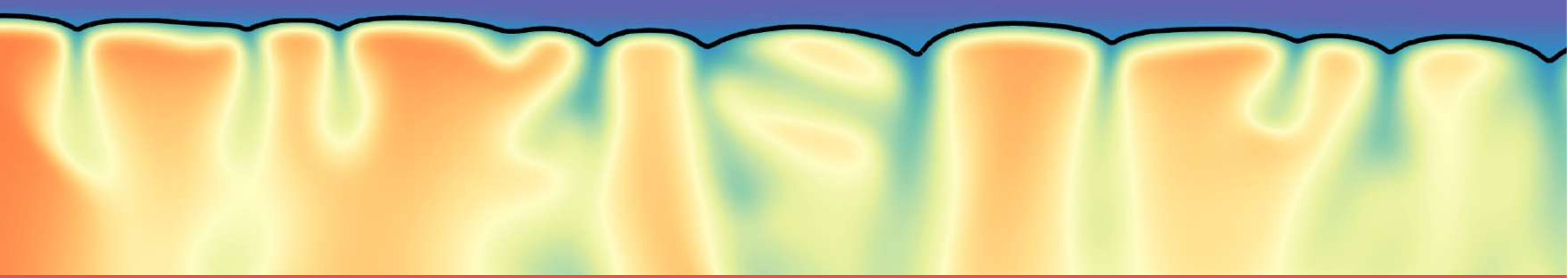
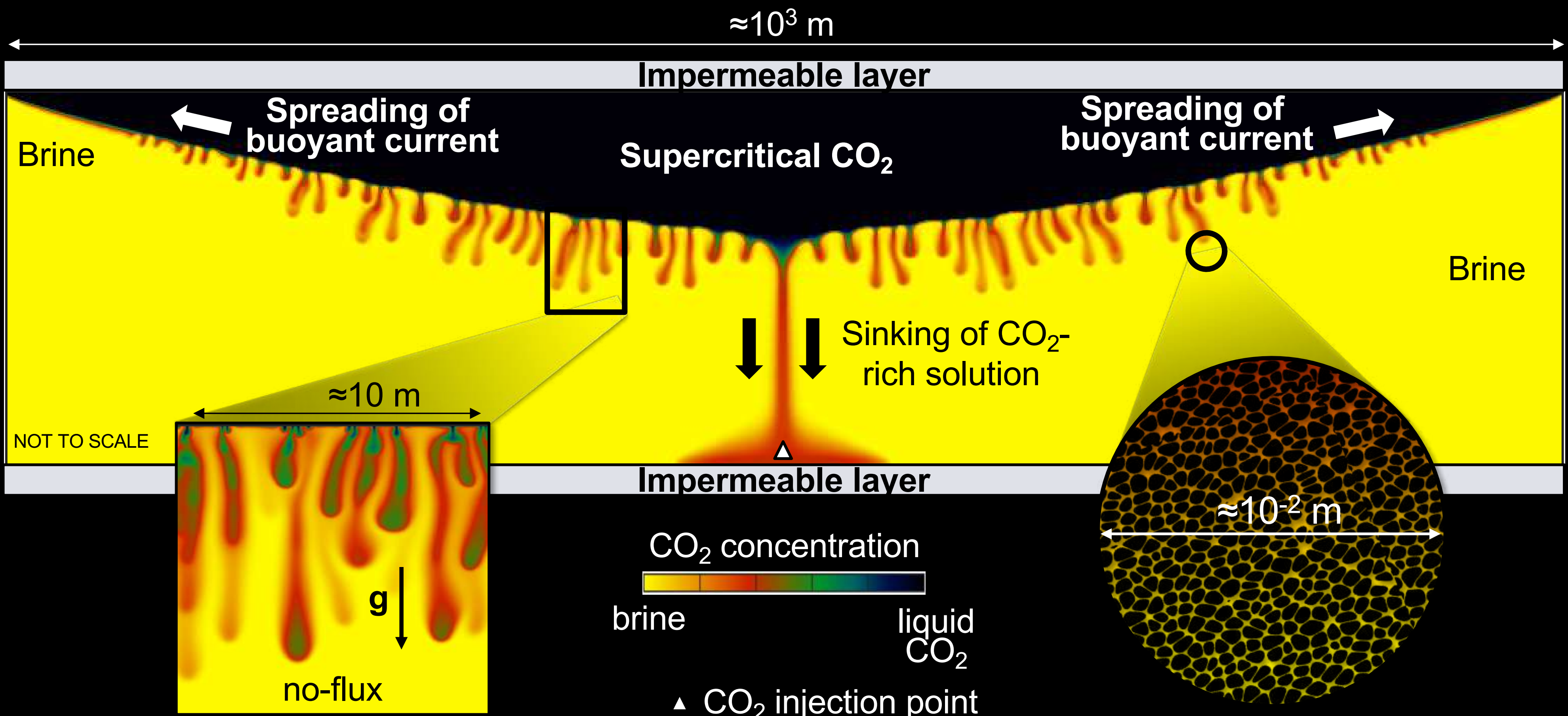
Numerical simulations of convective mixing with complex fluids



Marco De Paoli[1] & Sergio Pirozzoli[2]

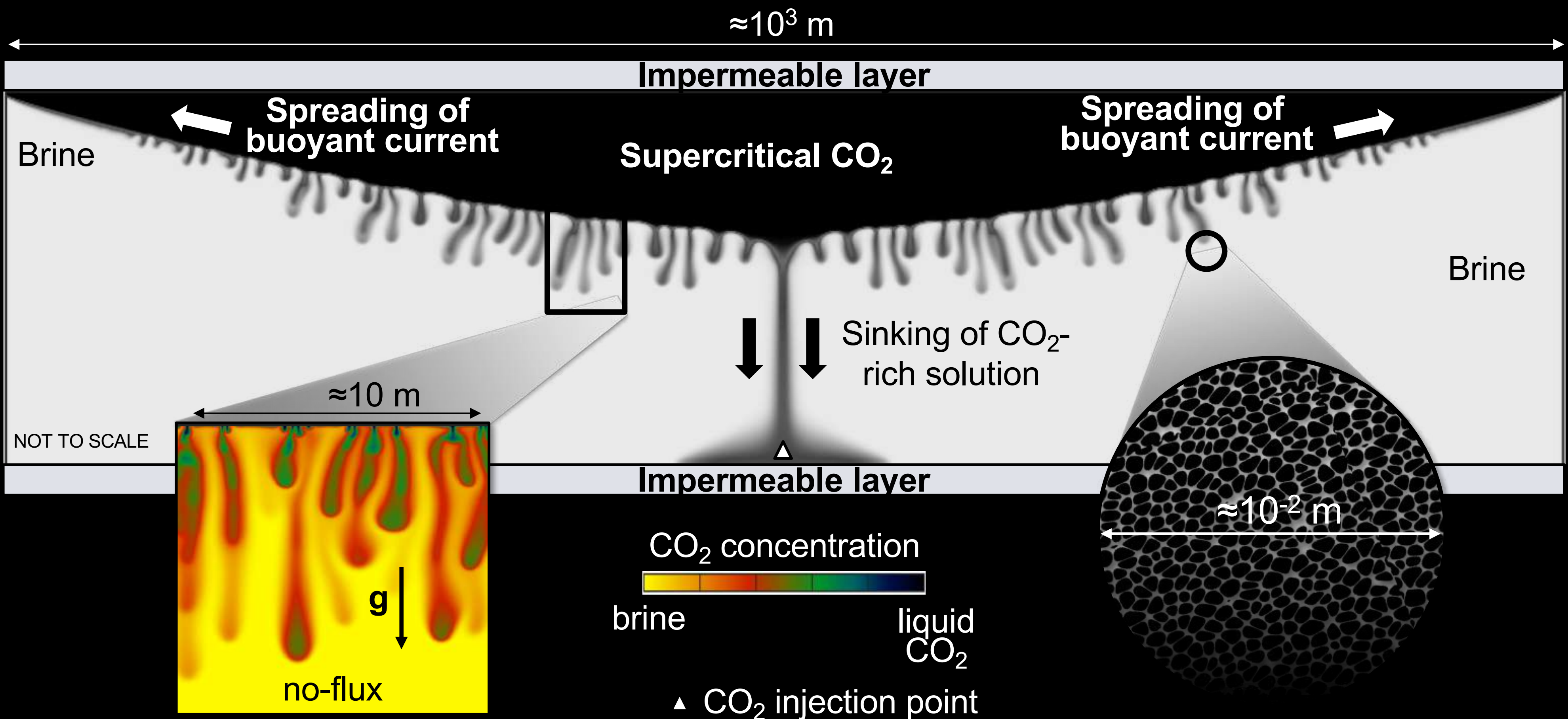
[1]TU Wien, Vienna, Austria
[2]Sapienza University, Rome, Italy
marco.de.paoli@tuwien.ac.at

Carbon Capture and Storage

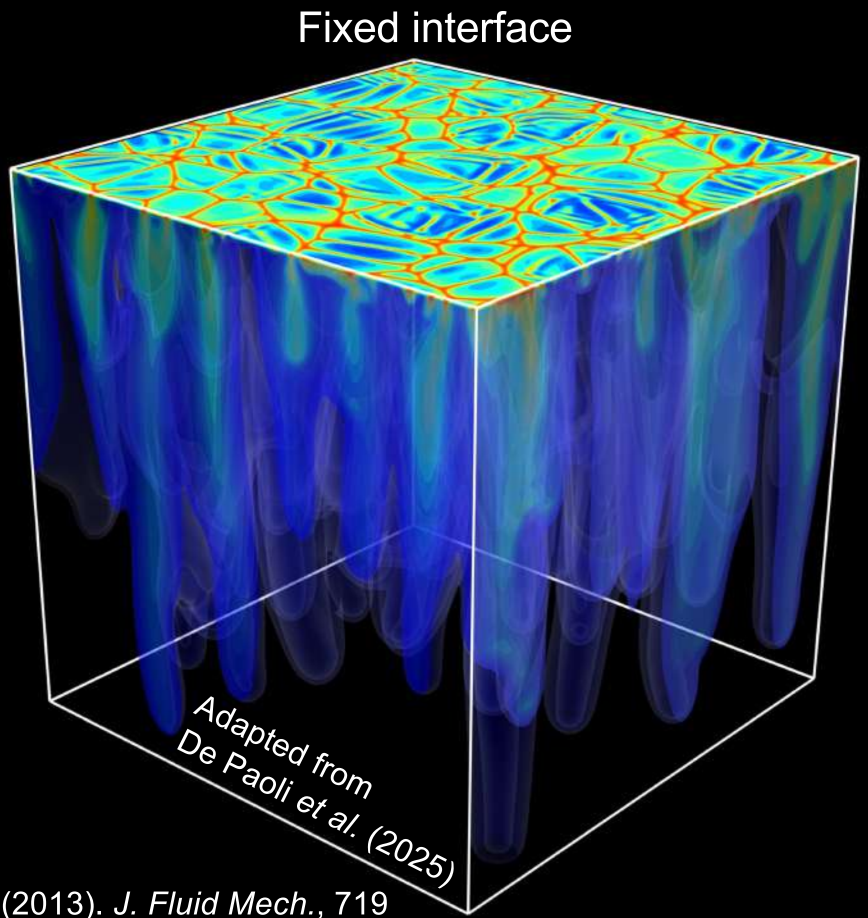


De Paoli, *Phys. Fluids* (2021)

Carbon Capture and Storage

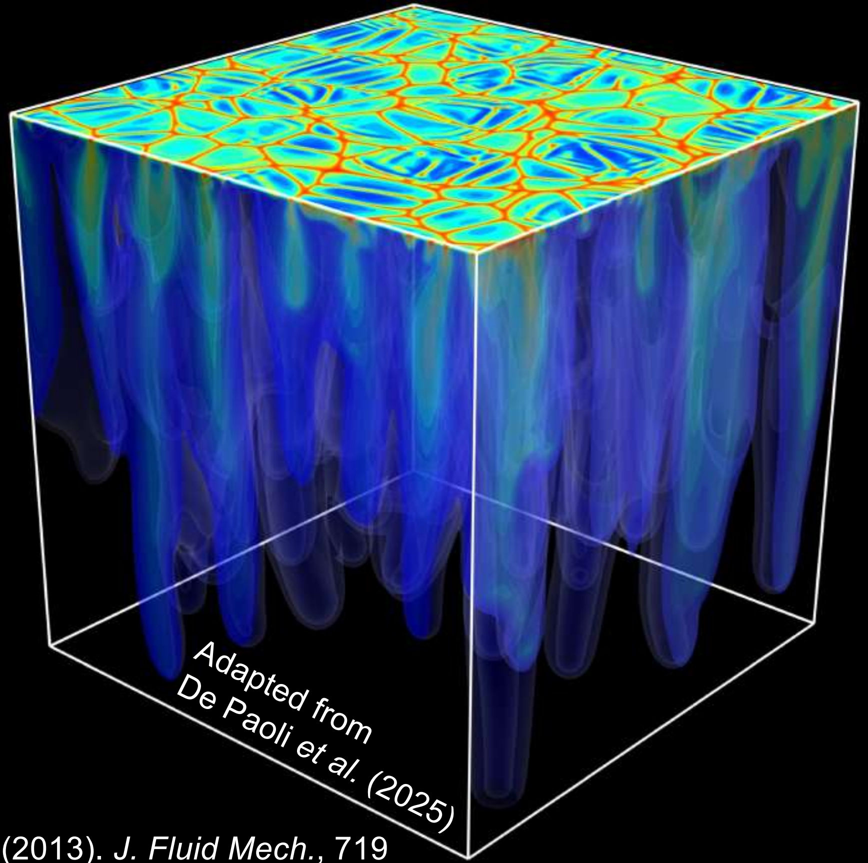


De Paoli, *Phys. Fluids* (2021)

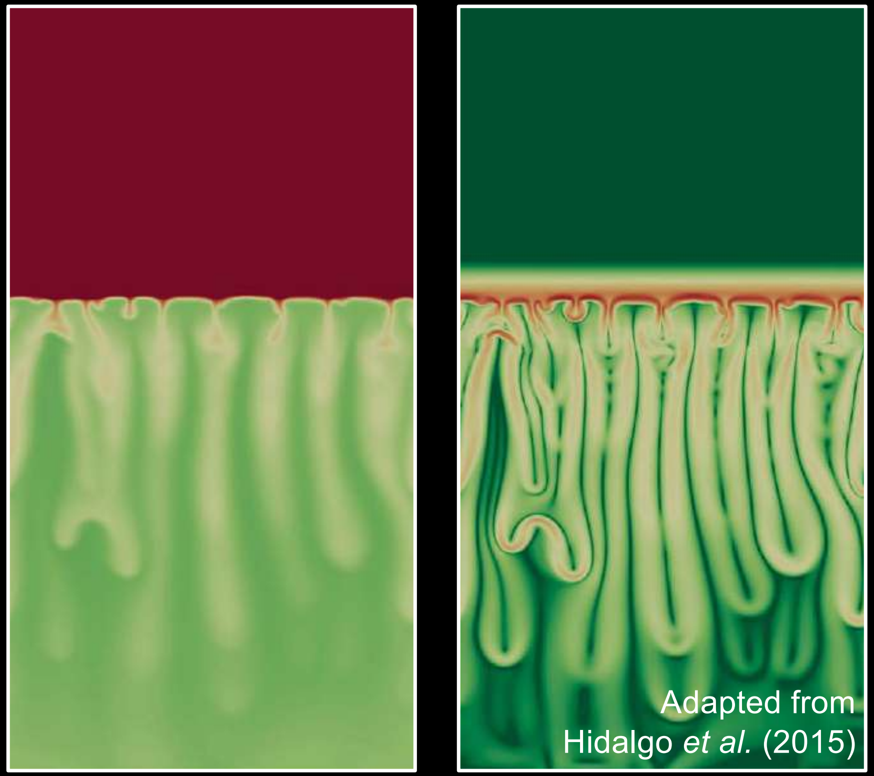


Hewitt *et al.* (2013). *J. Fluid Mech.*, 719
Slim, A. (2014). *J. Fluid Mech.*, 741
De Paoli *et al.* (2025). *Geophys. Res. Lett.*, 52 (7)

Fixed interface



Free interface



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Imuetinyan *et al.* (2026). The Eur. Phys. J. E, 49 (20)

What is the role of boundary conditions?

What is the role of boundary conditions?

What is the role of fluid model?

What is the role of boundary conditions?

What is the role of fluid model?

What is the role of dimensionality?

