Special Seminar

Modeling heat and mass transport in convective porous media flows: a multiscale approach

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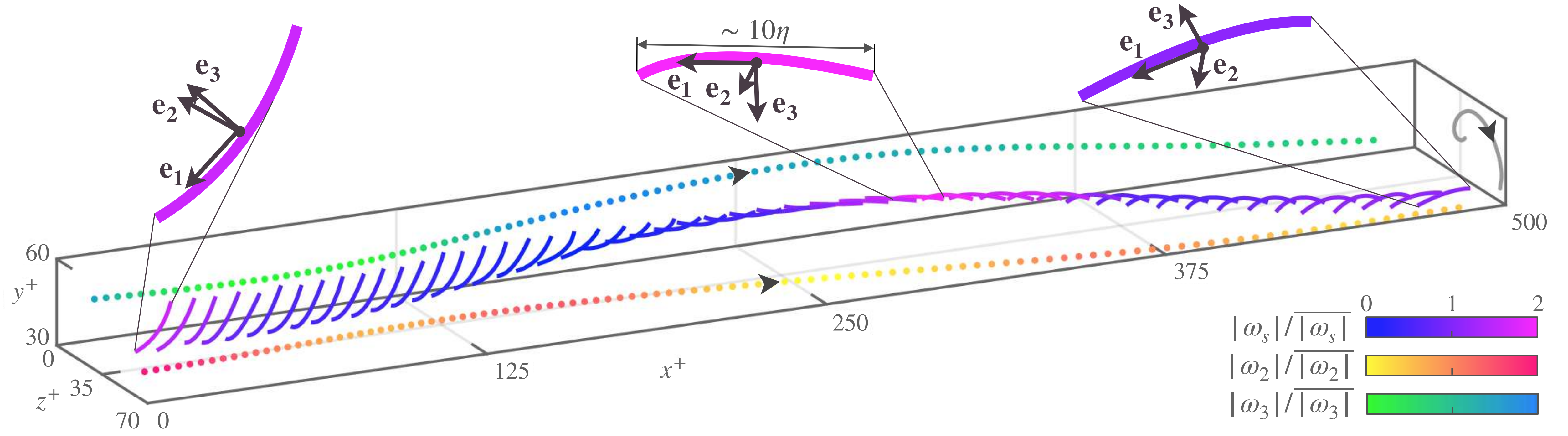
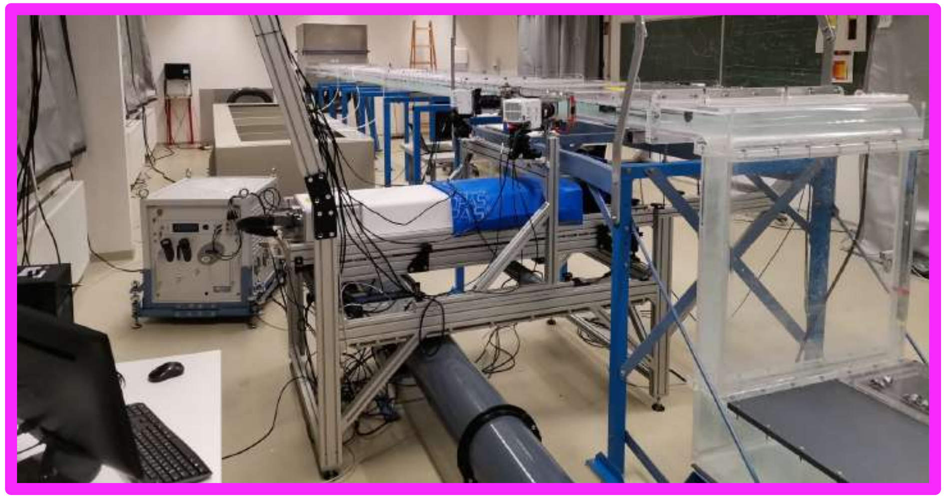
Physics of Fluids

TU WIEN



Full rotational dynamics of microplastic fibers in turbulence, Giurgiu V., Caridi G., De Paoli M. & Soldati A., *Physical Review Letters* (in press)



Acknowledgements

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Acknowledgements

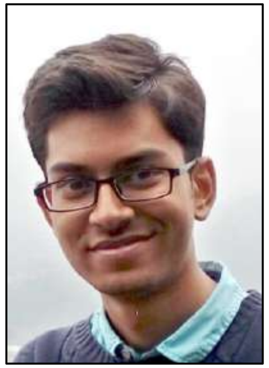
Physics of Fluids

MAX-PLANCK-GESELLSCHAFT

D. Lohse

C. Howland

G. Yerragolam



R. Verzicco

GSSI

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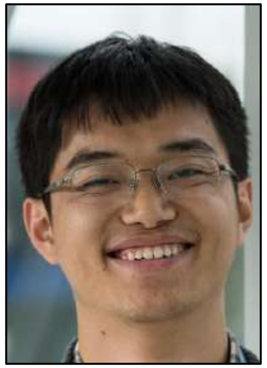

