal{C}(\mathbf{u}_h) = -\mathcal{C}^T(\mathbf{u}_h)$$

$$\Omega \mathbf{G} = -\mathbf{M}^T$$

Deconstructing the gradient model

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Continuous

$$\frac{\partial \mathbf{u}}{\partial t} + \mathcal{C}(\mathbf{u}, \mathbf{u}) = \nu \nabla^2 \mathbf{u} - \nabla p$$

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Discrete

$$\Omega \frac{d \mathbf{u}_h}{dt} + \mathcal{C}(\mathbf{u}_h) \mathbf{u}_h = \mathbf{D} \mathbf{u}_h - \mathbf{G} \mathbf{p}_h$$

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$$\Omega \mathbf{G} = -\mathbf{M}^T$$

$$\langle \nabla^2 \mathbf{a}, \mathbf{b} \rangle = \langle \mathbf{a}, \nabla^2 \mathbf{b} \rangle$$

$$\mathbf{D} = \mathbf{D}^T \quad \text{def -}$$

Deconstructing the gradient model

Continuous

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

Discrete

????

Deconstructing the gradient model

Continuous

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

$$-\nabla \cdot \mathbf{q}^{grad} =$$

Discrete

????

Deconstructing the gradient model

Continuous

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

$$-\nabla \cdot \mathbf{q}^{grad} =$$

Discrete

????

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

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

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

Deconstructing the gradient model

Continuous

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

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

Discrete

????

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

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Deconstructing the gradient model

Continuous

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

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

Discrete

????

$$-\mathbb{M}\mathbf{q}_h^{grad} = \mathcal{C}(\mathbf{u}_h)T_h + \mathbb{F}\mathcal{C}(\mathbf{u}_h)T_h \\ - \mathcal{C}(\mathbb{F}\mathbf{u}_h)T_h - \mathcal{C}(\mathbf{u}_h)\mathbb{F}T_h$$