Flow

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

$$\mathbf{u} = -\left(\nabla p + \rho \mathbf{k}\right)$$

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \frac{1}{Ra_0} \nabla^2 C$$

De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

Flow

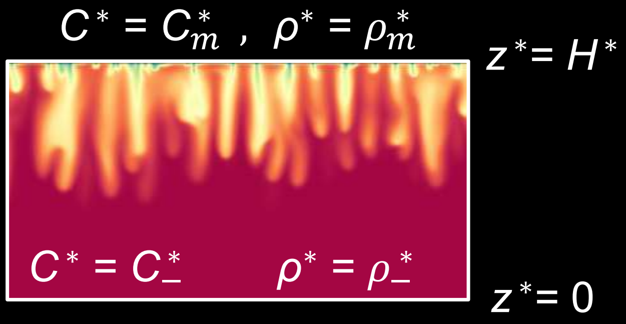
$$\nabla \cdot \mathbf{u} = 0 \qquad \mathbf{u} = -(\nabla p + \rho \mathbf{k}) \qquad \frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \frac{1}{Ra_0} \nabla^2 C$$

Fluid

Fixed interface

$$\rho = 1 + C \quad , \quad -1 \leqslant C \leqslant 0$$

$$\rho = 1 - C^2 \quad , \quad -1 \leqslant C \leqslant 0$$



De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

Fluid models

Flow

$$\nabla \cdot \mathbf{u} = 0 \qquad \mathbf{u} = -\left(\nabla p + \rho \mathbf{k}\right) \qquad \frac{\partial C}{\partial t} + \mathbf{u}\cdot\nabla C = \frac{1}{Ra_0}\nabla^2 C$$

Fluid

Fixed interface

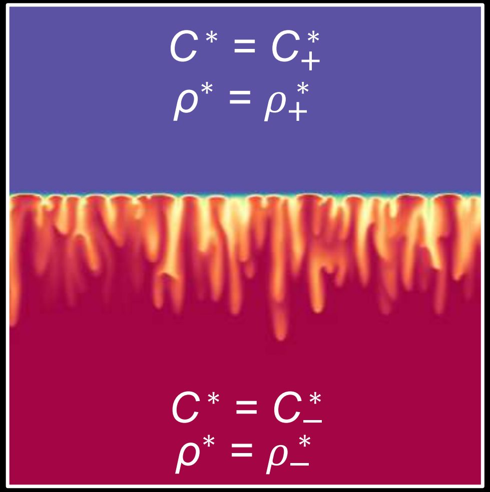
$$\rho = 1 + C \quad , \quad -1 \leqslant C \leqslant 0$$

$$\rho = 1 - C^2 \quad , \quad -1 \leqslant C \leqslant 0$$

Free interface

$$\rho = \begin{cases} 1 - C^2 \quad , \quad -1 \leqslant C \leqslant 0 \\ 1 - (1+\beta)\left(1 - \frac{1}{\alpha}\right)^2 C^2 \end{cases}$$

$$Ra_0 = \frac{\mathscr{U}^* H^*}{\phi D} \quad , \quad \alpha = \frac{C_+^* - C_m^*}{C_+^* - C_-^*} \quad , \quad \beta = \frac{\rho_-^* - \rho_+^*}{\rho_m^* - \rho_-^*}$$

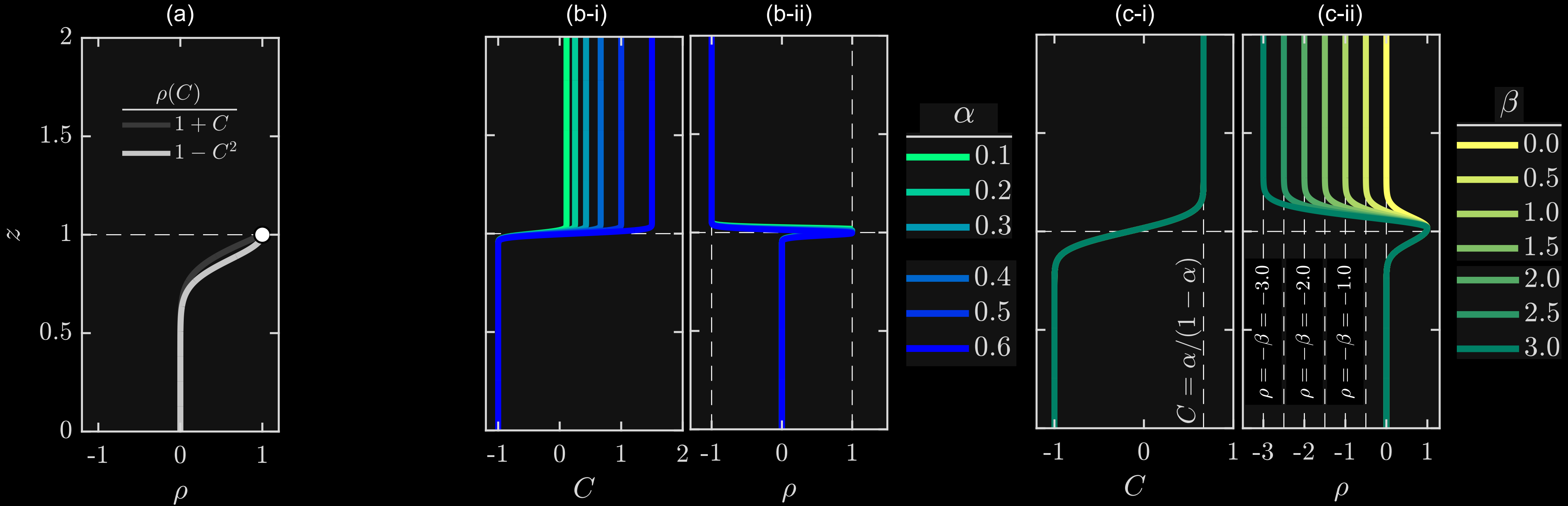


$$0 < C \leqslant C_+ = \frac{\alpha}{1-\alpha}$$

De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

fixed interface

free interface



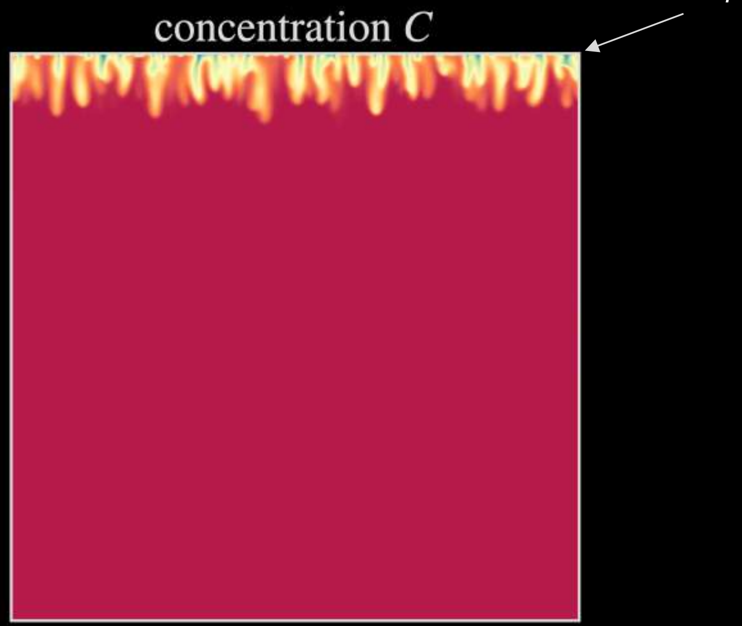
$$\alpha = \frac{C_+^* - C_m^*}{C_+^* - C_-^*} \quad , \quad \beta = \frac{\rho_-^* - \rho_+^*}{\rho_m^* - \rho_-^*}$$

De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

Fixed interface: 3D faster mixing than 2D

$\rho = 1 + C$

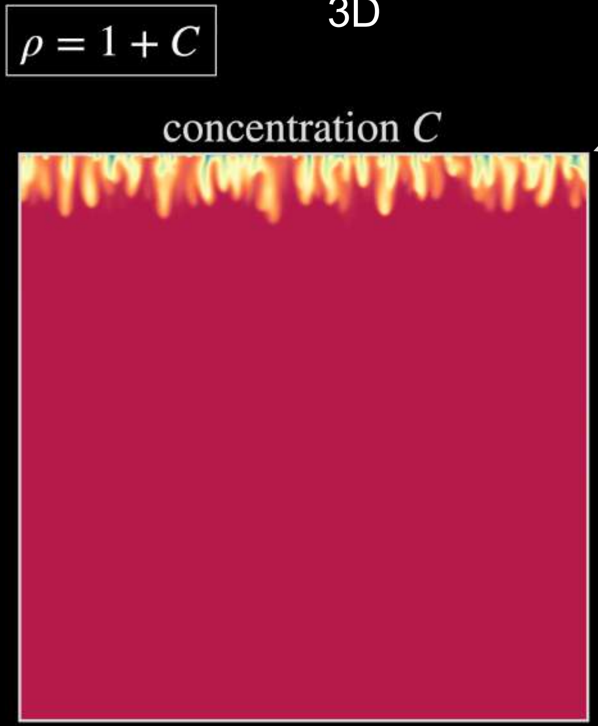
3D

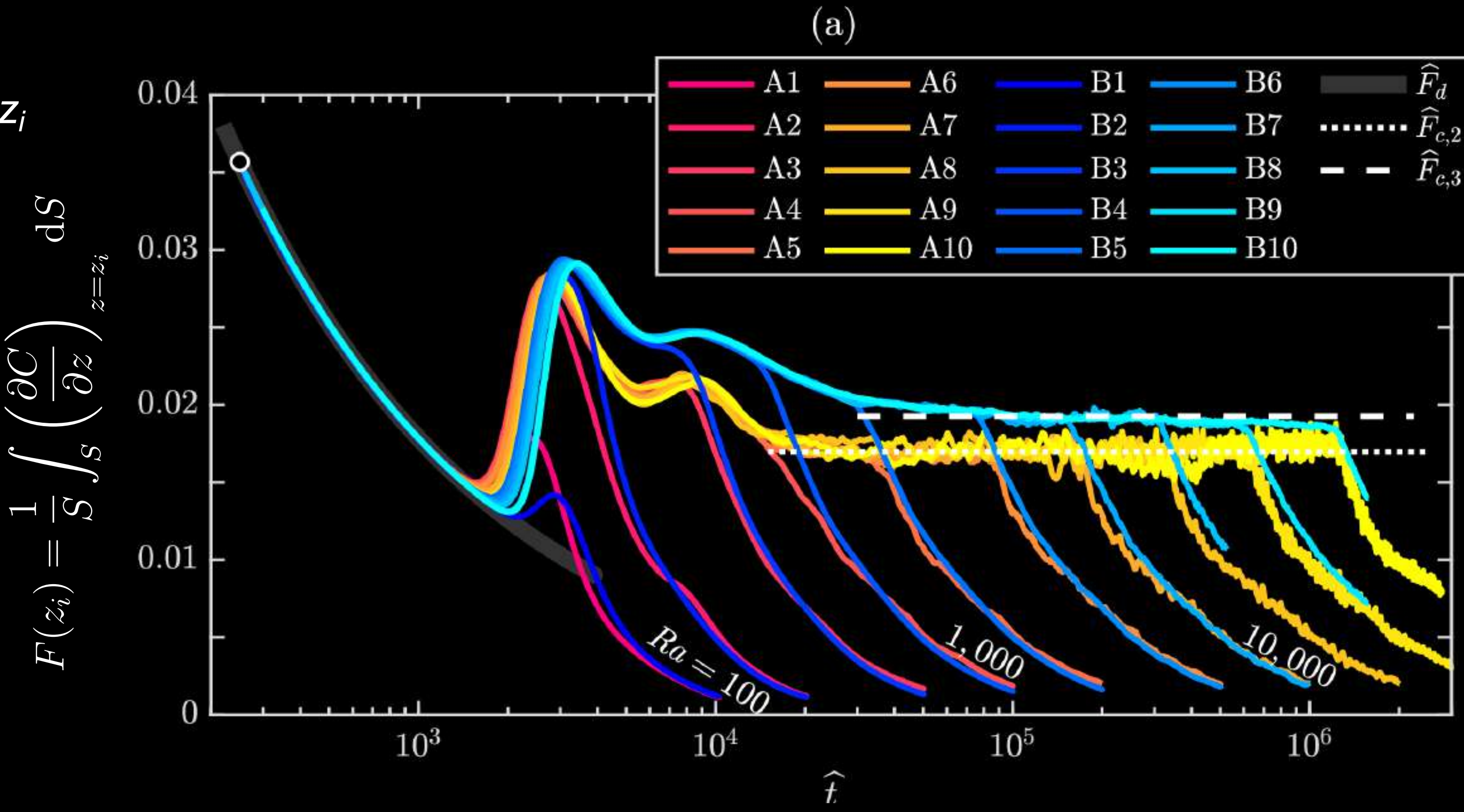


De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

Fixed interface: 3D faster mixing than 2D

3D



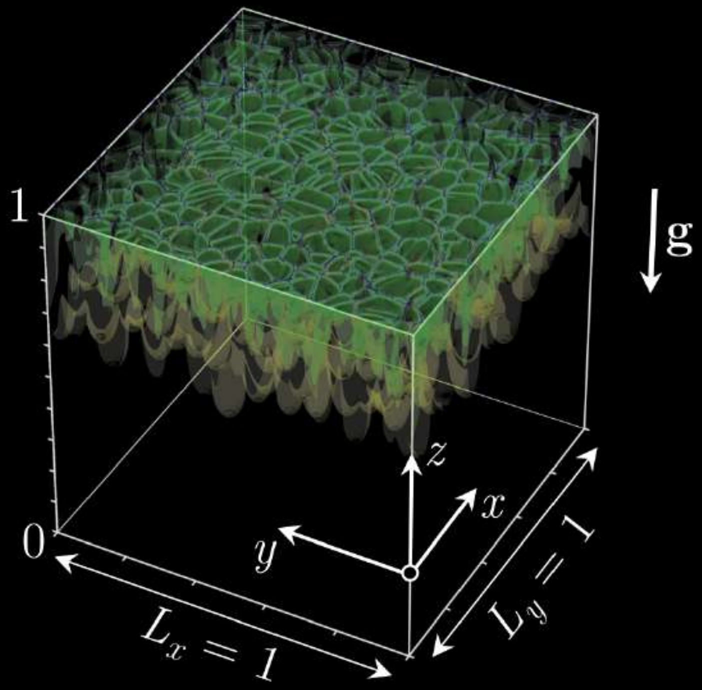


De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

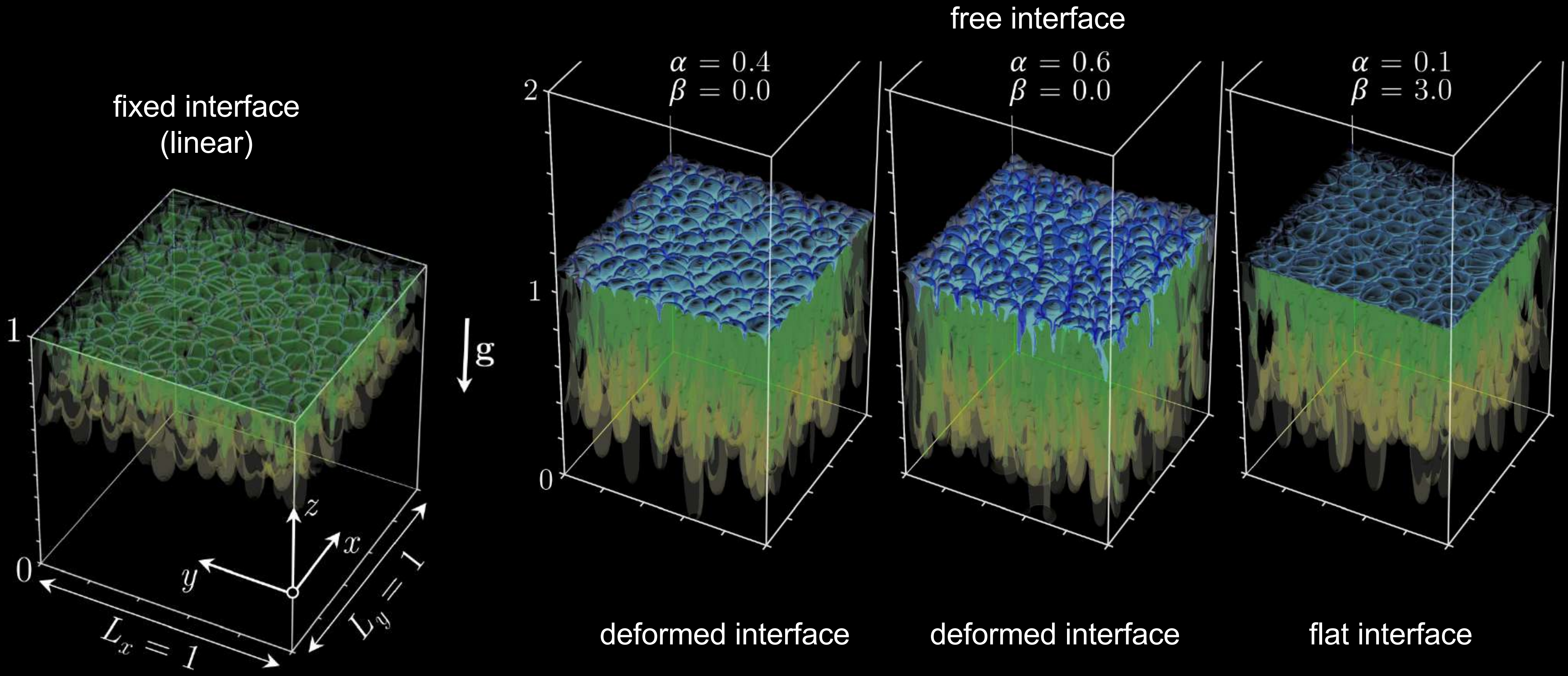
De Paoli, Zonta, Enzenberger, Coliban, & Pirozzoli (2025). *Geophysical Research Letters*.

Fixed vs. free interface

fixed interface
(linear)



Fixed vs. free interface

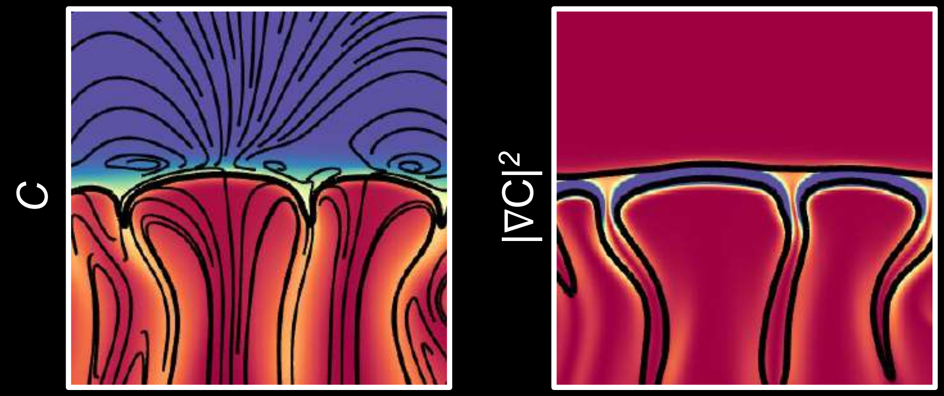


Mixing

Mean scalar dissipation

$$\chi = \langle |\nabla C|^2 \rangle$$

with $\langle \quad \rangle$ = volume average



Jha, B., Cueto-Felgueroso, L., & Juanes, R. (2011). *Phys. Rev. E*, 84 (6), 066312
Hidalgo, J., Fe, J., Cueto-Felgueroso, L., & Juanes, R. (2012). *Phys. Rev. Lett.,* 109 (26), 264503.
Hidalgo, J., Dentz, M., Cabeza, Y., & Carrera, J. (2015). *Geophys. Res. Lett.,* 42 (15), 6357–6364.