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Presentation outline

1. Motivation
2. Reservoir-scale: multiphase gravity currents
3. Darcy-scale: simulations, experiments and finite-size effects
4. Pore-scale modelling and dispersion
5. Conclusions and outlook

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2. Reservoir-scale: multiphase gravity currents
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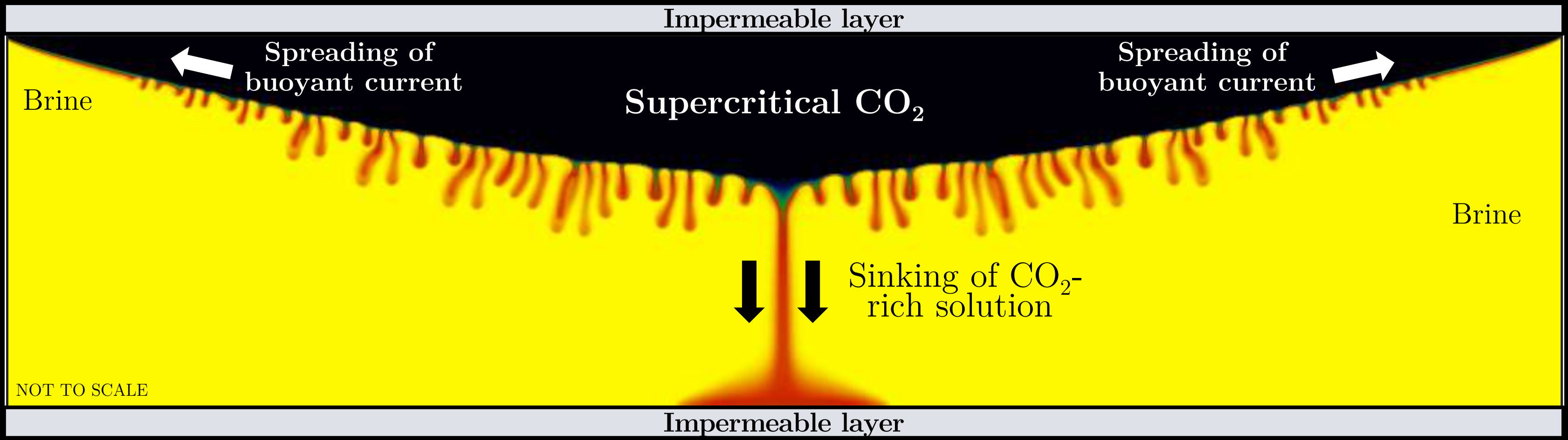
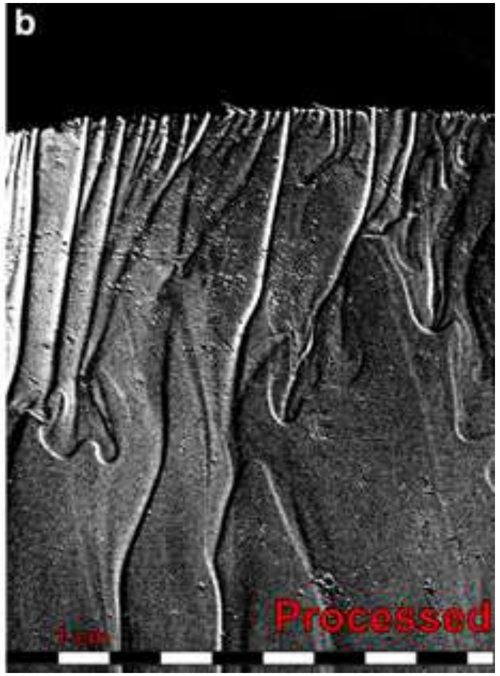
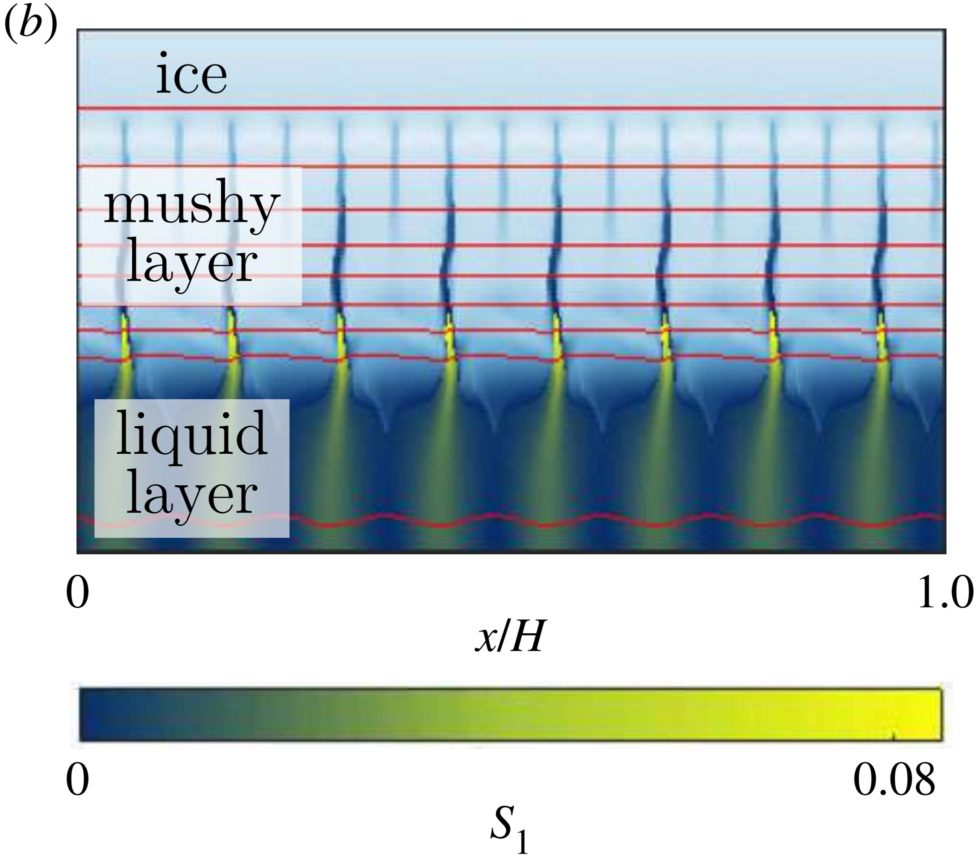