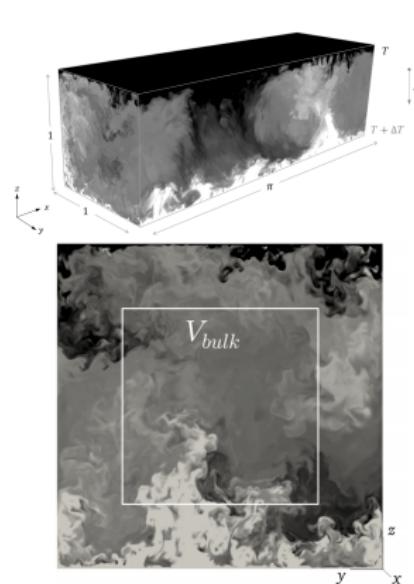
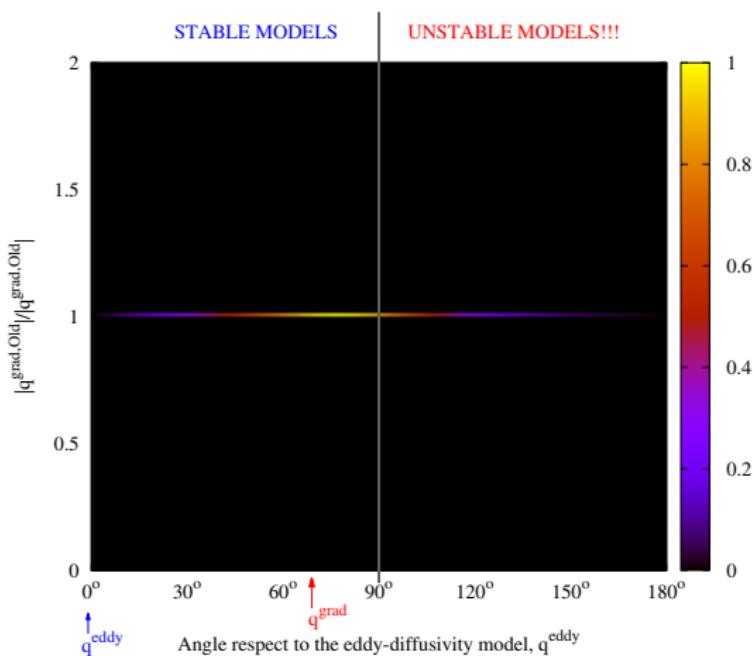
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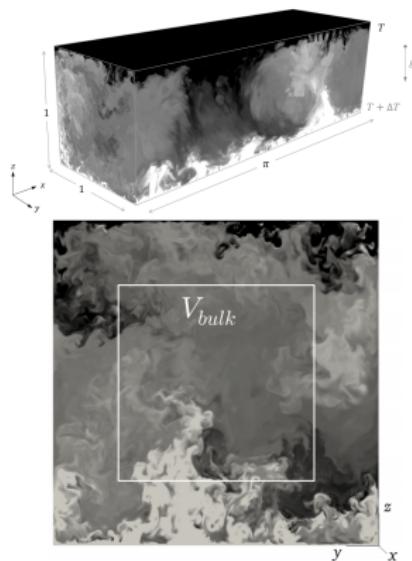
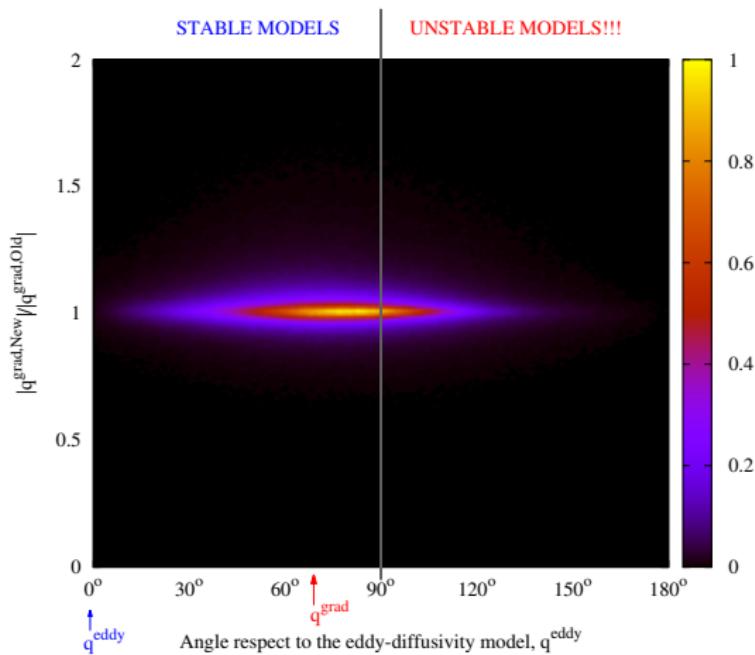
Deconstructing the gradient model

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



Deconstructing the gradient model

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



Deconstructing the gradient model

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Deconstructing the gradient model

$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathbf{C}(\mathbf{u}_h)\mathbf{T}_h + \mathbf{F}\mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h - \mathbf{C}(\mathbf{u}_h)\mathbf{F}\mathbf{T}_h$$

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

Deconstructing the gradient model

$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathbf{C}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$

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

Alternatively, it can be expressed as follows

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

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

Deconstructing the gradient model

$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathbf{C}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$

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

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

$$-\mathbf{T}_h \cdot \mathbf{M}\mathbf{q}_h^{grad} = \mathbf{T}_h \cdot (\mathbf{R}\mathbf{C} - \mathbf{C}\mathbf{R})\mathbf{T}_h$$

Deconstructing the gradient model

$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathbf{C}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$