Mean scalar dissipation

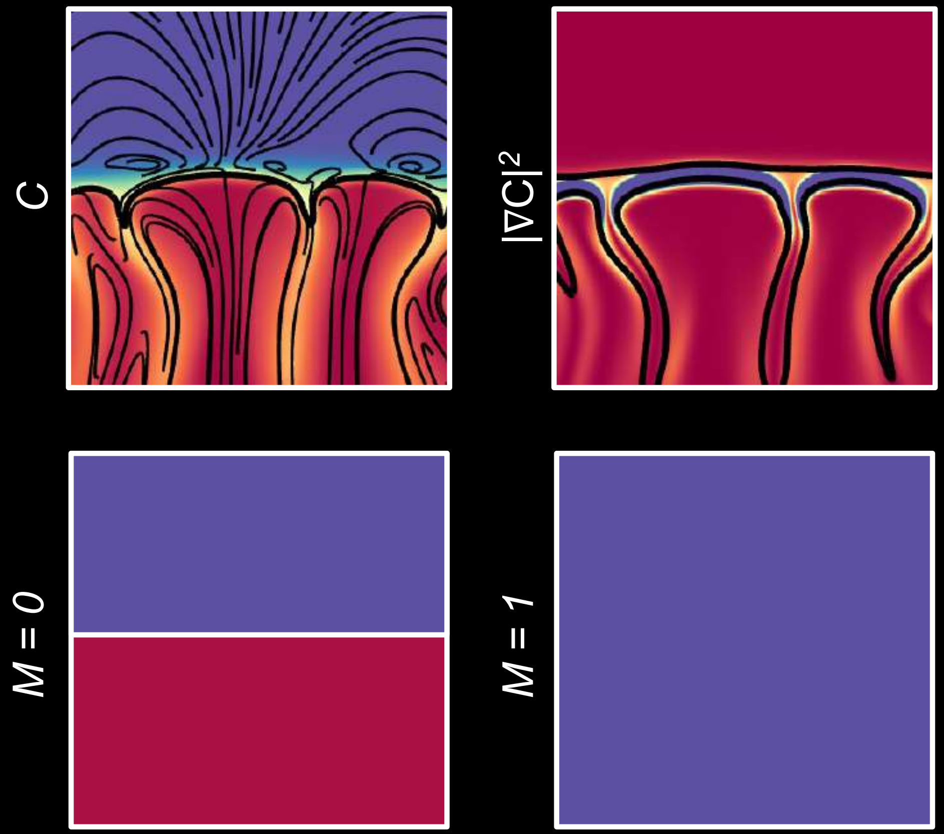
$$\chi = \langle |\nabla C|^2 \rangle$$

with ⟨ ⟩ = volume average

Degree of mixing

$$M(t) = 1 - \frac{\sigma^2(t)}{\sigma^2_{\max}} = \frac{8(1-\alpha)^2}{Ra} \int_0^t \chi \, \mathrm{d}t$$

$$\sigma^2 = \langle C^2 \rangle - \langle C \rangle^2$$



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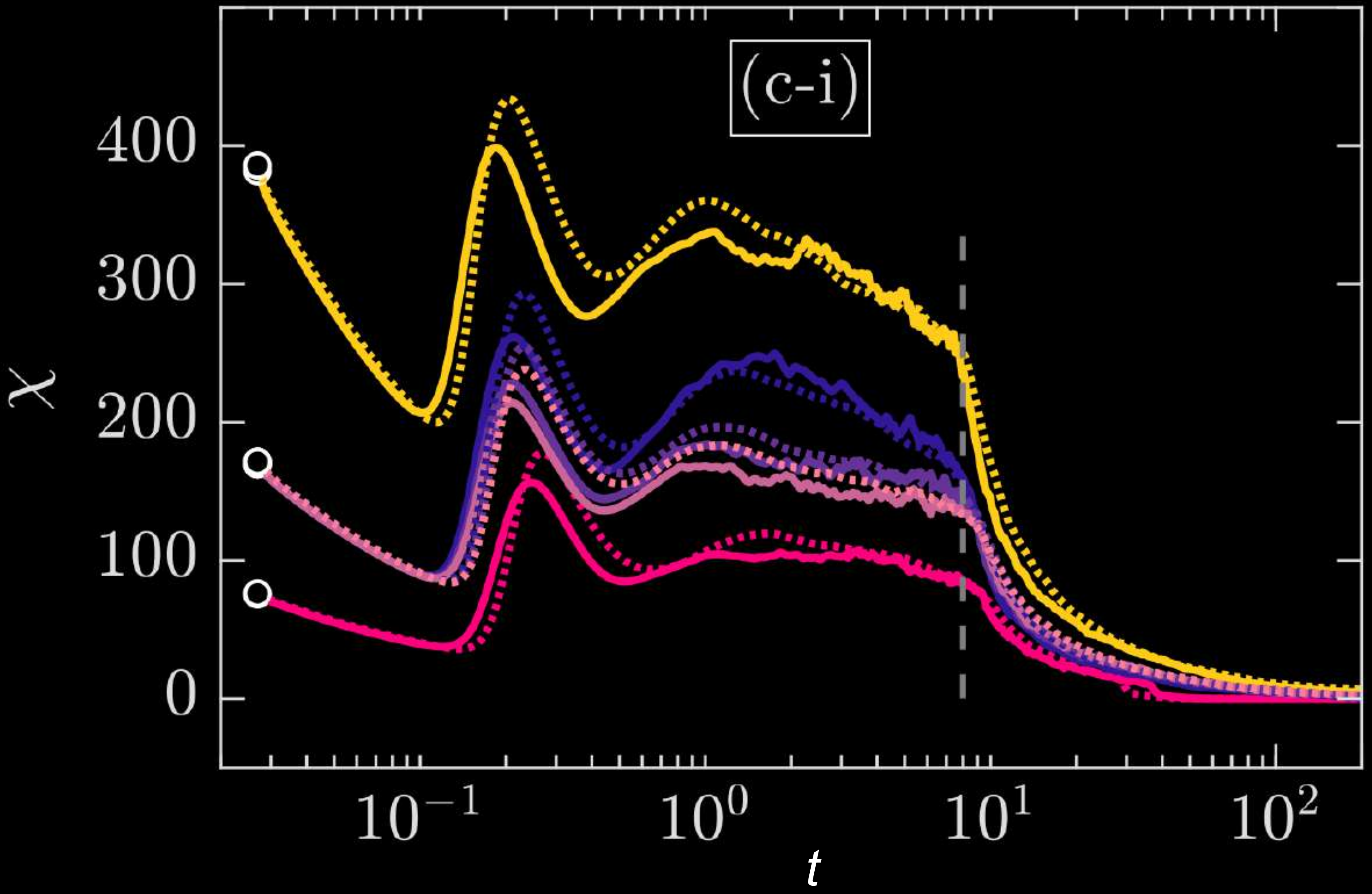
Mean dissipation and mixing



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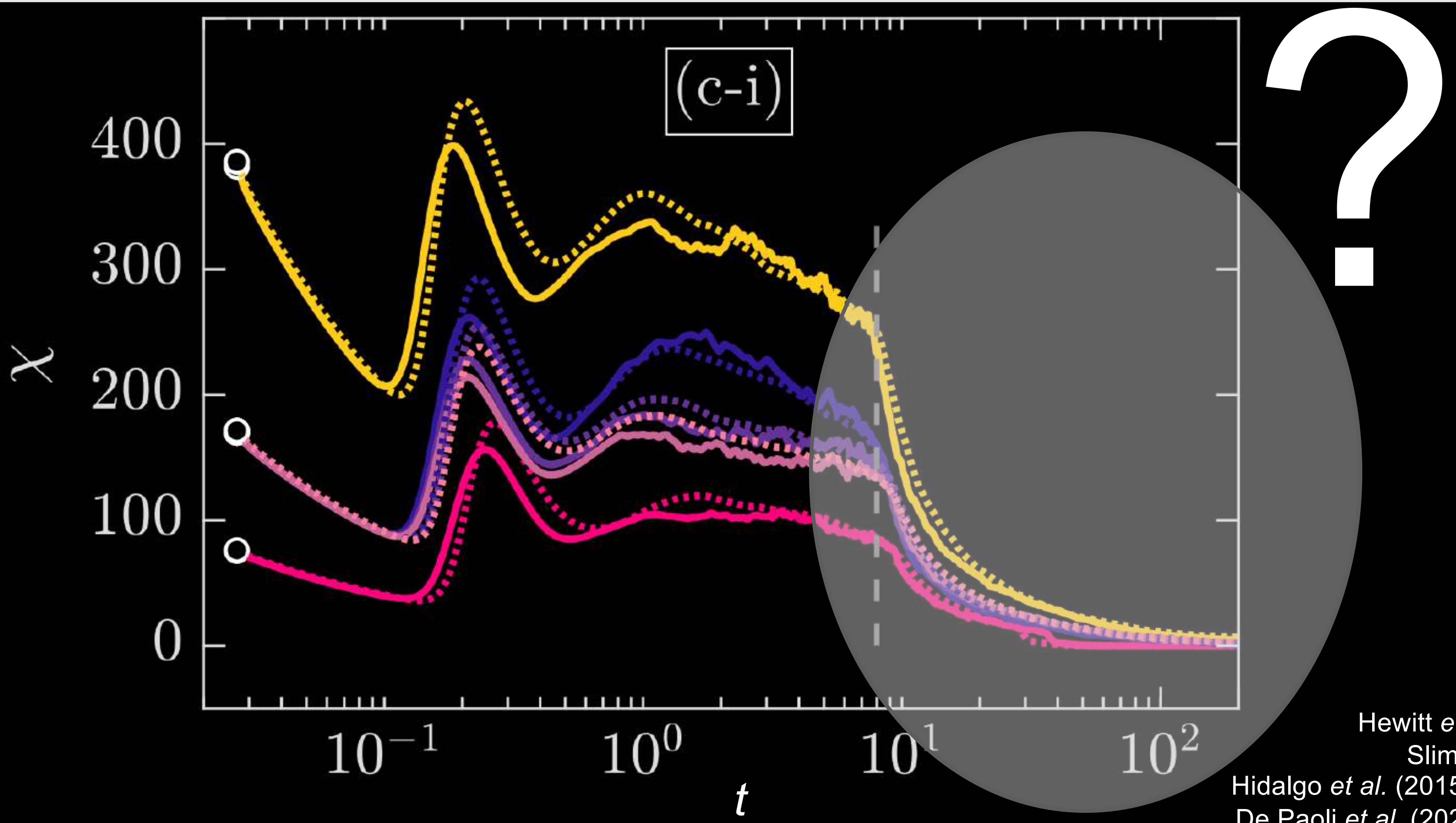

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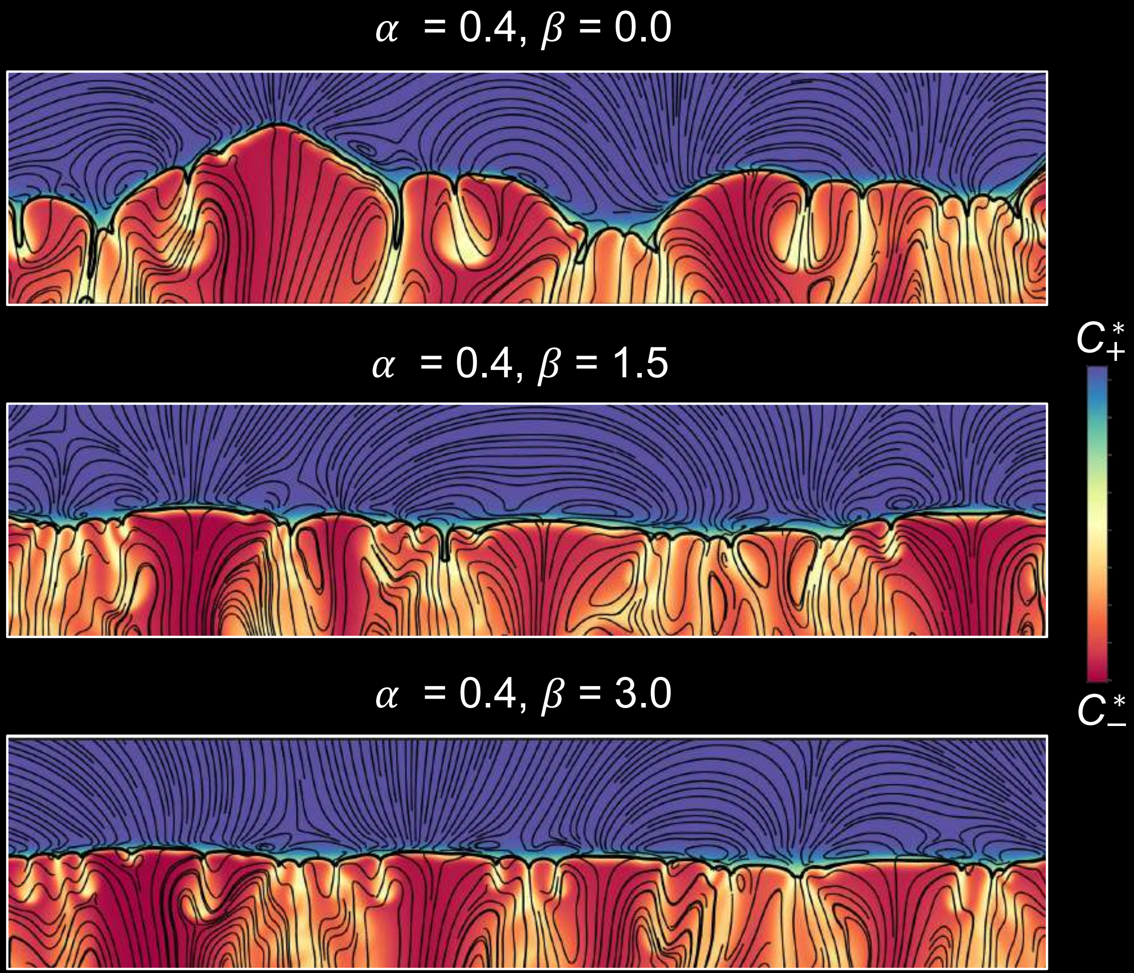
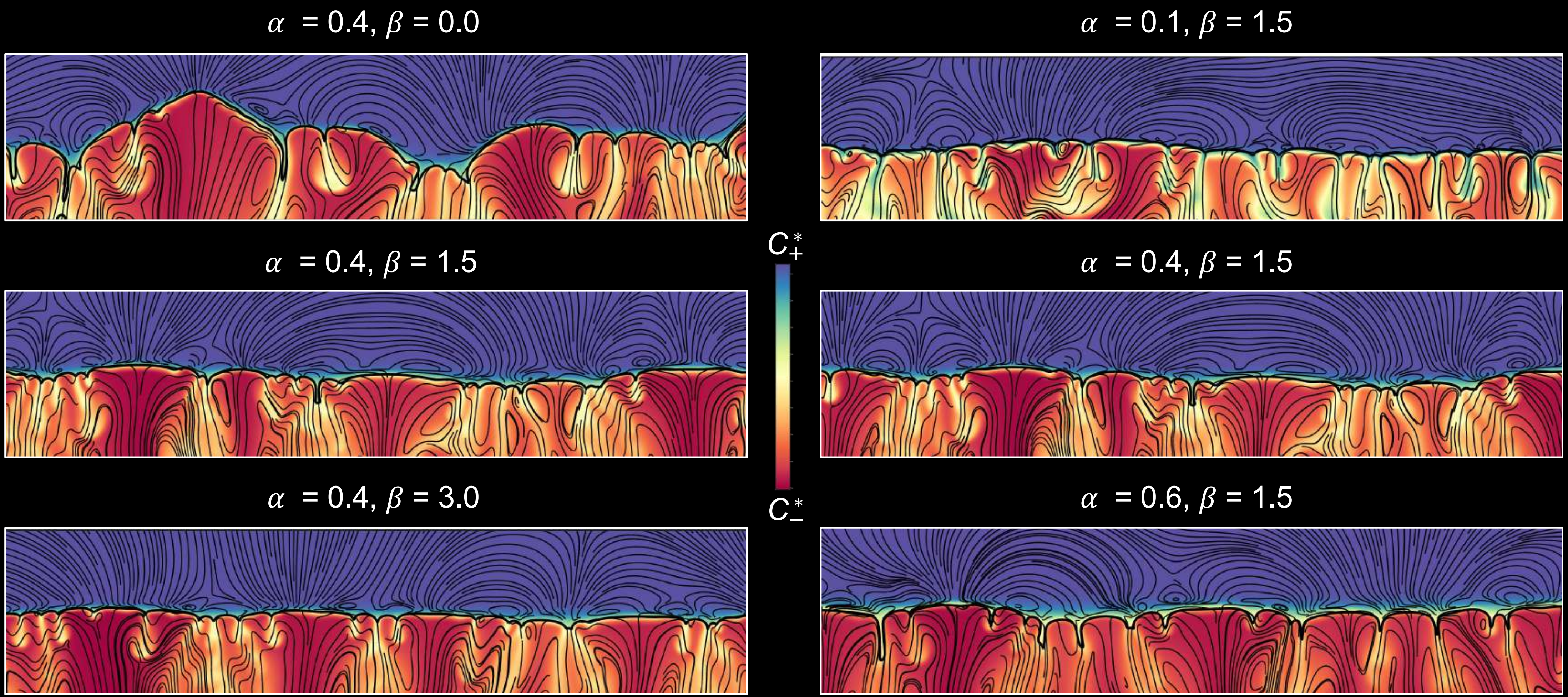
Influence of fluid models on the interface



Influence of fluid models on the interface

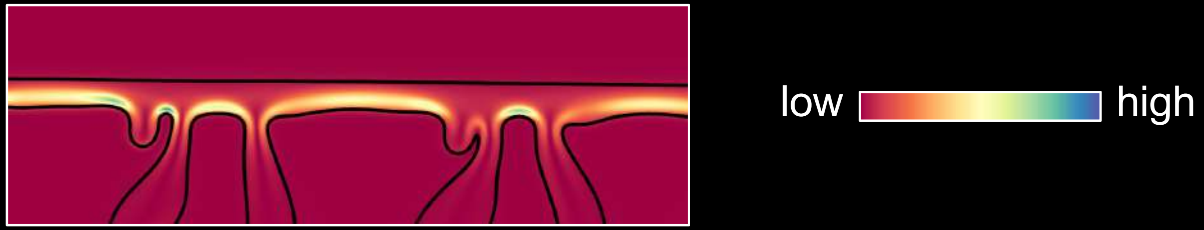


Mean dissipation and mixing

Model for dissipation during shutdown of convection $\chi = \langle |\nabla C|^2 \rangle$

1. Estimate local dissipation $|\nabla C|^2$

$$|\partial_x C| \approx |\partial_y C| \ll |\partial_z C|$$



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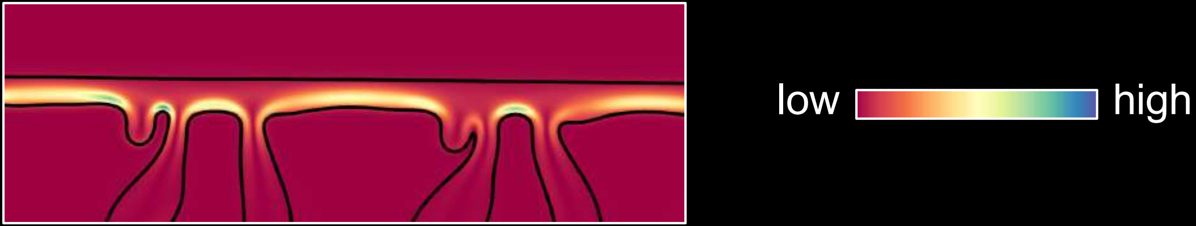

2. Estimate boundary layer thickness

$$\delta(t) = (C_+ - C_-)\, f(t) = \frac{f(t)}{1-\alpha}$$

$$C_+ - C_- = 1/(1-\alpha)$$

$$f(t) = [a_1 + (t - t_s)]/a_2$$

Interface deformation model
by Hidalgo et al. (2015)

Hidalgo, J., Dentz, M., Cabeza, Y., & Carrera, J. (2015). *Geophys. Res. Lett.*, 42 (15), 6357–6364.