Sea ice formation



Middleton et al., “ Visualizing brine channel development and convective processes during artificial sea-ice growth using Schlieren optical methods”. *J. Glaciology* (2016).



Wells AJ, Hitchen JR, Parkinson JRG., «Mushy-layer growth and convection, with application to sea ice» 2019 *Phil. Trans. R. Soc. A*

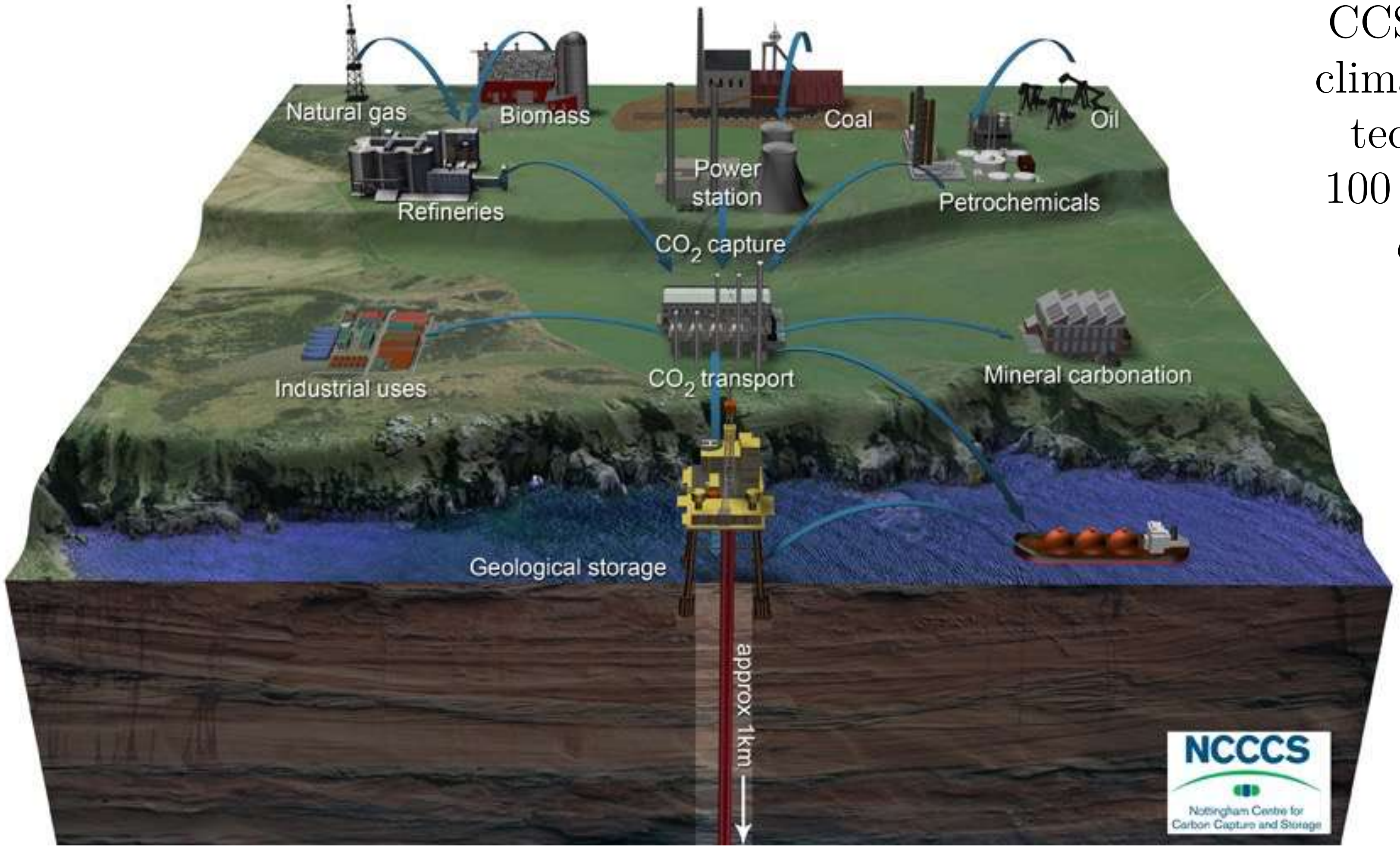
Other applications