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

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

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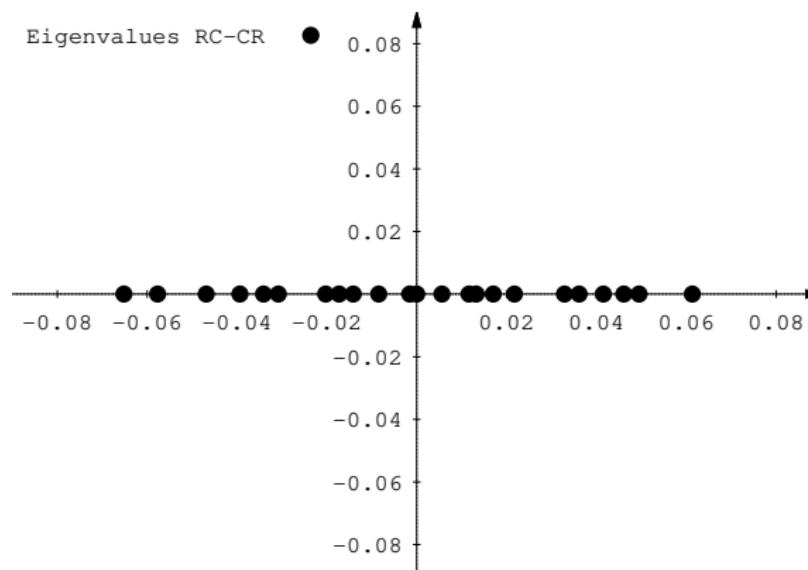
where $\mathbf{F} = \mathbf{I} - \mathbf{R}$. Recalling that $\mathbf{C} = -\mathbf{C}^T$ and $\mathbf{F} = \mathbf{F}^T$, leads to

$$-\mathbf{T}_h \cdot \mathbf{M}\mathbf{q}_h^{grad} = \mathbf{T}_h \cdot (\mathbf{RC} - \mathbf{CR})\mathbf{T}_h$$

Stabilizing the gradient model

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

Stability is determined by the sign of the Rayleigh quotient of $\mathbf{R} \mathbf{C} - \mathbf{C} \mathbf{R}$