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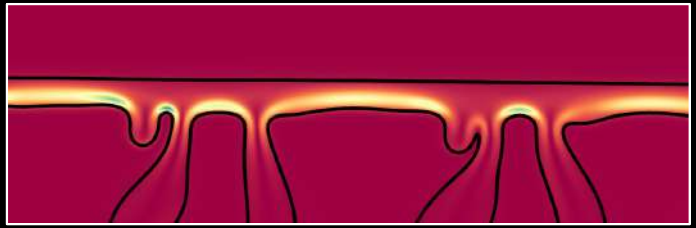

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Interface deformation model by Hidalgo et al. (2015)

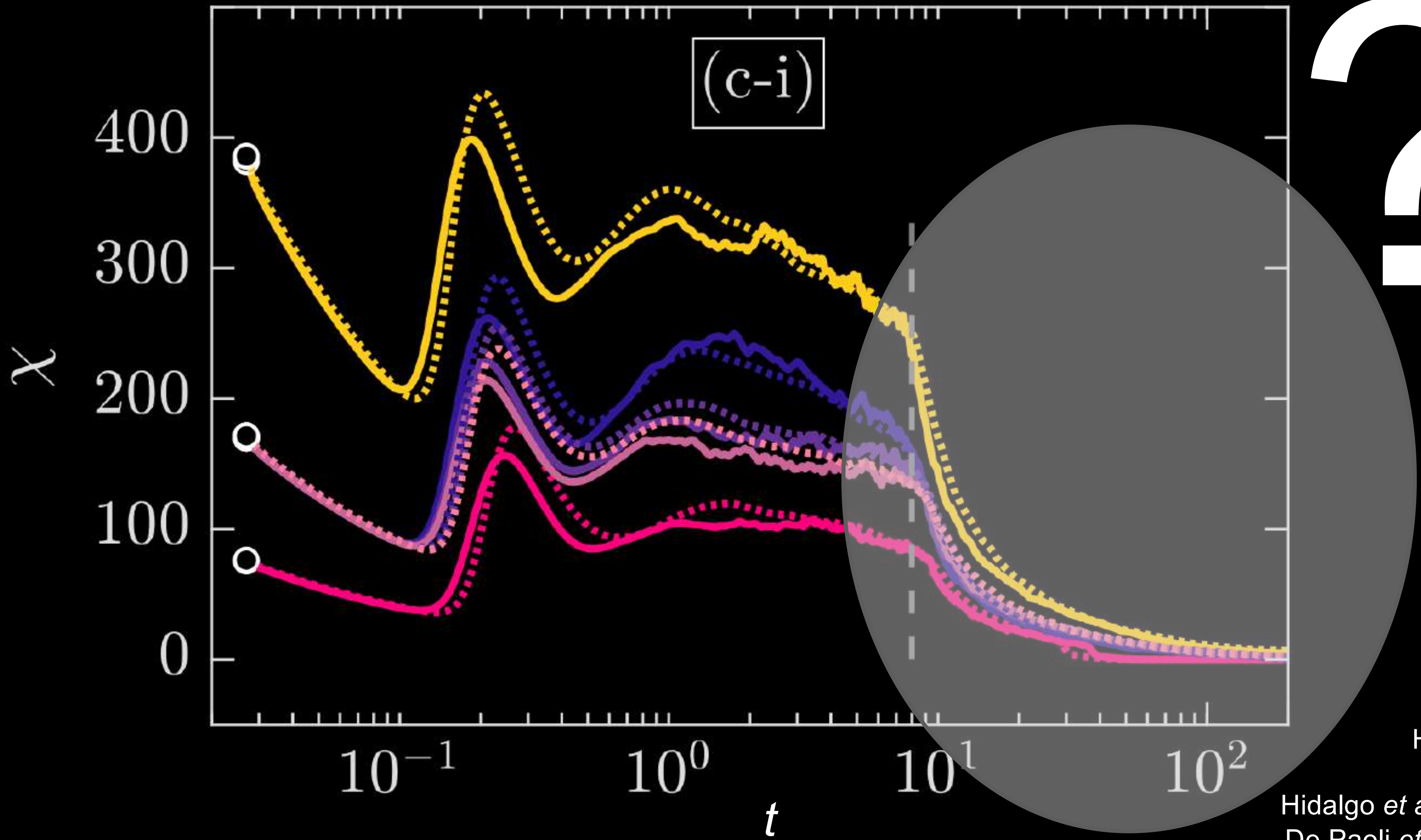
3. Combine and find dissipation

$$\chi = \langle|\nabla C|^2\rangle \approx \frac{\delta}{L_z}\left(\frac{C_+ - C_-}{\delta}\right)^2$$

$$\chi_{sd}(t) = \frac{1}{2(1-\alpha)f(t)}$$

Hidalgo, J., Dentz, M., Cabeza, Y., & Carrera, J. (2015). *Geophys. Res. Lett.*, 42 (15), 6357–6364.

Mean dissipation and mixing



?

Hewitt *et al.* (2013). *J. Fluid Mech.*, 719
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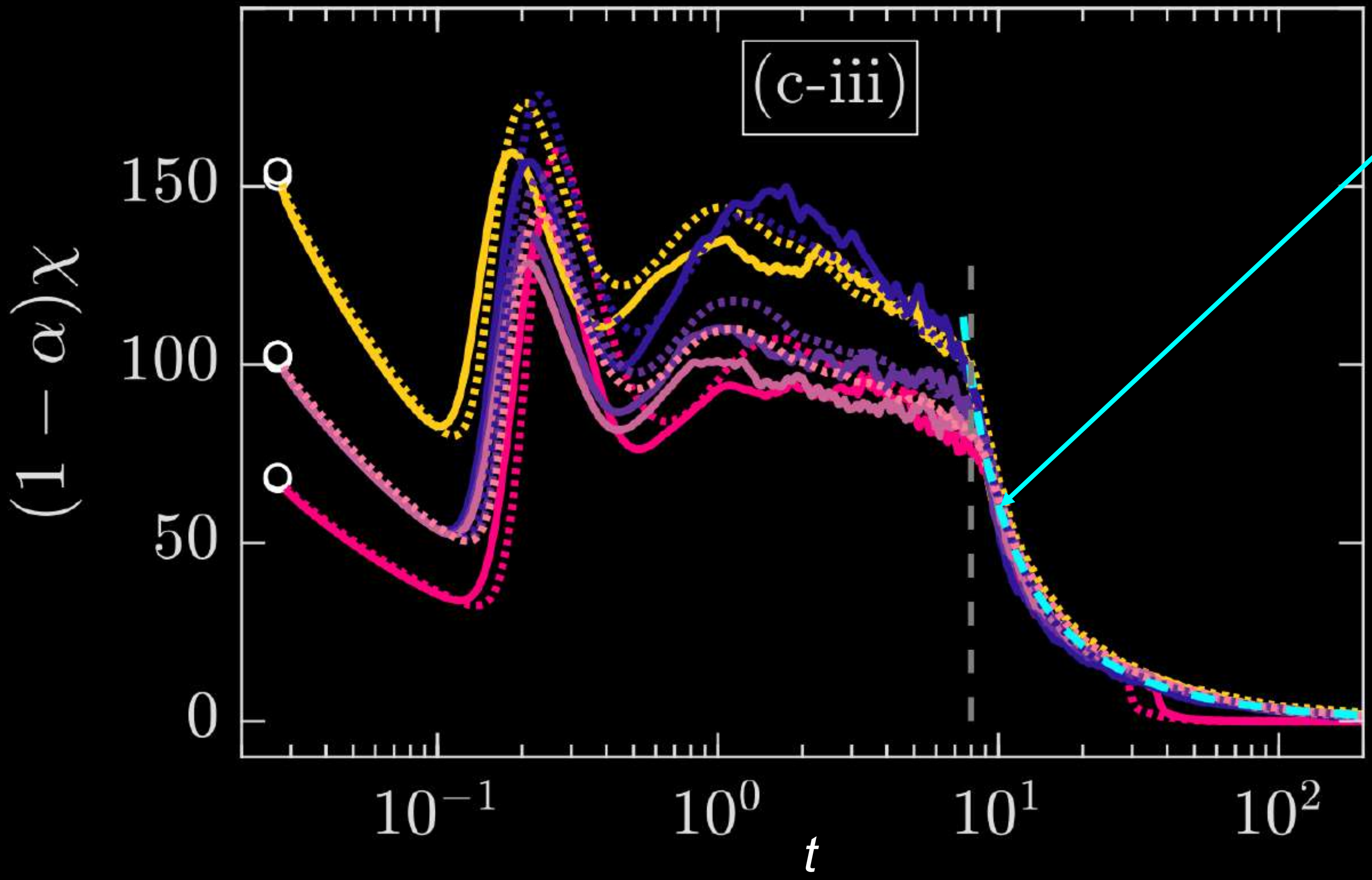
Mean dissipation and mixing

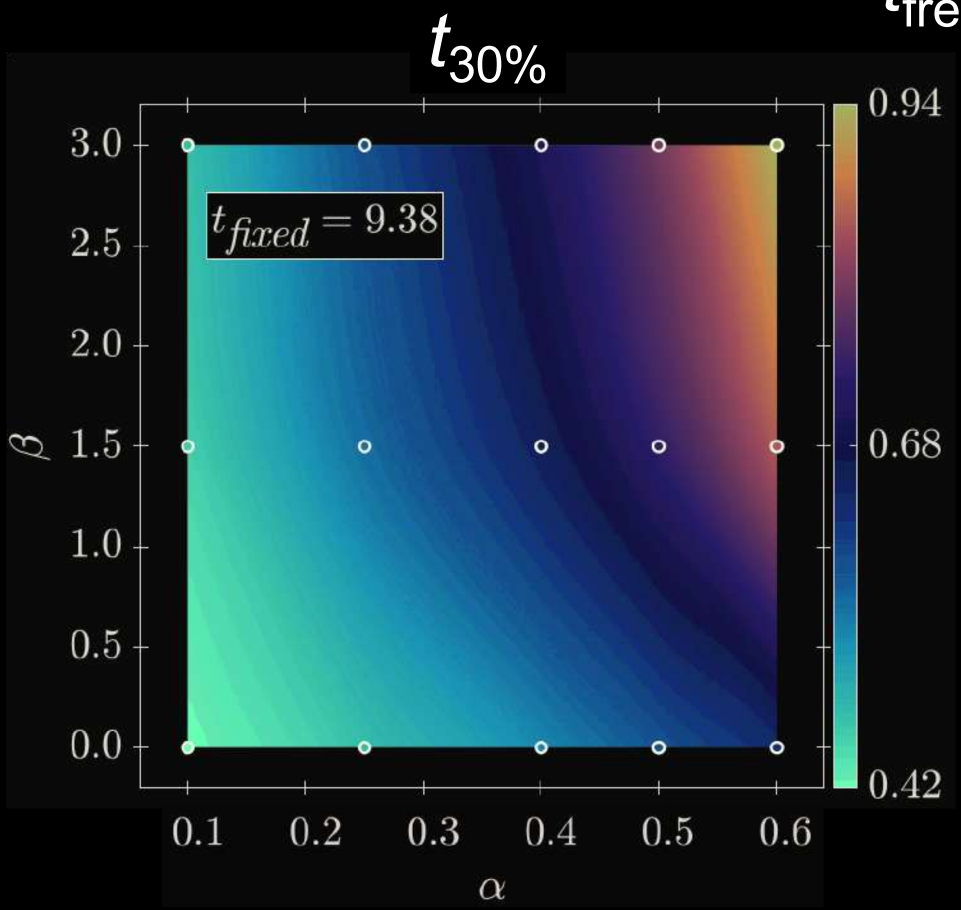


$$\chi_{sd}(t) = \frac{1}{2(1-\alpha)f(t)}$$

$$f(t) = [a_1 + (t - t_s)]/a_2$$

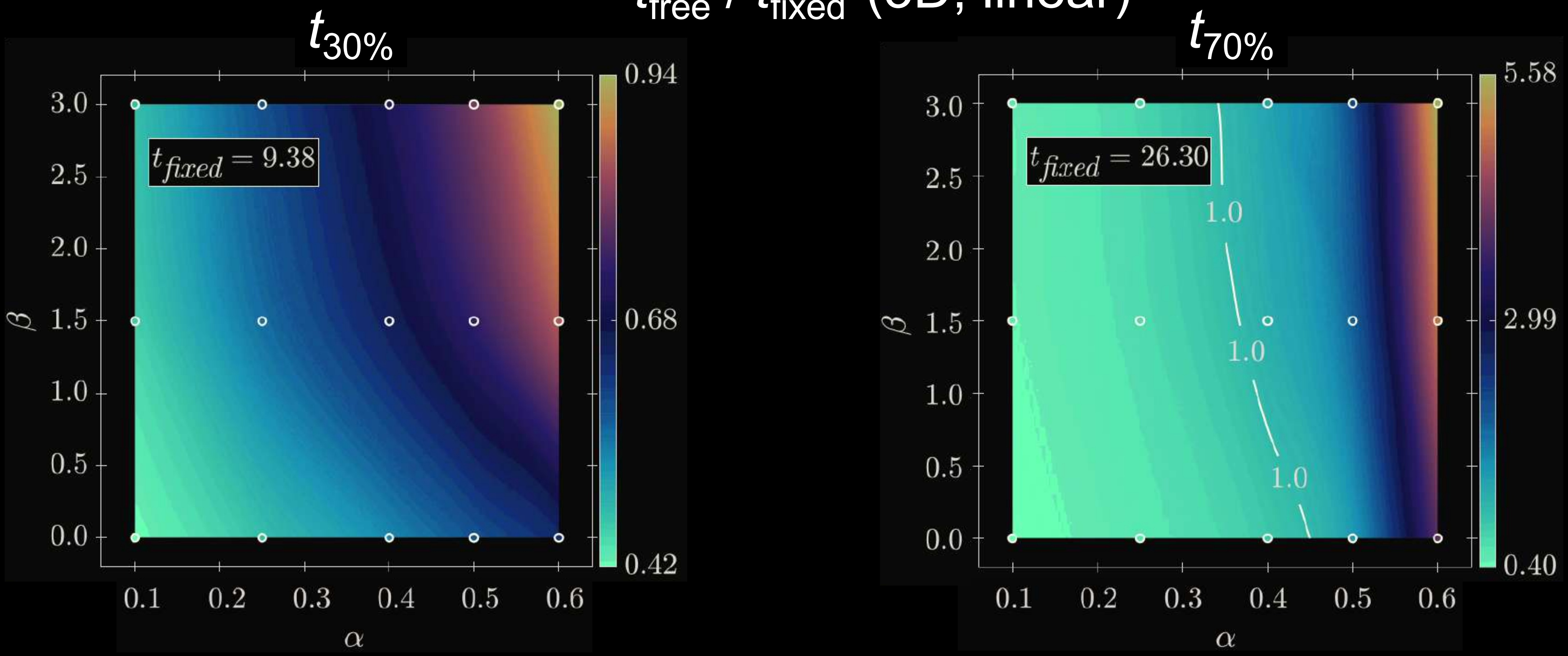
Time for mixing

t_{free} / t_{fixed} (3D, linear)



Time for mixing

t_{free} / t_{fixed} (3D, linear)



TU WIEN

Conclusions

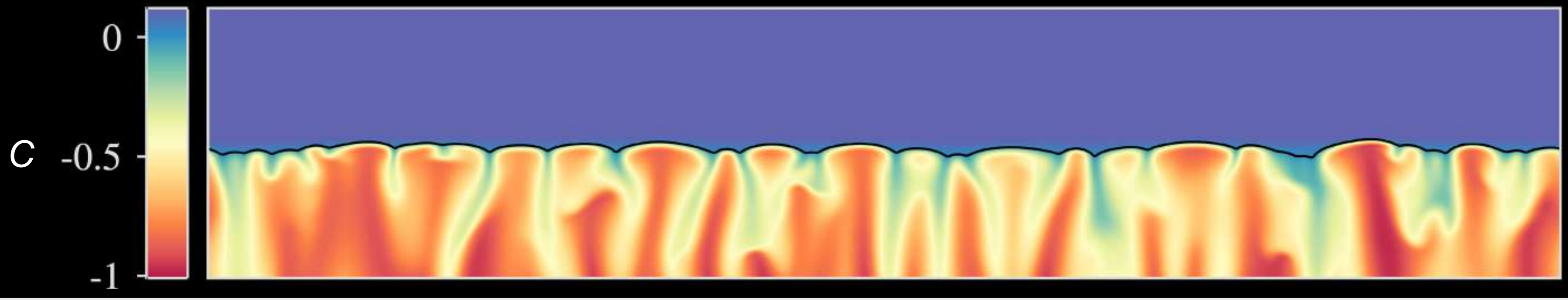
InterPore

Theoretical framework for comparison of system with different b.c. and fluid models

De Paoli & Pirozzoli (*arXiv:2604.23199*

preprint

data



α = 0.1
β = 1.5

Conclusions

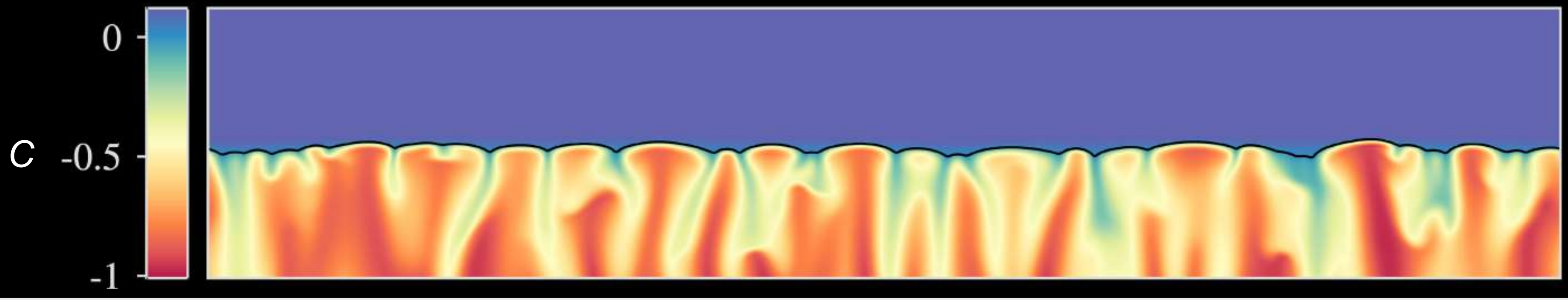
Theoretical framework for comparison of system with different b.c. and fluid models