Simmons et al., “Variable-density groundwater flow and solute transport in heterogeneous porous media: approaches, resolutions and future challenges,” *J. Contam. Hydrol.* (2001).

Molen et al., “Transport of solutes in soils and aquifers,” *J. Hydrol.* (1988).

LeBlanc, *Sewage plume in a sand and gravel aquifer, Cape Cod, Massachusetts* (US Geological Survey, 1984).

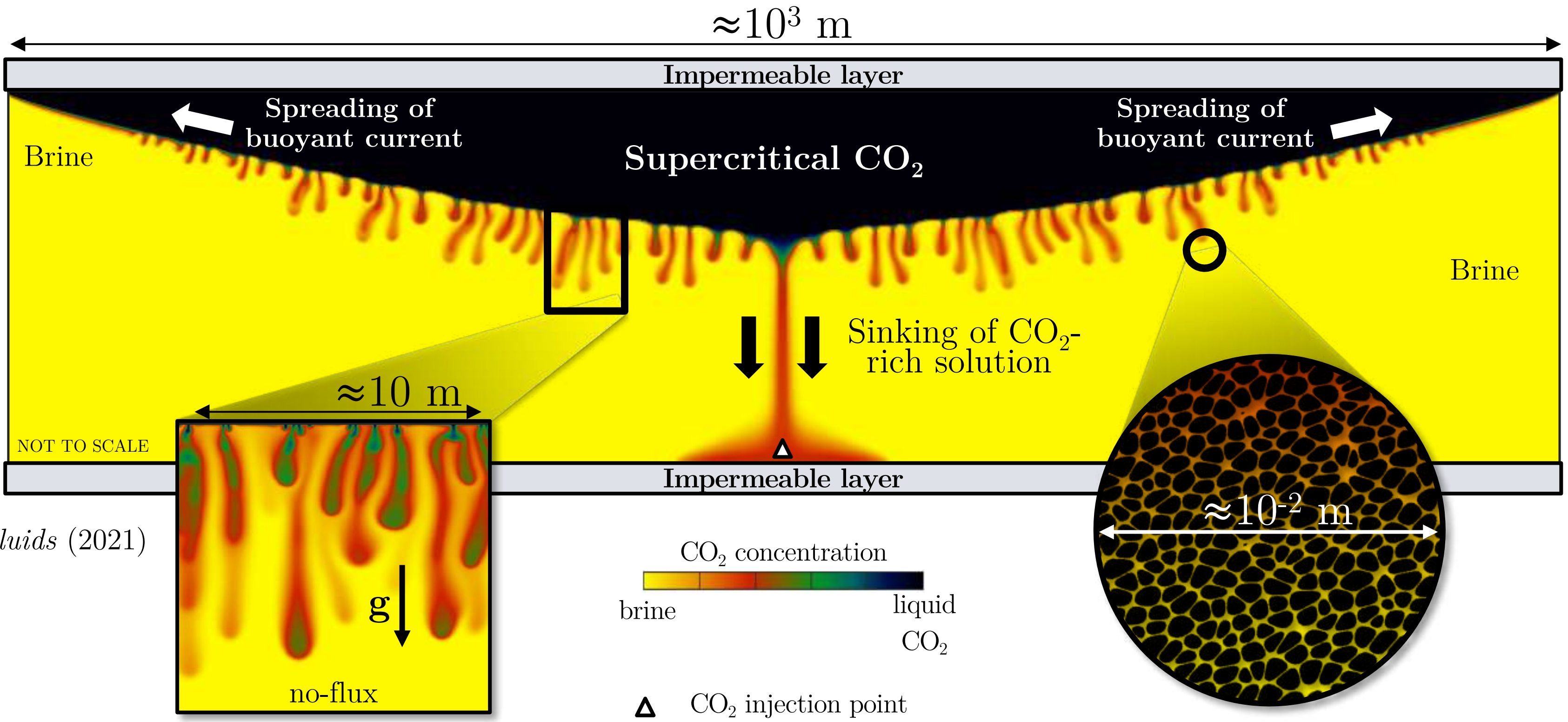
Carbon Capture and Storage (CCS)