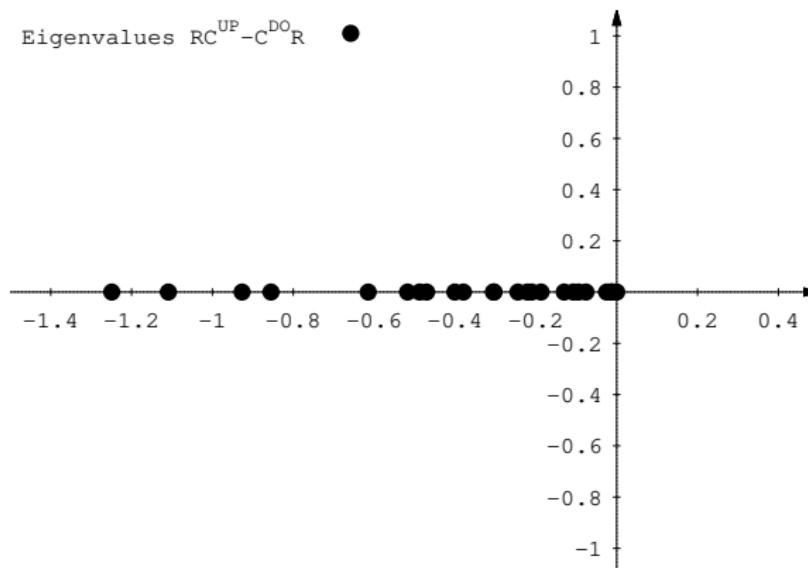


$\mathbf{R} \mathbf{C} - \mathbf{C} \mathbf{R}$

Stabilizing the gradient model

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

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

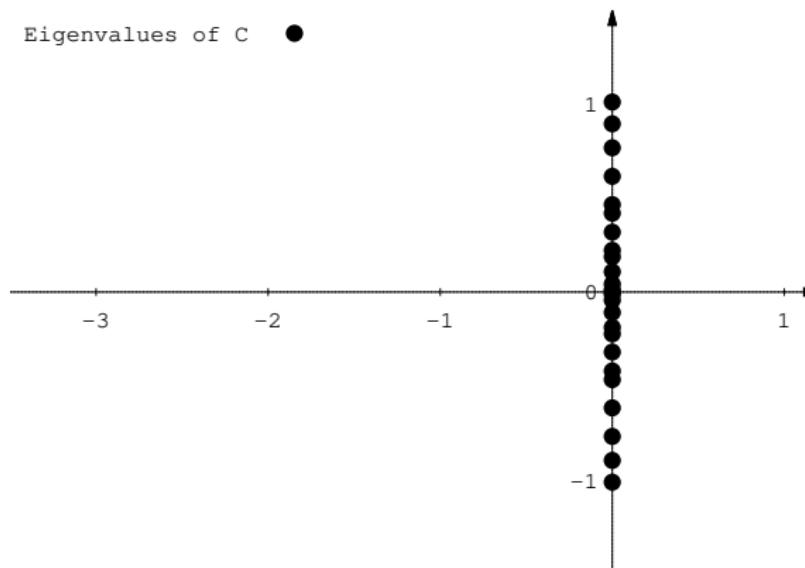


Idea: $\mathbf{RC}^{UP} - \mathbf{C}^{DO} \mathbf{R}$ instead of $\mathbf{RC} - \mathbf{CR}$ guarantees stability

Stabilizing the gradient model

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Stability is determined by the sign of the Rayleigh quotient of $\mathbf{R}\mathbf{C} - \mathbf{C}\mathbf{R}$

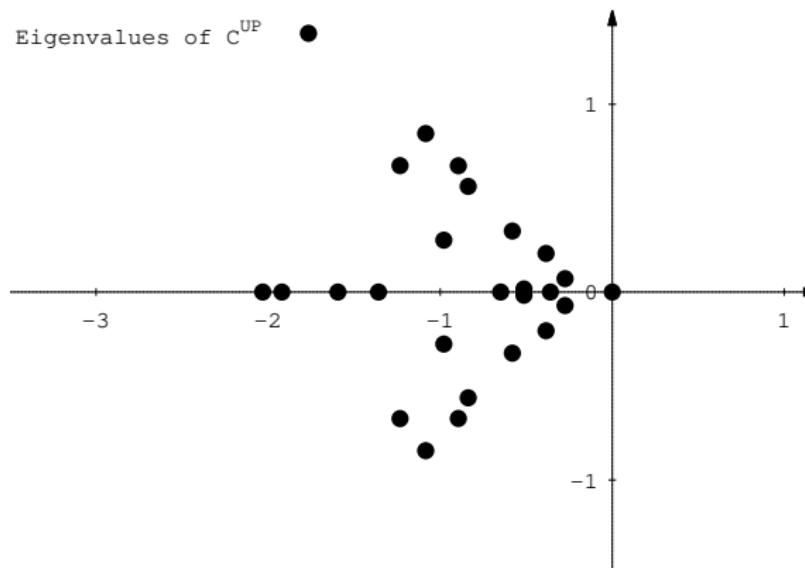


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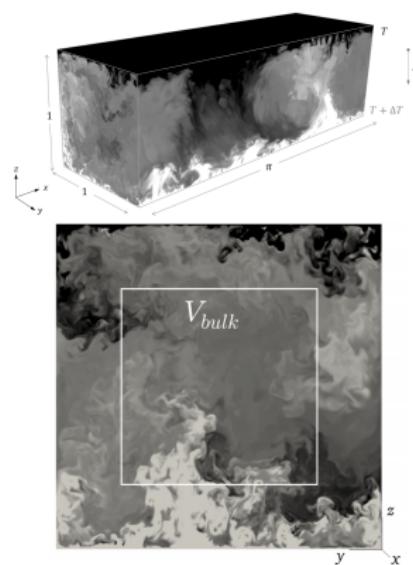
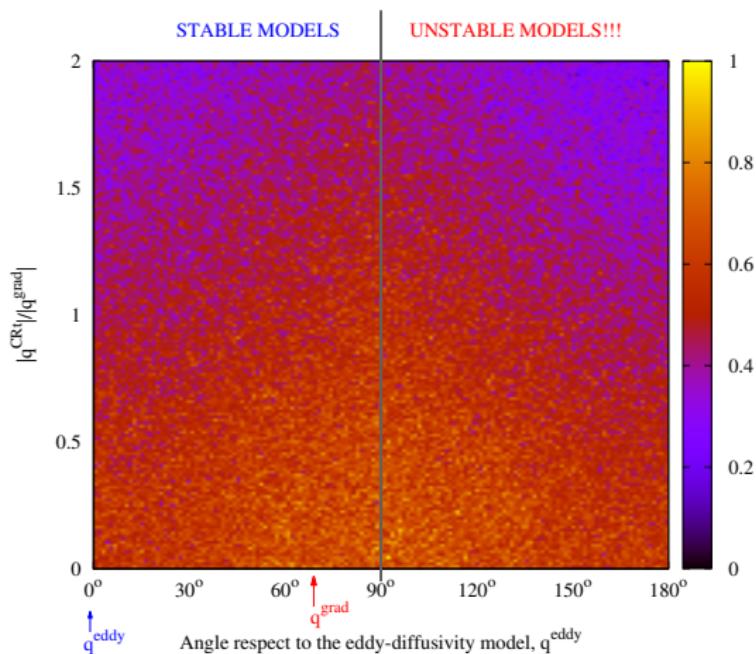
Stability is determined by the sign of the Rayleigh quotient of $\mathbf{R}\mathbf{C} - \mathbf{C}\mathbf{R}$