Understanding and modelling of mixing dynamics

De Paoli & Pirozzoli (*arXiv:2604.23199*)

preprint

data



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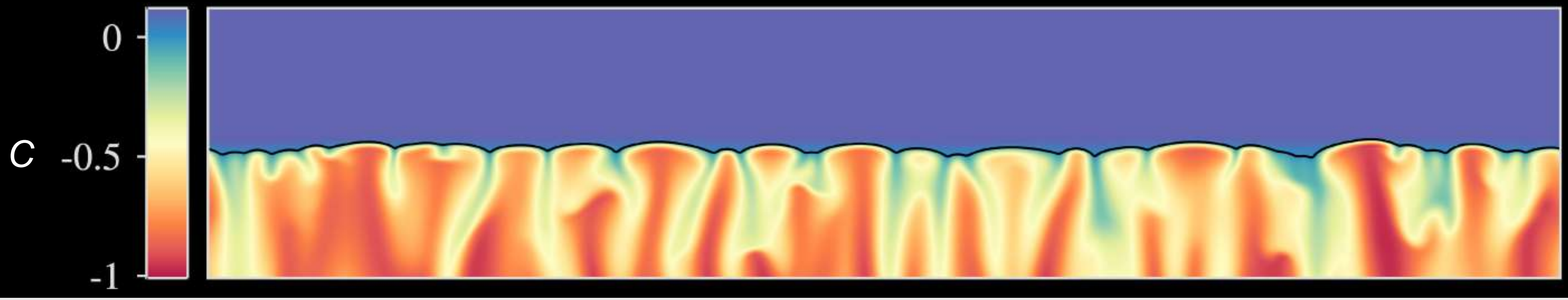

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Understanding and modelling of mixing dynamics

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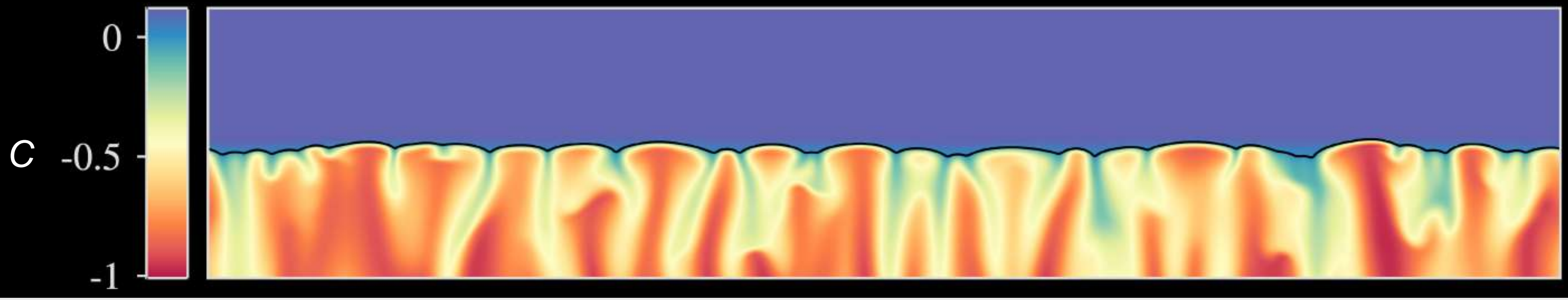
Funded by the European Union (ERC, MORPHOS, 101163625). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them. The results presented have been achieved using in part the Vienna Scientific Cluster (VSC).

De Paoli & Pirozzoli
(*arXiv:2604.23199*)

preprint

data



$\alpha = 0.1$
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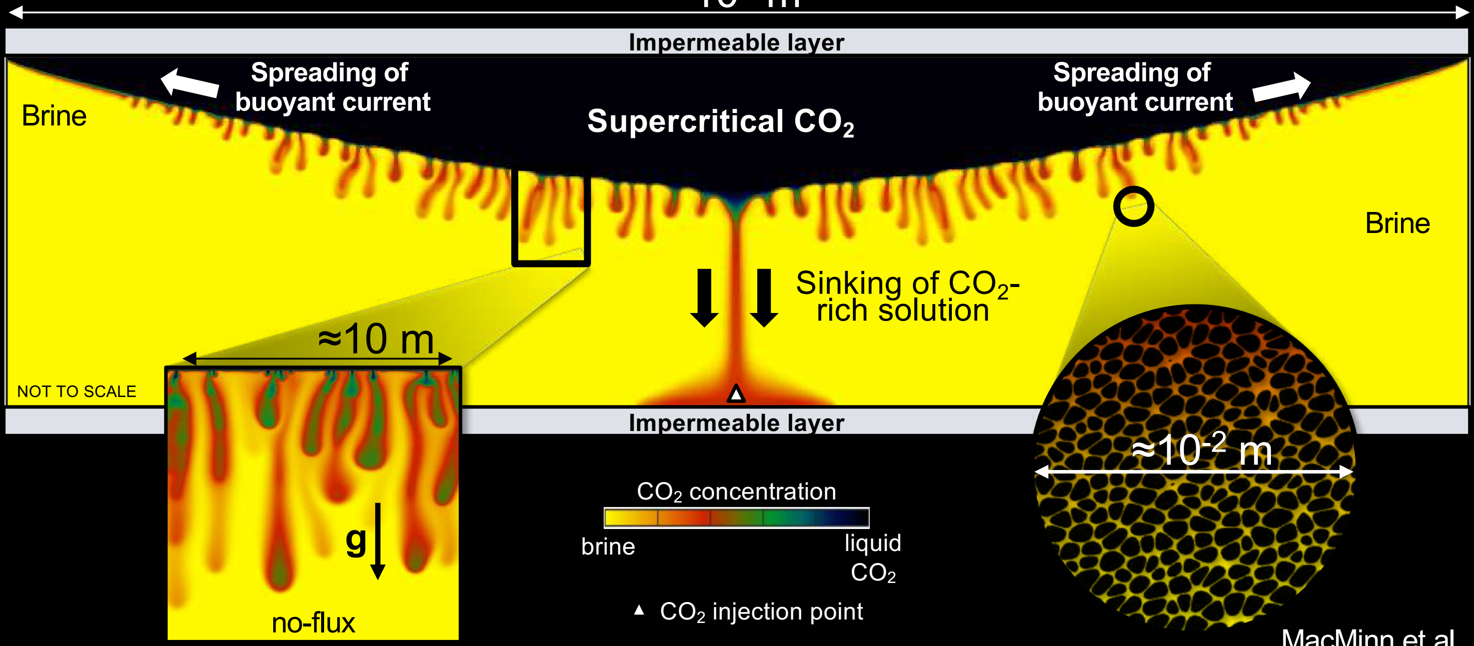
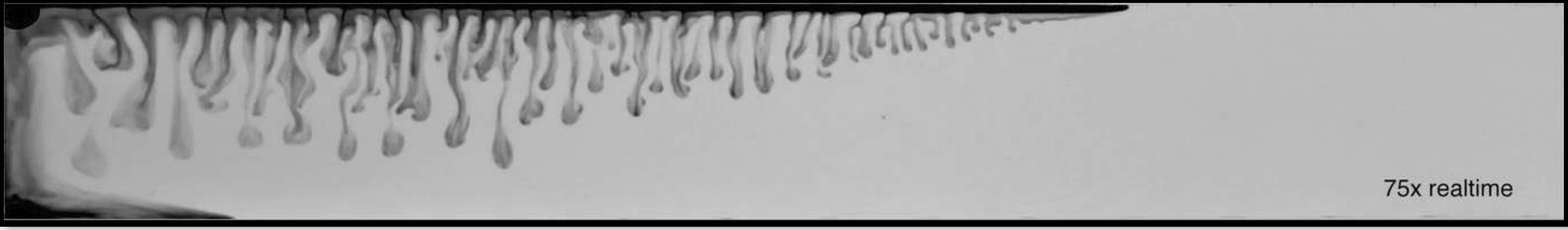
Backup slides

Carbon Capture and Storage

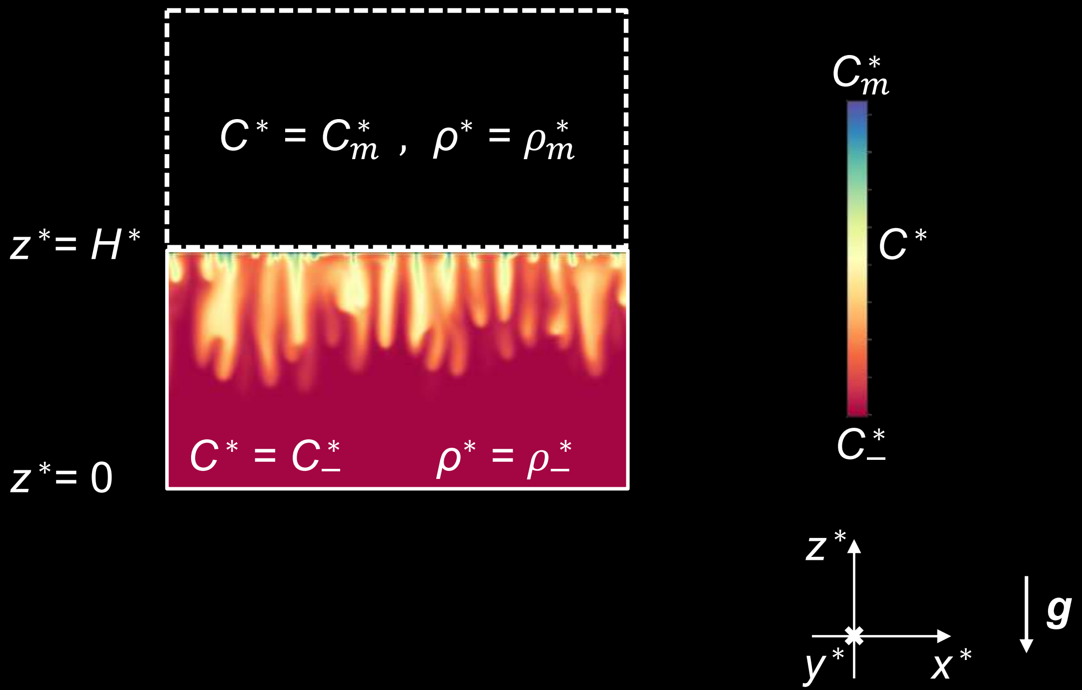
De Paoli, *Phys. Fluids* (2021)



MacMinn et al., *Geophys. Res. Lett.* (2013)



(a) fixed interface



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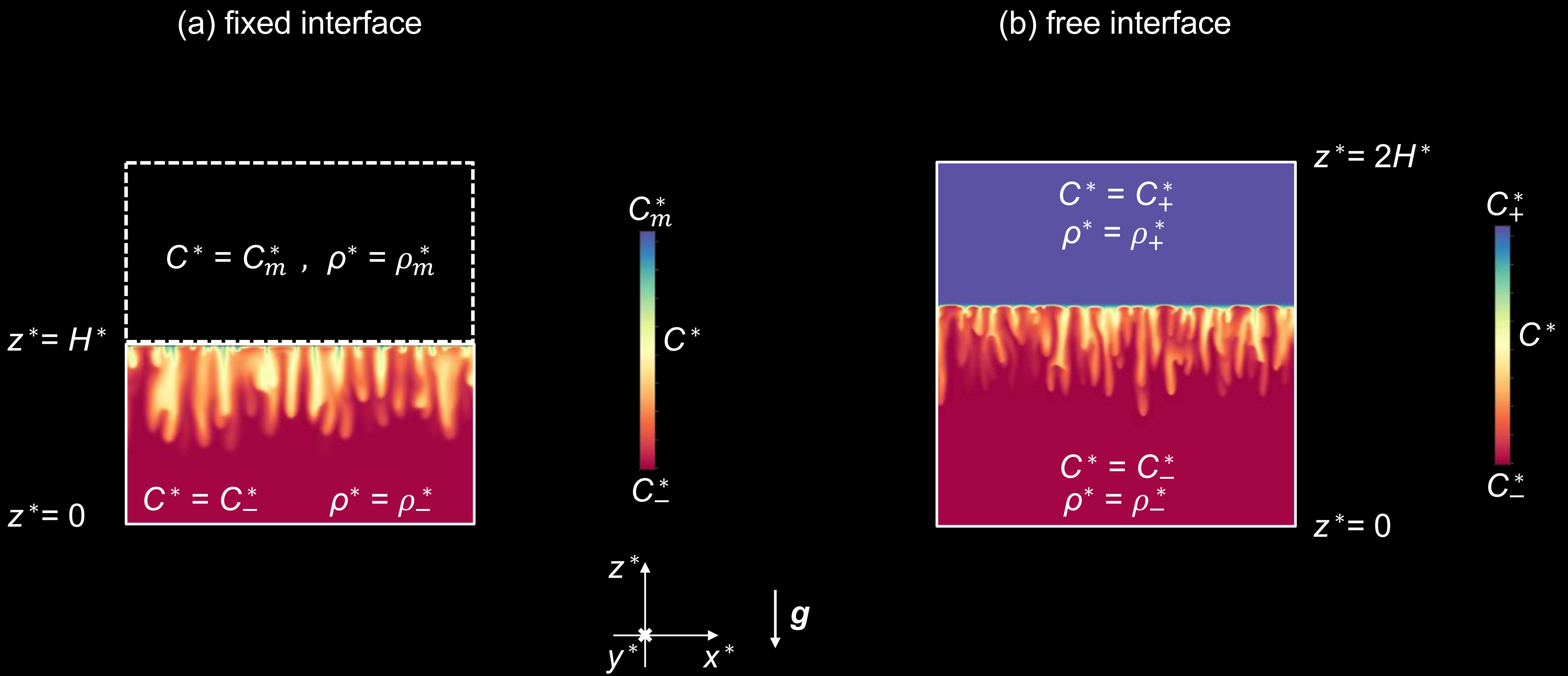
Boundary conditions



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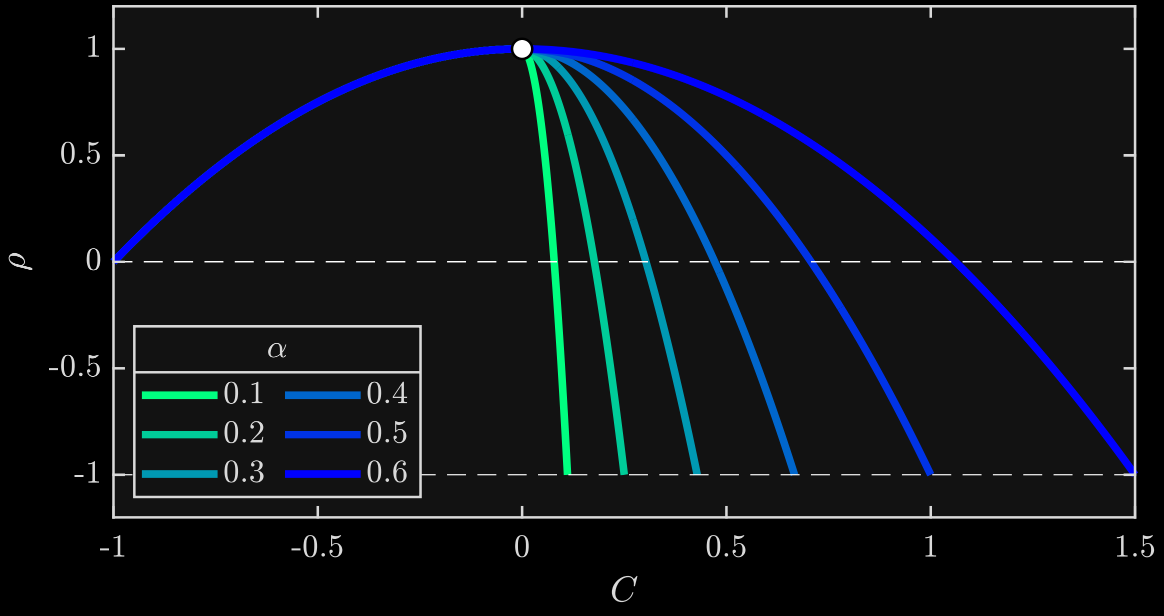
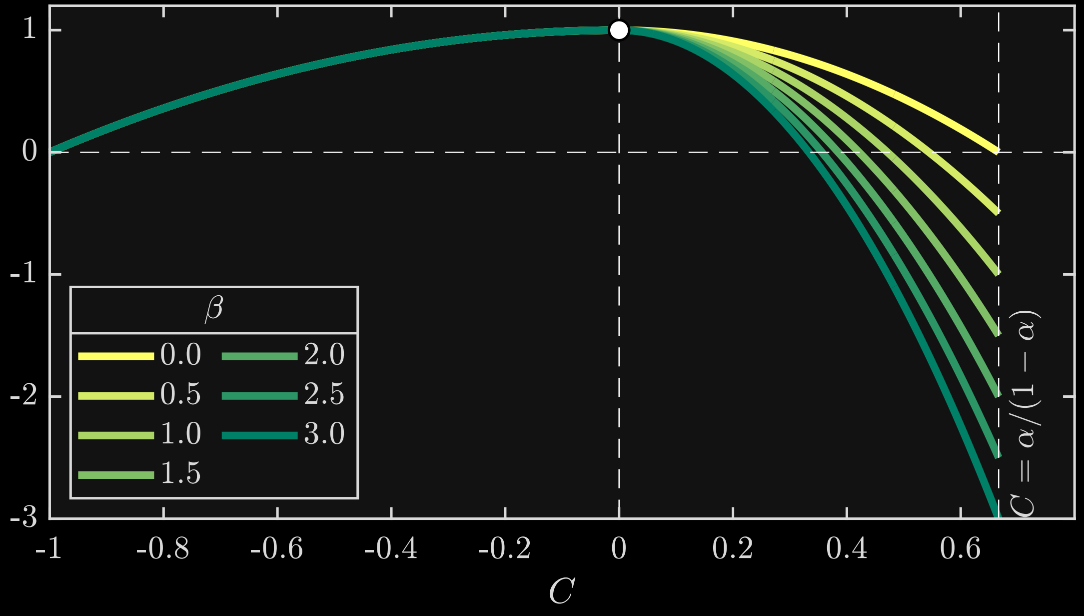
Fluid models