Injection point

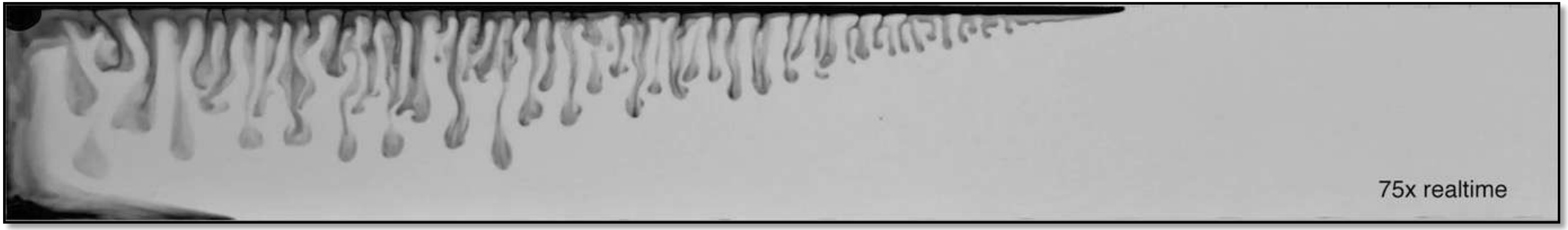
CCS can work as unique climate change mitigation technology for at least 100 years [Szulczewski *et al.*, *(PNAS)* 2012]

Carbon Capture and Storage

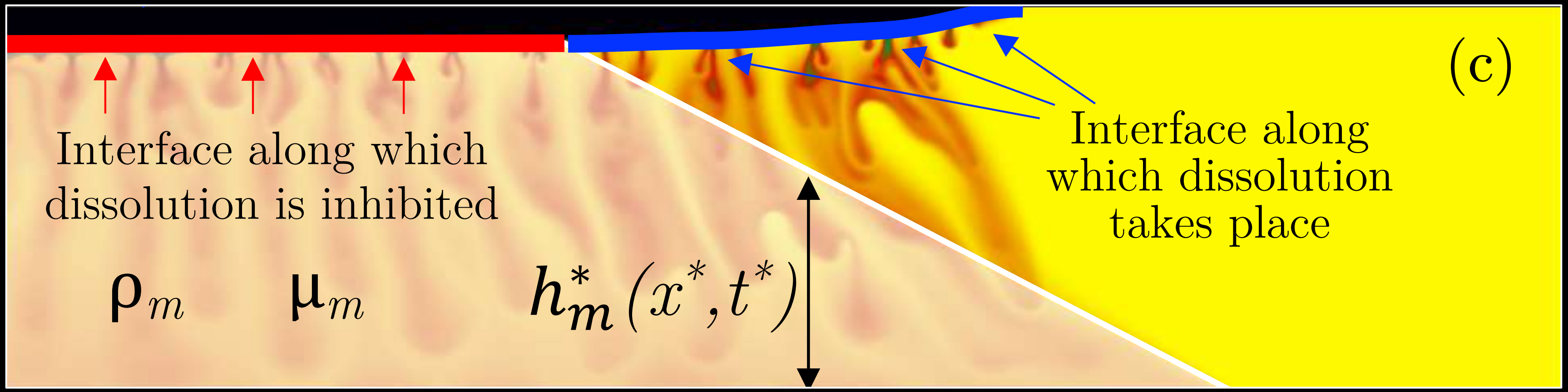


De Paoli, *Phys. Fluids* (2021)