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

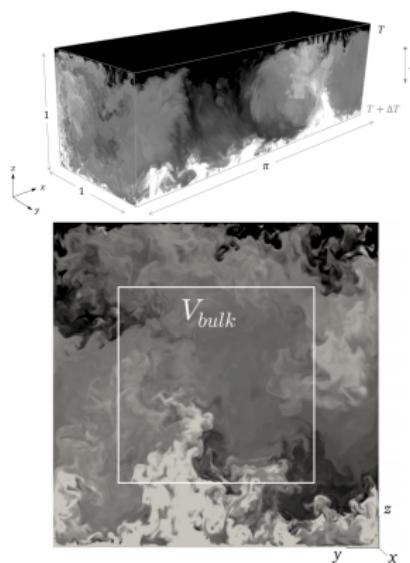
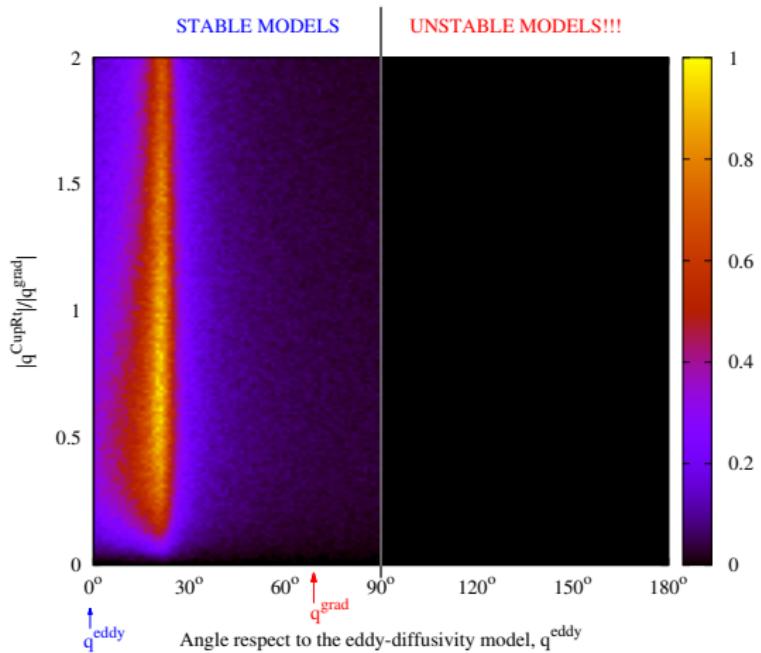
Stabilizing the gradient model

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



Stabilizing the gradient model

$$-\mathbf{M} \mathbf{q}_h^{grad} = \mathbf{C}(\mathbf{u}_h) T_h \left[-\mathbf{R} \mathbf{C}^{UP}(\mathbf{u}_h) T_h \right] - \mathbf{C}(\mathbf{F} \mathbf{u}_h) T_h \left[+\mathbf{C}^{DO}(\mathbf{u}_h) \mathbf{R} T_h \right]$$