Effect of α



Effect of β

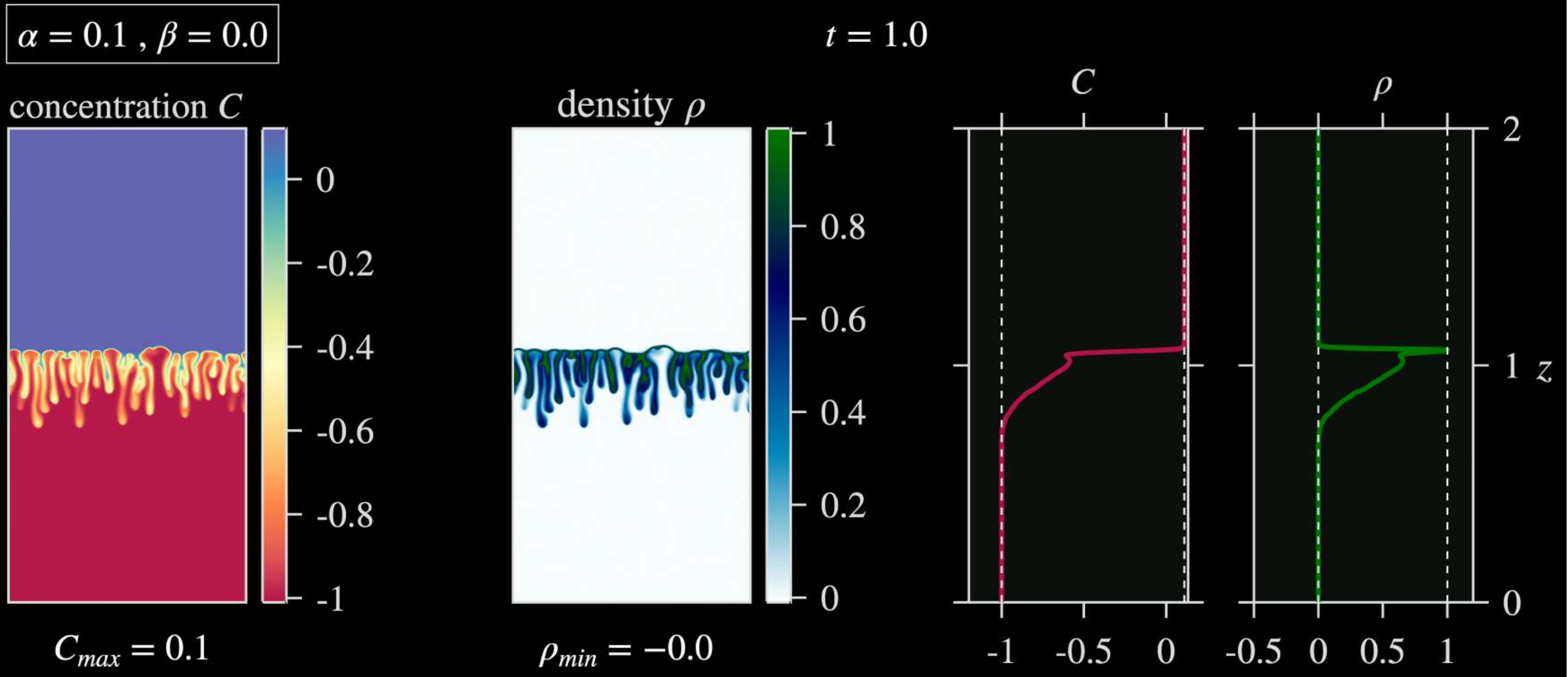


$$Ra_0 = \frac{\mathscr{U}^* H^*}{\phi D} \quad , \quad \alpha = \frac{C_+^* - C_m^*}{C_+^* - C_-^*} \quad , \quad \beta = \frac{\rho_-^* - \rho_+^*}{\rho_m^* - \rho_-^*}$$

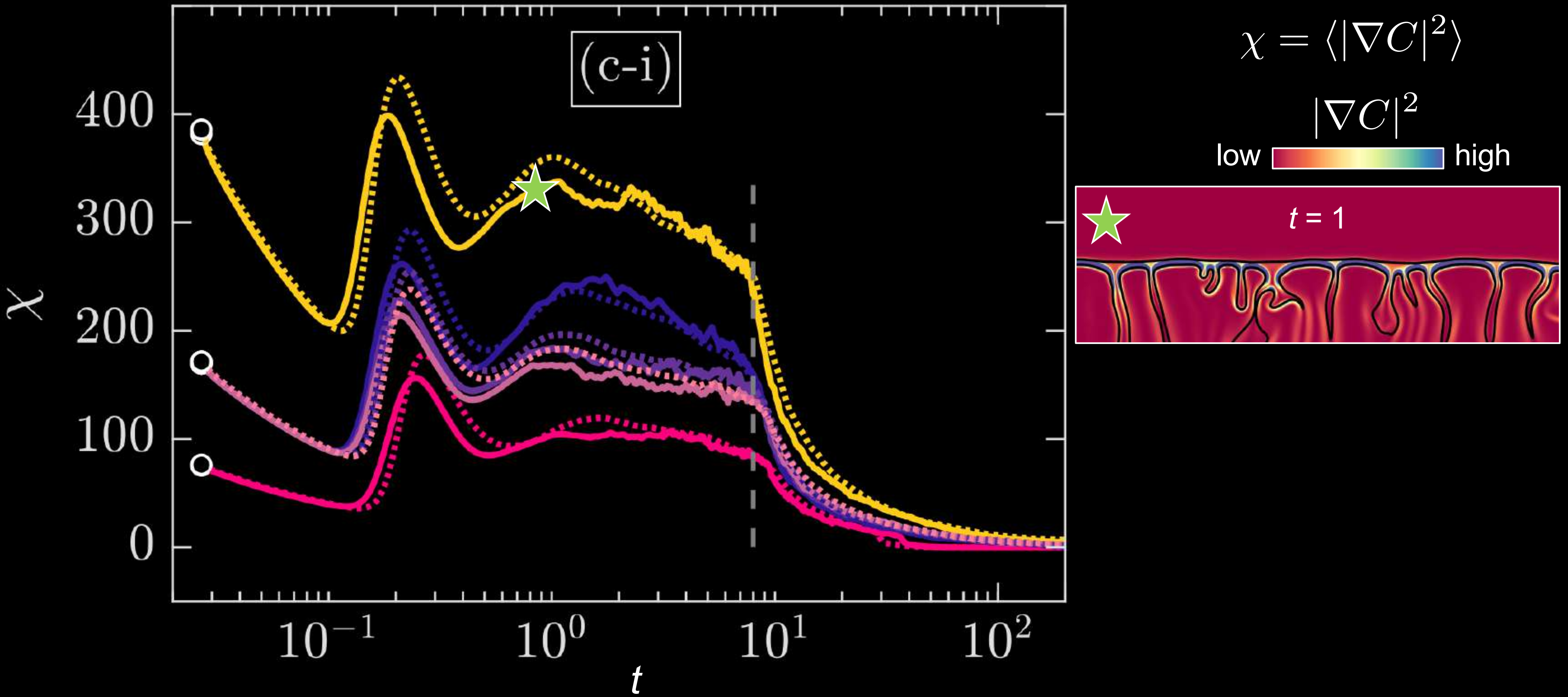
In this work
Ra_0 = 10^4

De Paoli & Pirozzoli (2026), *arXiv:2604.23199*

Free-interface dynamics (2D)

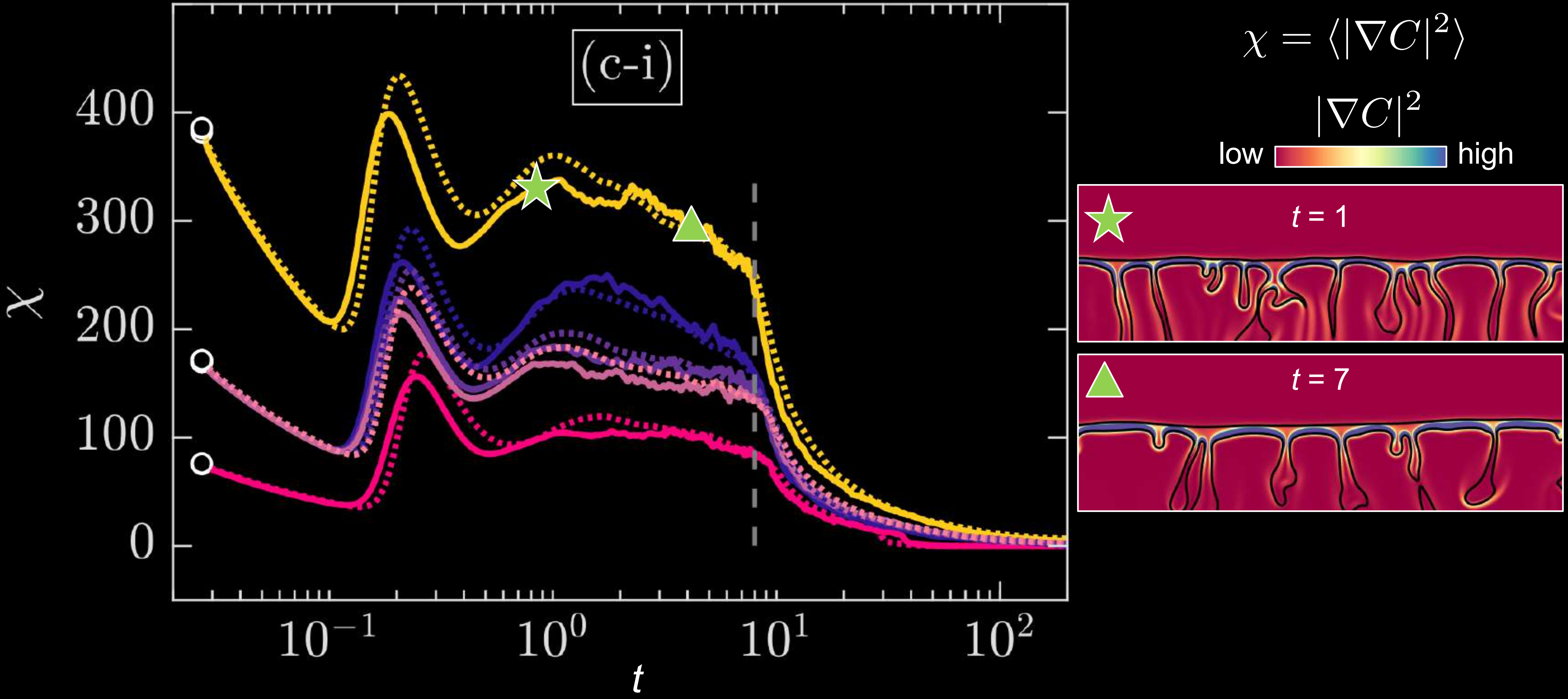


Mean dissipation and mixing



Mean dissipation and mixing

$$\chi = \langle |\nabla C|^2 \rangle$$



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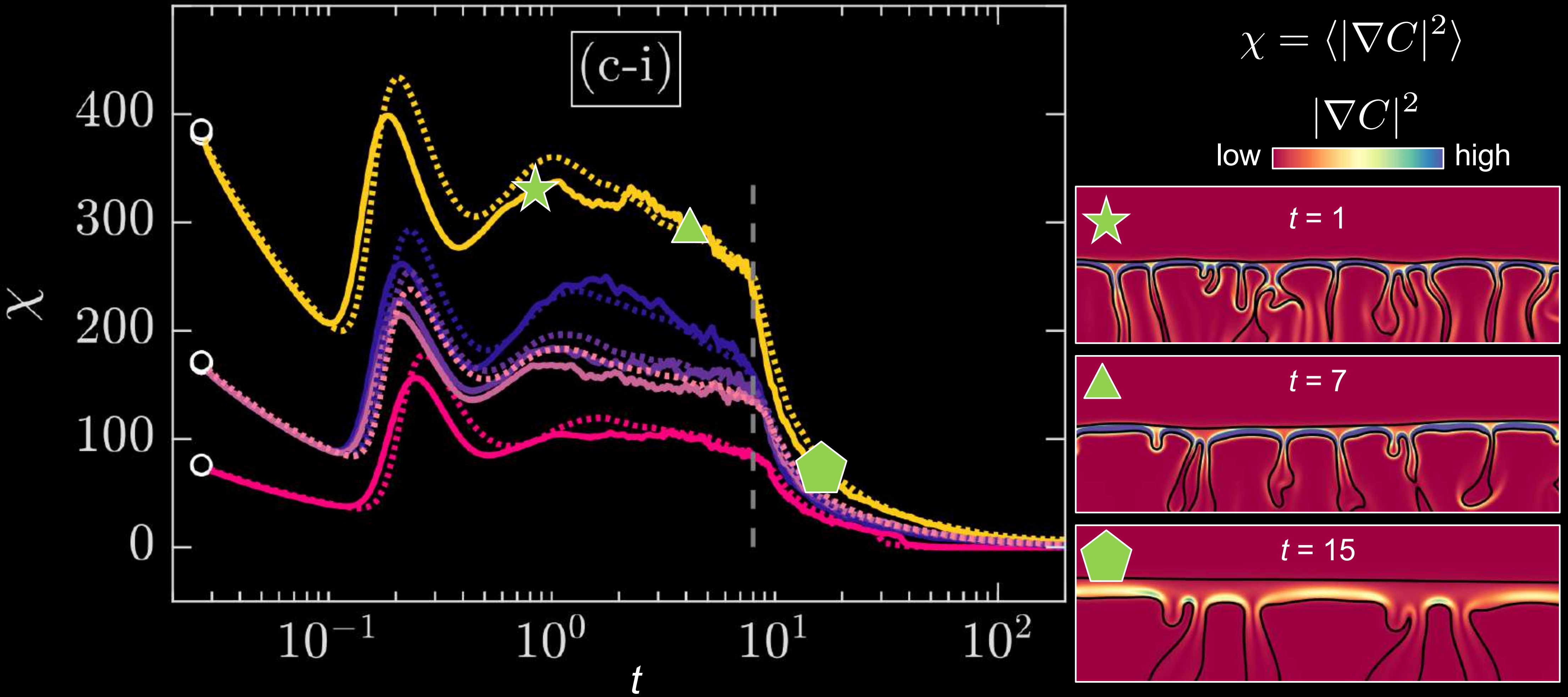
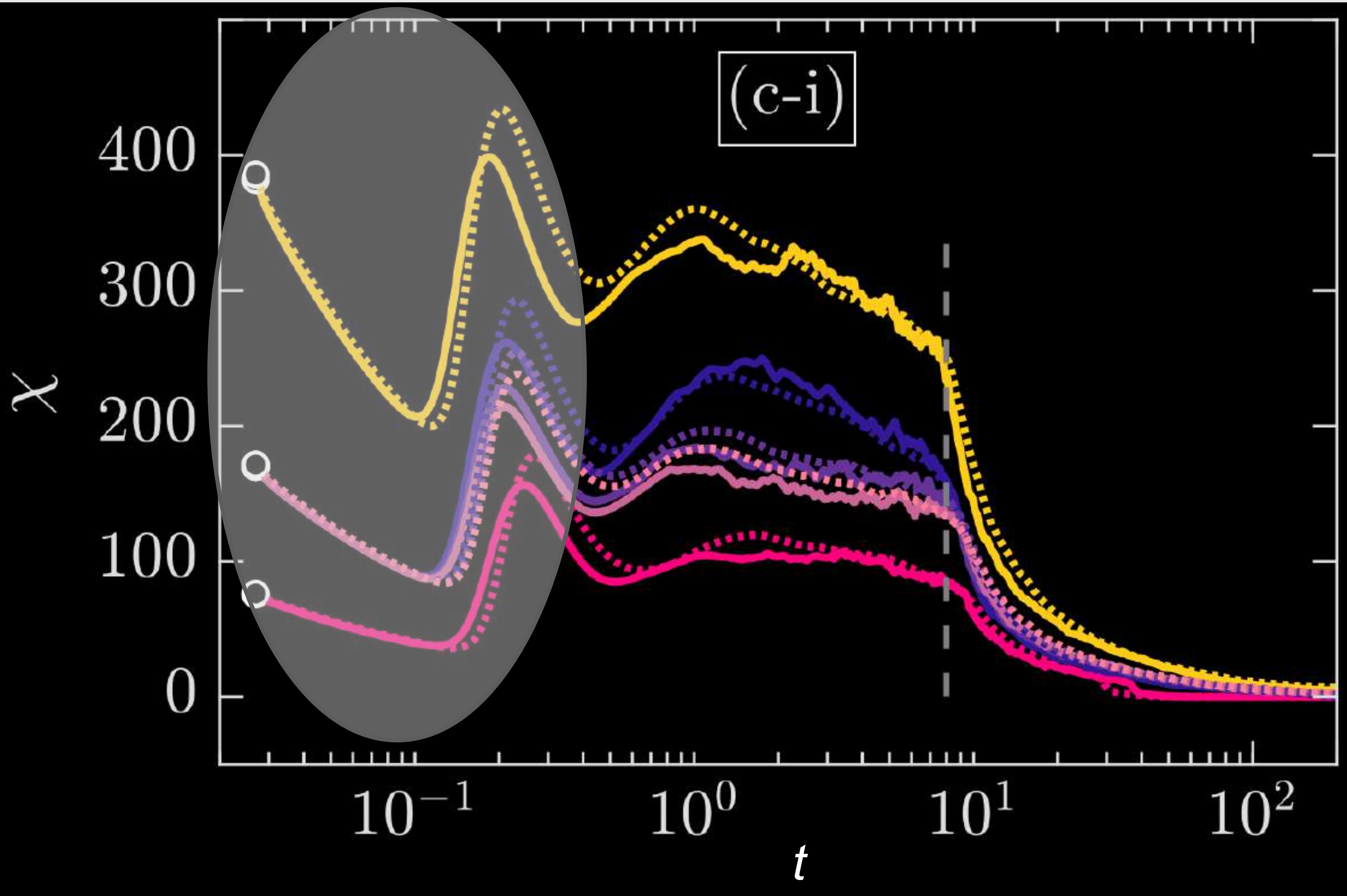