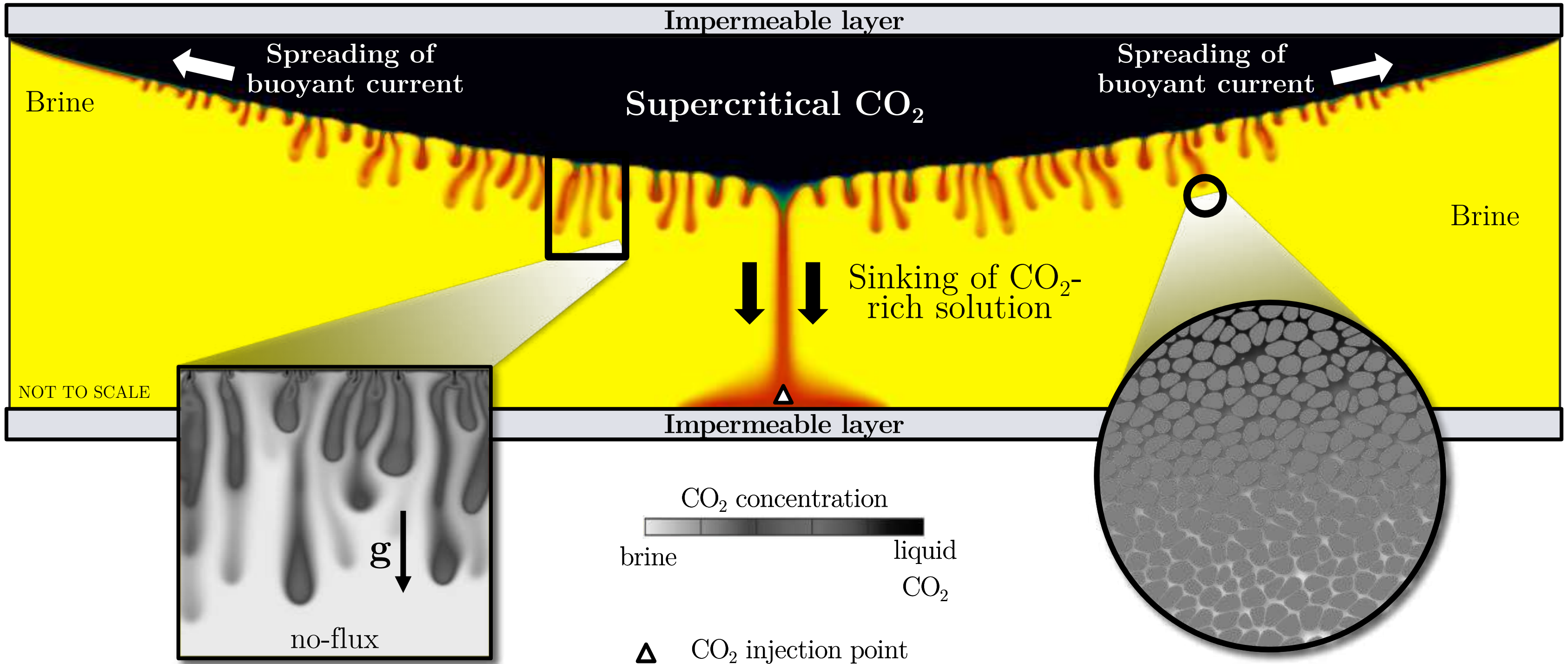
MacMinn et al., *Geophys. Res. Lett.* (2013)



1. Motivation
2. **Reservoir-scale: multiphase gravity currents**
3. Darcy-scale: simulations, experiments and finite-size effects
4. Pore-scale modelling and dispersion
5. Conclusions and outlook