Stabilizing the gradient model

Test-case: passive scalar in a 2D channel flow

Stabilizing the gradient model

Test-case: passive scalar in a 2D channel flow

Stabilizing the gradient model

Test-case: passive scalar in a 2D channel flow

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Stabilizing the gradient model

Test-case: passive scalar in a 2D channel flow

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Concluding remarks

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

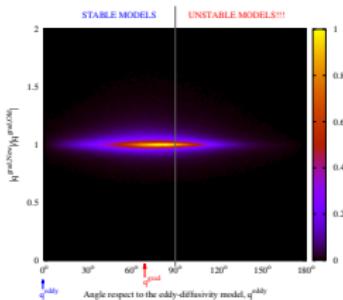
$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathbf{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathbf{C}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$

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- Good *a priori* alignment trends ✓



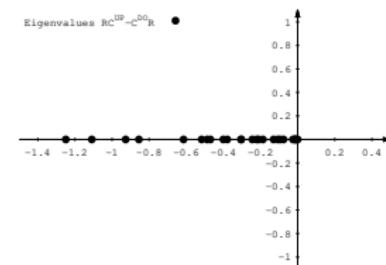
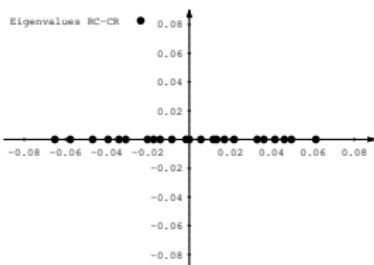
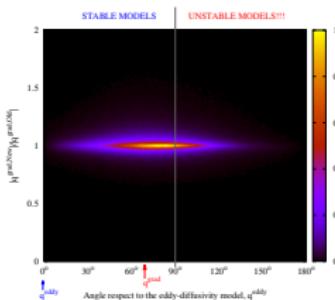
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$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathcal{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathcal{C}(\mathbf{u}_h)\mathbf{T}_h - \mathcal{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathcal{C}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$

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

$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathcal{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathcal{C}^{UP}(\mathbf{u}_h)\mathbf{T}_h - \mathcal{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathcal{C}^{DO}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$



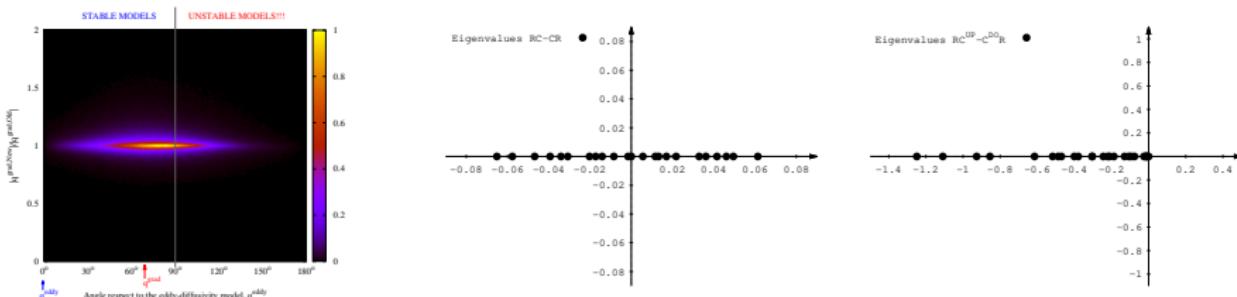
Concluding remarks

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$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathcal{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathcal{C}(\mathbf{u}_h)\mathbf{T}_h - \mathcal{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathcal{C}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$

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

$$-\mathbf{M}\mathbf{q}_h^{grad} = \mathcal{C}(\mathbf{u}_h)\mathbf{T}_h - \mathbf{R}\mathcal{C}^{UP}(\mathbf{u}_h)\mathbf{T}_h - \mathcal{C}(\mathbf{F}\mathbf{u}_h)\mathbf{T}_h + \mathcal{C}^{DO}(\mathbf{u}_h)\mathbf{R}\mathbf{T}_h$$



- Discrete operators must be **consistently discretized** ✓

Thank you for your attendance