Mean dissipation and mixing



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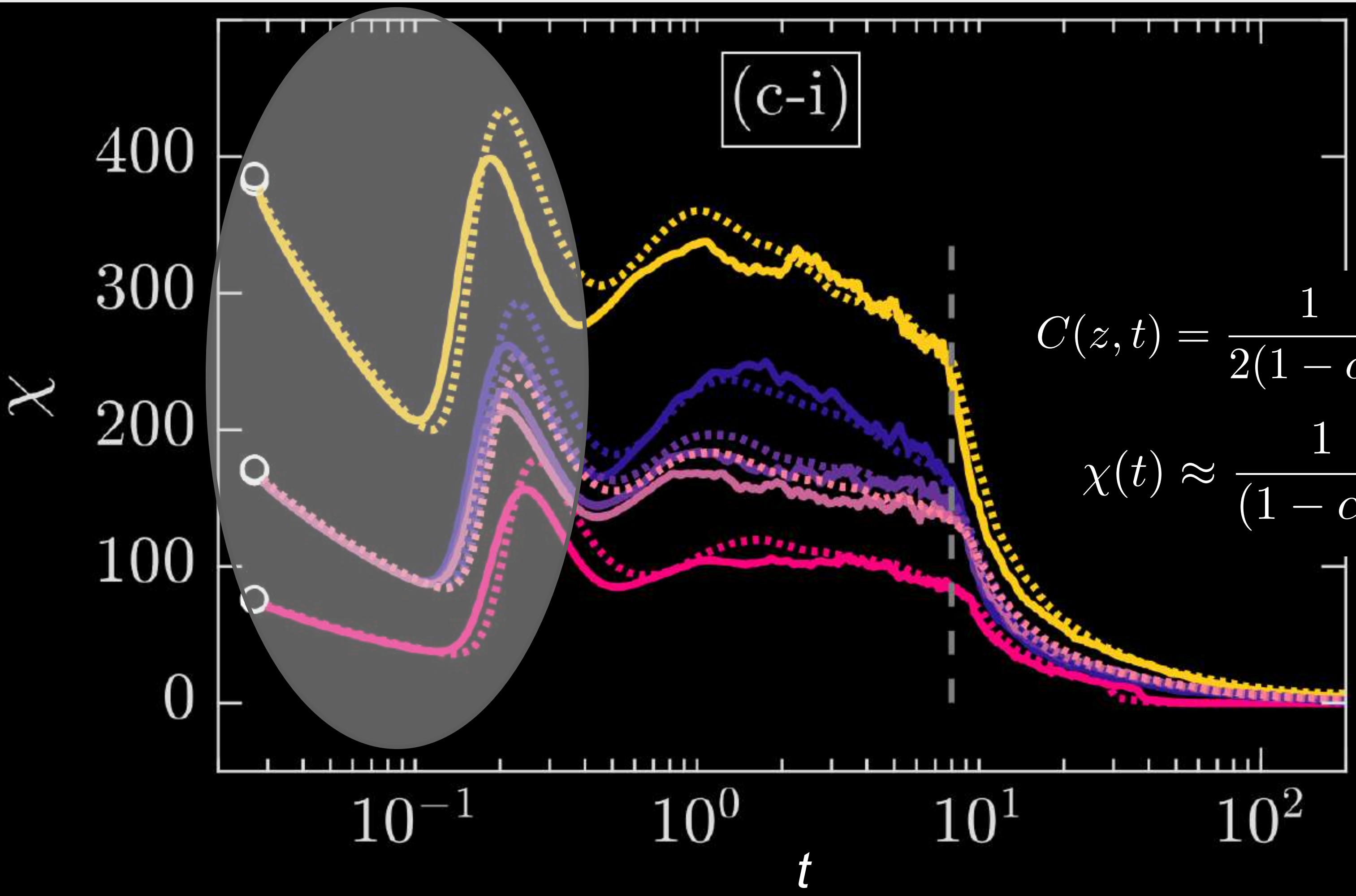
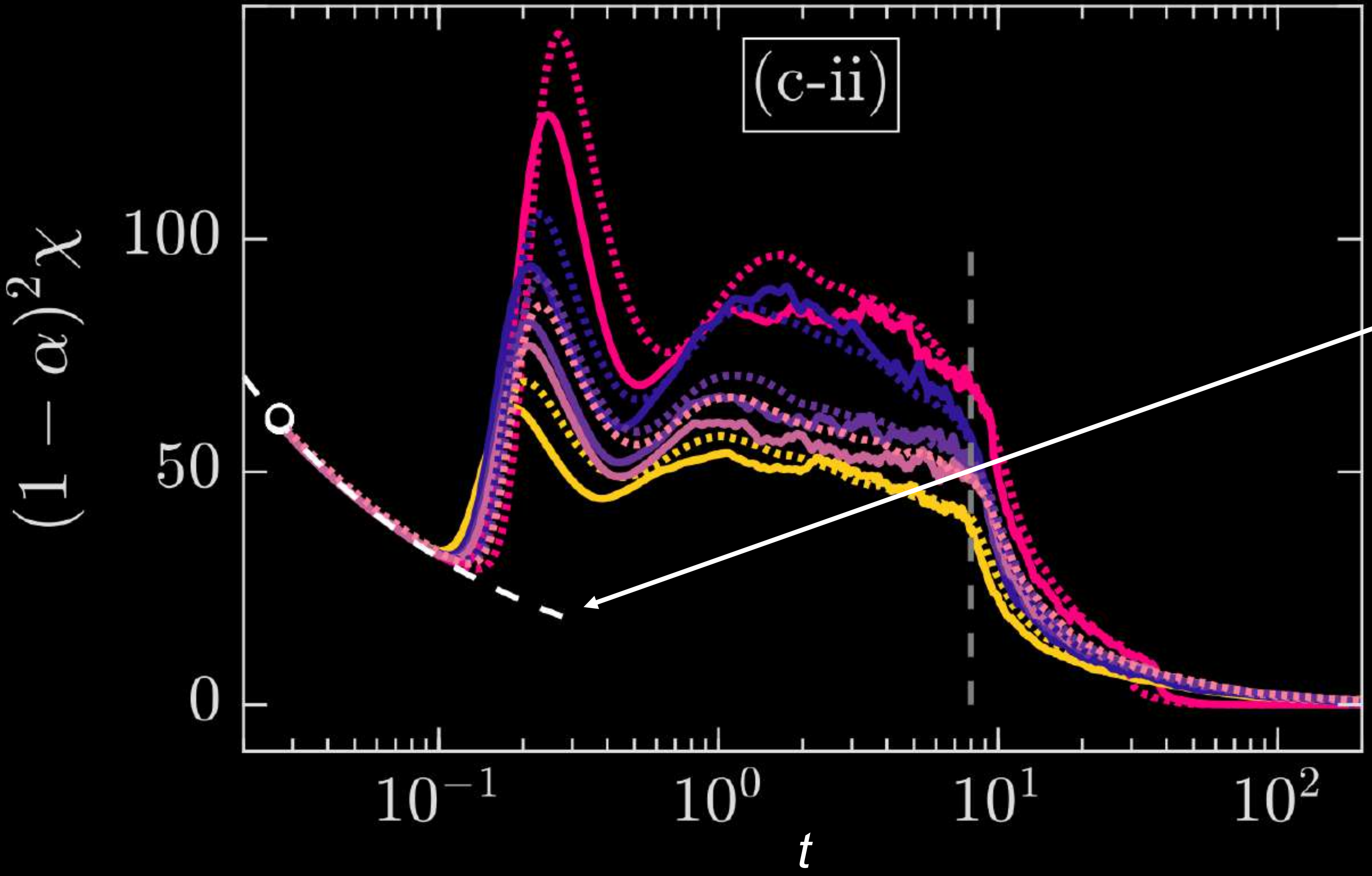


$$\chi = \langle |\nabla C|^2 \rangle$$

Diffusive solution

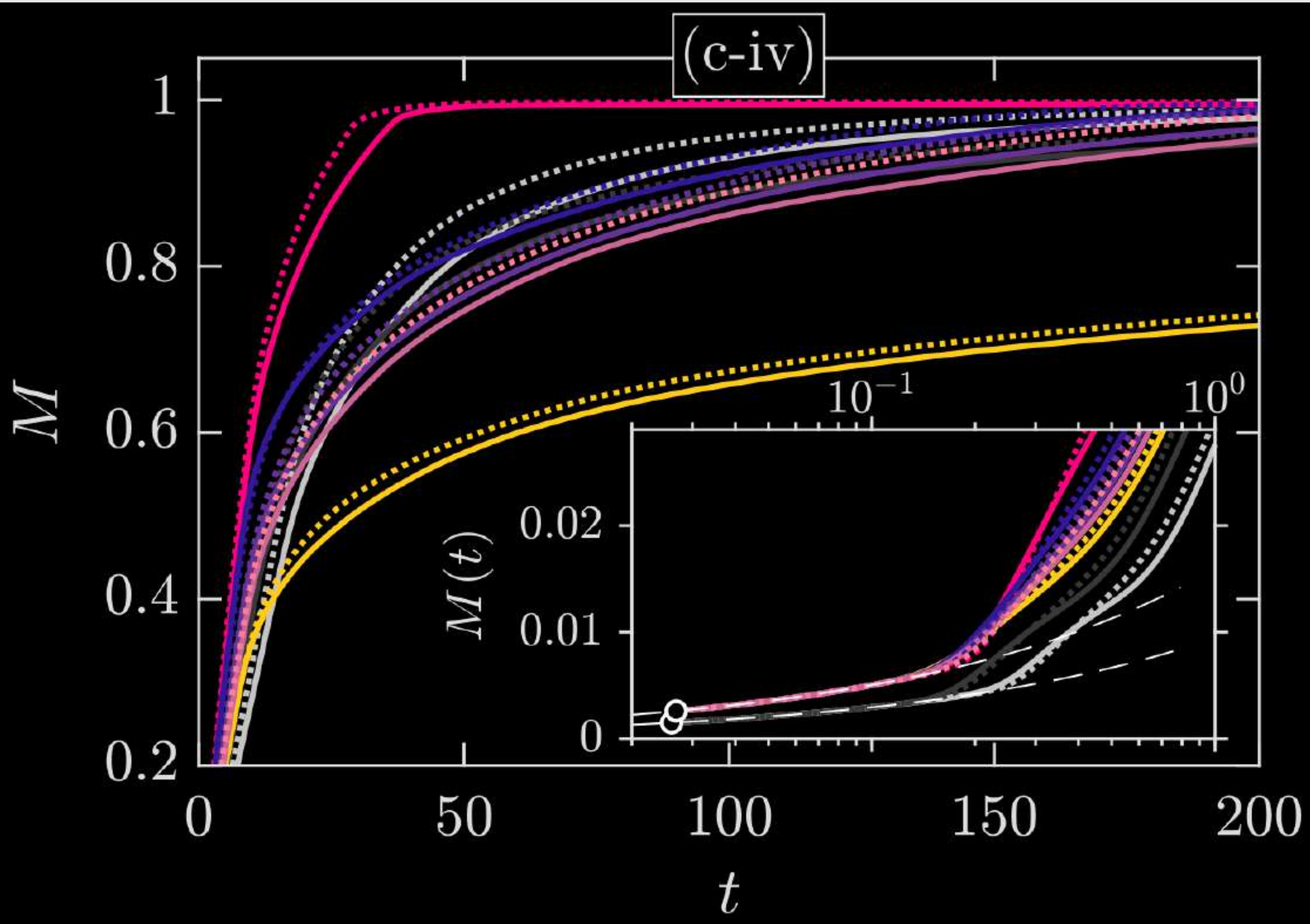
$$C(z,t) = \frac{1}{2(1-\alpha)}\left[2\alpha - 1 + \mathrm{erf}\left(\frac{(z-1)\,Ra}{2\sqrt{t\,Ra}}\right)\right]$$

$$\chi(t) \approx \frac{1}{(1-\alpha)^2}\frac{1}{4}\sqrt{\frac{Ra}{2\pi t}}.$$



$$\chi(t) \approx \frac{1}{(1-\alpha)^2}\frac{1}{4}\sqrt{\frac{Ra}{2\pi t}}.$$

Degree of mixing



$$M(t) = \frac{8(1-\alpha)^2}{Ra} \int_0^t \chi \, \mathrm{d}t$$

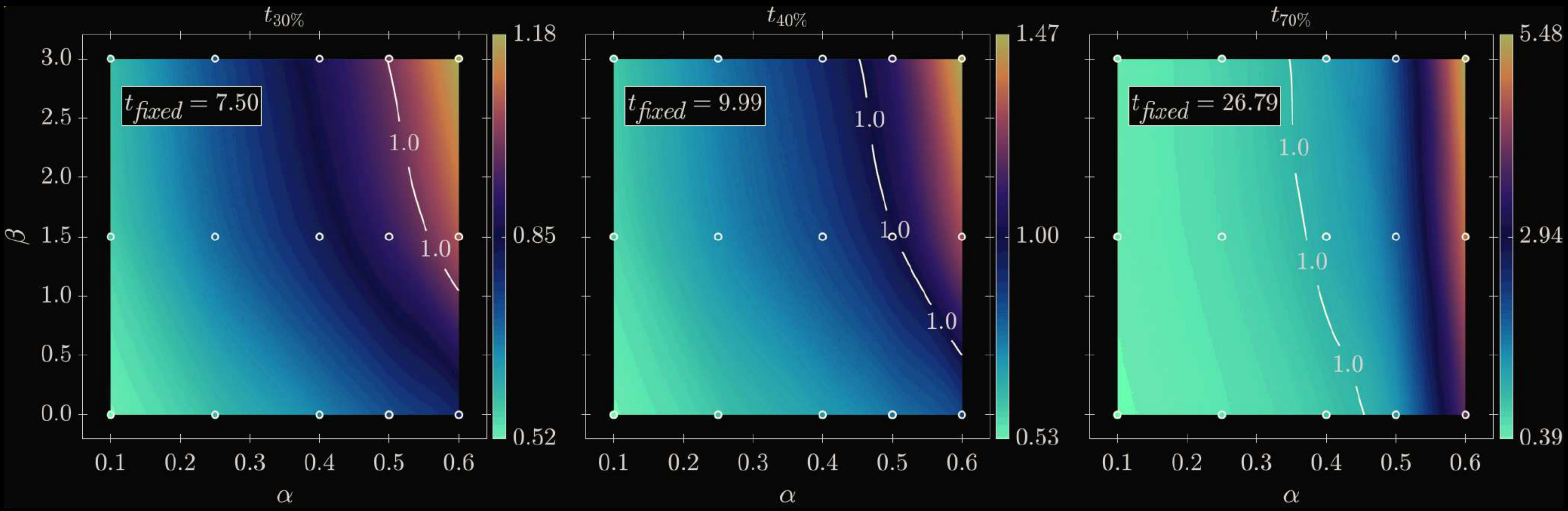
fixed interface

A1 (2D) A3 (3D)
A2 (2D) A4 (3D)

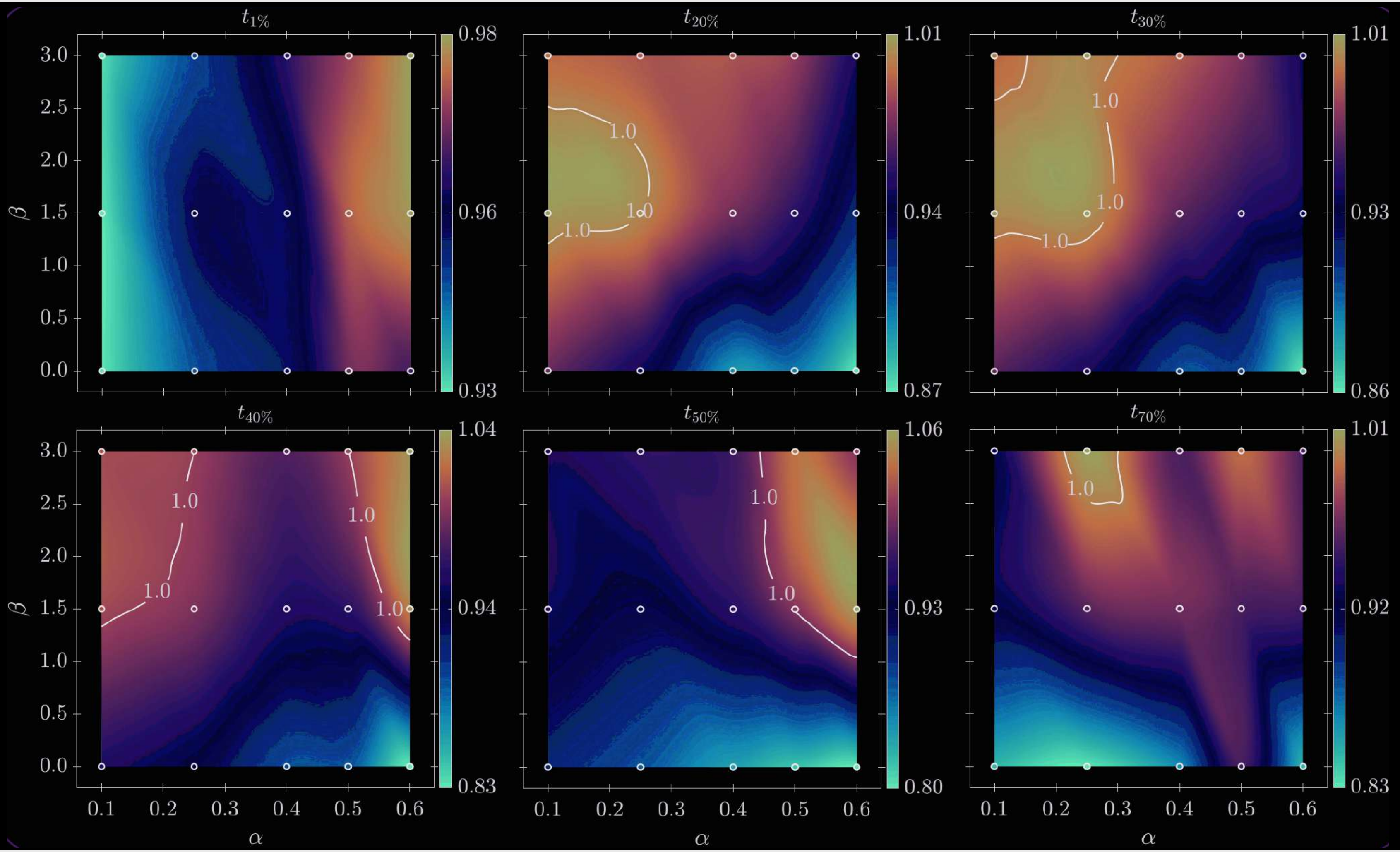
free interface

B1 (2D) B4 (3D)
B2 (2D) B5 (3D)
B3 (2D) B6 (3D)
C1 (2D) C4 (3D)
C2 (2D) C5 (3D)
C3 (2D) C6 (3D)

t_{free} / t_{fixed} (3D, parabolic)