Carbon Capture and Storage

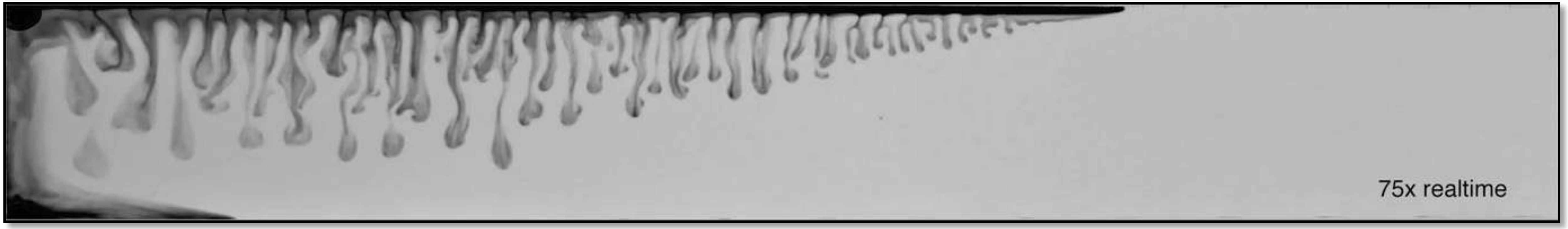


De Paoli, *Phys. Fluids* (2021)

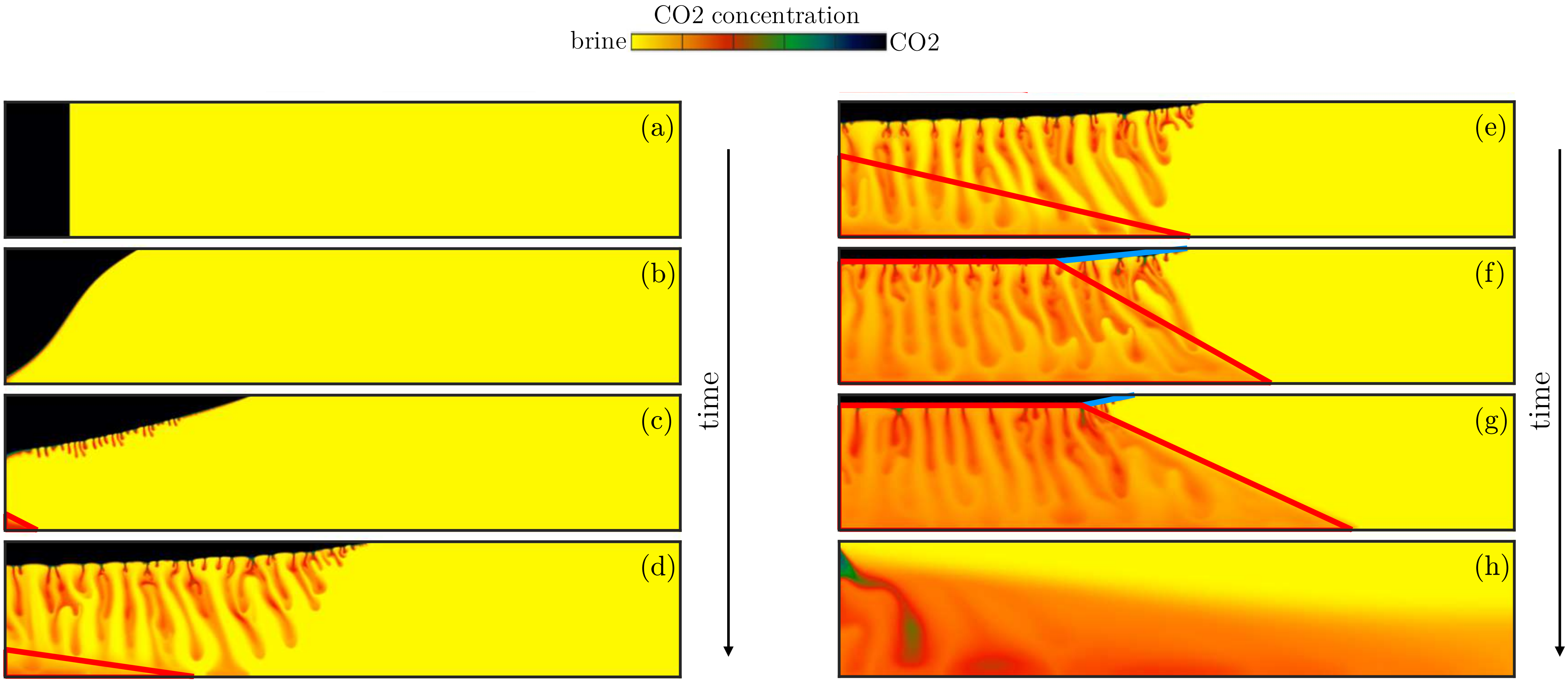
Reservoir properties

- anisotropy and heterogeneities
- finite size of confining layers
- effects of rock properties (mechanical dispersion)
- chemical dissolution and morphology variations
- ...