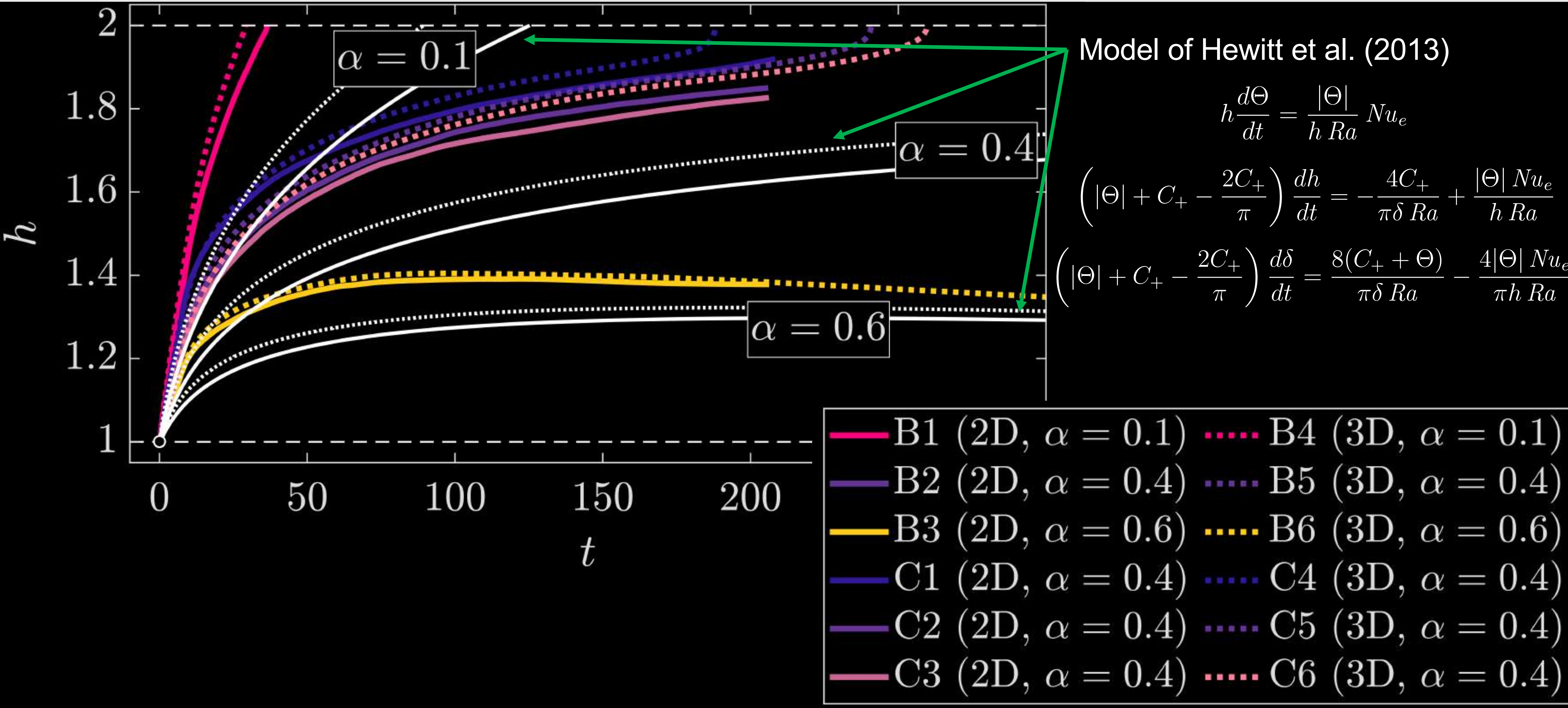


Time for mixing



t_{2D} / t_{3D}
(free interface)

Interface position



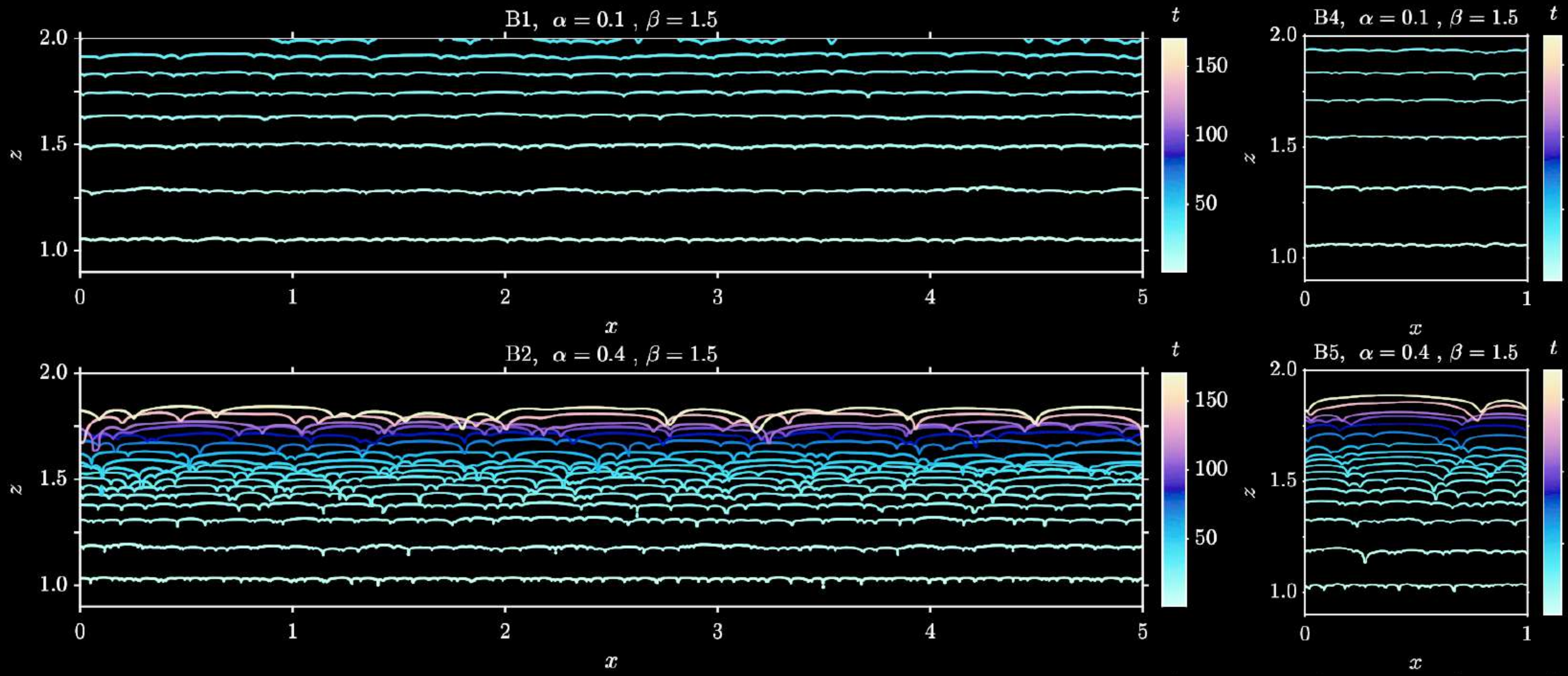
Model of Hewitt et al. (2013)

$$h\frac{d\Theta}{dt} = \frac{|\Theta|}{h\,Ra} Nu_e$$

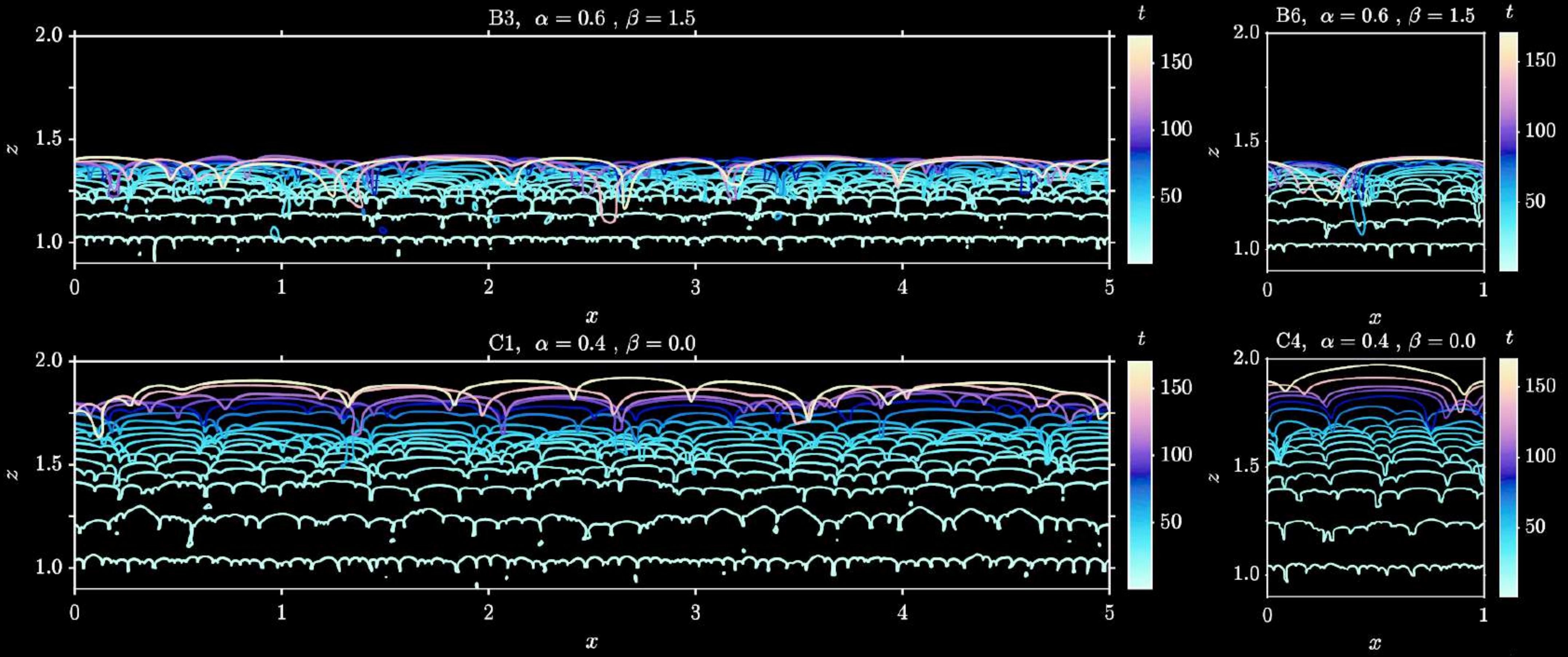
$$\left(|\Theta| + C_+ - \frac{2C_+}{\pi}\right)\frac{dh}{dt} = -\frac{4C_+}{\pi\delta\,Ra} + \frac{|\Theta|\,Nu_e}{h\,Ra}$$

$$\left(|\Theta| + C_+ - \frac{2C_+}{\pi}\right)\frac{d\delta}{dt} = \frac{8(C_+ + \Theta)}{\pi\delta\,Ra} - \frac{4|\Theta|\,Nu_e}{\pi h\,Ra}$$

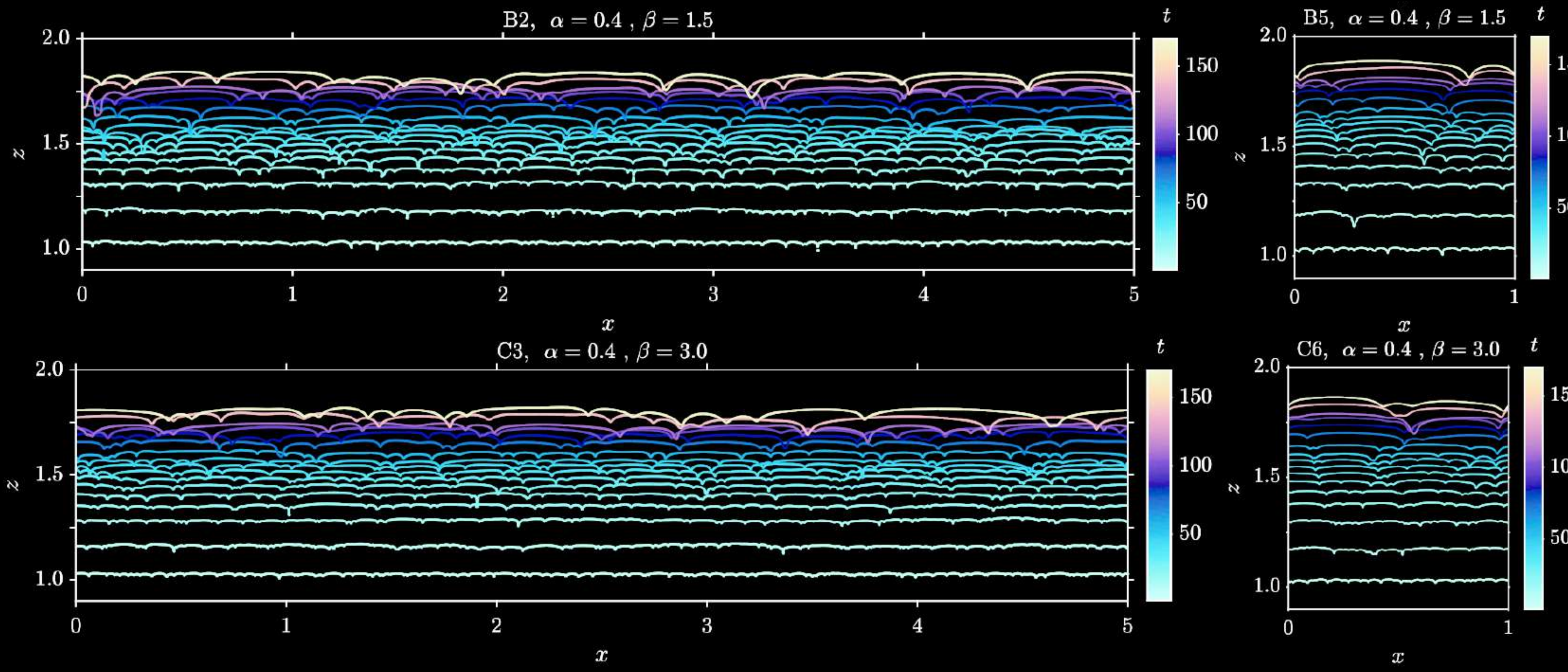
Interface dynamics



Interface dynamics



Interface dynamics



Simulations details

Sim.	interface/b.c.	Ra	$\rho(C)$	α	β	L_x	L_y	L_z	N_x	N_y	N_z
A1	fixed/(8)	1×10^4	linear (S6)	-	-	5	-	1	5120	1	256
A2	fixed/(8)	1×10^4	parabolic (S7)	-	-	5	-	1	5120	1	256
A3	fixed/(8)	1×10^4	linear (S6)	-	-	1	1	1	1024	1024	256
A4	fixed/(8)	1×10^4	parabolic (S7)	-	-	1	1	1	1024	1024	256
B1	free/(9)	1×10^4	piecewise (S8)	0.1	1.5	5	-	2	5120	1	1024
B2≡C2	free/(9)	1×10^4	piecewise (S8)	0.4	1.5	5	-	2	5120	1	1024
B3	free/(9)	1×10^4	piecewise (S8)	0.6	1.5	5	-	2	5120	1	1024
B4	free/(9)	1×10^4	piecewise (S8)	0.1	1.5	1	1	2	1024	1024	1024
B5≡C5	free/(9)	1×10^4	piecewise (S8)	0.4	1.5	1	1	2	1024	1024	1024
B6	free/(9)	1×10^4	piecewise (S8)	0.6	1.5	1	1	2	1024	1024	1024
C1	free/(9)	1×10^4	piecewise (S8)	0.4	0.0	5	-	2	5120	1	1024
C2≡B2	free/(9)	1×10^4	piecewise (S8)	0.4	1.5	5	-	2	5120	1	1024
C3	free/(9)	1×10^4	piecewise (S8)	0.4	3.0	5	-	2	5120	1	1024
C4	free/(9)	1×10^4	piecewise (S8)	0.4	0.0	1	1	2	1024	1024	1024
C5≡B5	free/(9)	1×10^4	piecewise (S8)	0.4	1.5	1	1	2	1024	1024	1024
C6	free/(9)	1×10^4	piecewise (S8)	0.4	3.0	1	1	2	1024	1024	1024

Simulations details

Sim.	interface/b.c.	Ra	$\rho(C)$	α	β	L_x	L_y	L_z	N_x	N_y	N_z
D1	free/(9)	1×10^4	piecewise (S8)	0.25	0.0	5	-	2	5120	1	1024
D2	free/(9)	1×10^4	piecewise (S8)	0.25	1.5	5	-	2	5120	1	1024
D3	free/(9)	1×10^4	piecewise (S8)	0.25	3.0	5	-	2	5120	1	1024
D4	free/(9)	1×10^4	piecewise (S8)	0.5	0.0	5	-	2	5120	1	1024
D5	free/(9)	1×10^4	piecewise (S8)	0.5	1.5	5	-	2	5120	1	1024
D6	free/(9)	1×10^4	piecewise (S8)	0.5	3.0	5	-	2	5120	1	1024
D7	free/(9)	1×10^4	piecewise (S8)	0.25	0.0	1	1	2	1024	1024	1024
D8	free/(9)	1×10^4	piecewise (S8)	0.25	1.5	1	1	2	1024	1024	1024
D9	free/(9)	1×10^4	piecewise (S8)	0.25	3.0	1	1	2	1024	1024	1024
D10	free/(9)	1×10^4	piecewise (S8)	0.5	0.0	1	1	2	1024	1024	1024
D11	free/(9)	1×10^4	piecewise (S8)	0.5	1.5	1	1	2	1024	1024	1024
D12	free/(9)	1×10^4	piecewise (S8)	0.5	3.0	1	1	2	1024	1024	1024
E1	free/(9)	1×10^4	piecewise (S8)	0.1	0.0	5	-	2	5120	1	1024
E2	free/(9)	1×10^4	piecewise (S8)	0.6	0.0	5	-	2	5120	1	1024
E3	free/(9)	1×10^4	piecewise (S8)	0.1	3.0	5	-	2	5120	1	1024
E4	free/(9)	1×10^4	piecewise (S8)	0.6	3.0	5	-	2	5120	1	1024
E5	free/(9)	1×10^4	piecewise (S8)	0.1	0.0	1	1	2	1024	1024	1024
E6	free/(9)	1×10^4	piecewise (S8)	0.6	0.0	1	1	2	1024	1024	1024
E7	free/(9)	1×10^4	piecewise (S8)	0.1	3.0	1	1	2	1024	1024	1024
E8	free/(9)	1×10^4	piecewise (S8)	0.6	3.0	1	1	2	1024	1024	1024