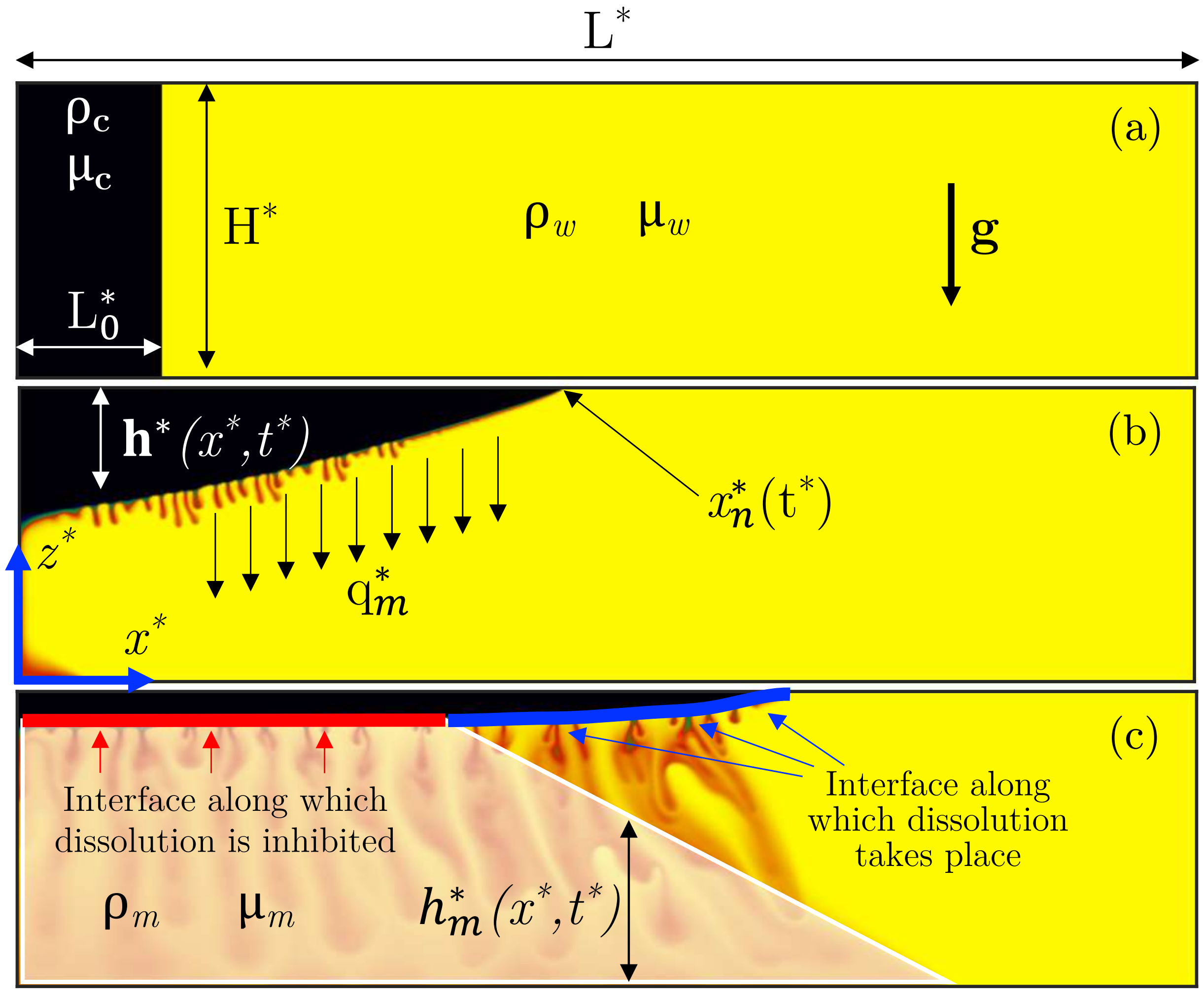
MacMinn & Juanes., *Geophys. Res. Lett.* (2013)



Multiphase gravity currents with dissolution



De Paoli, *Phys. Fluids.* (2021)



De Paoli, *Phys. Fluids.* (2021)

$$\frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left[(1-f)h\frac{\partial h}{\partial x} - \delta f h_m \frac{\partial h_m}{\partial x}\right] = -\varepsilon_0,$$

$$\frac{\partial h_m}{\partial t} - \frac{\partial}{\partial x}\left[\delta(1-f_m)h_m\frac{\partial h_m}{\partial x} - f_m h \frac{\partial h}{\partial x}\right] = \frac{\varepsilon_0}{X_v}$$

$$f = \frac{Mh^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

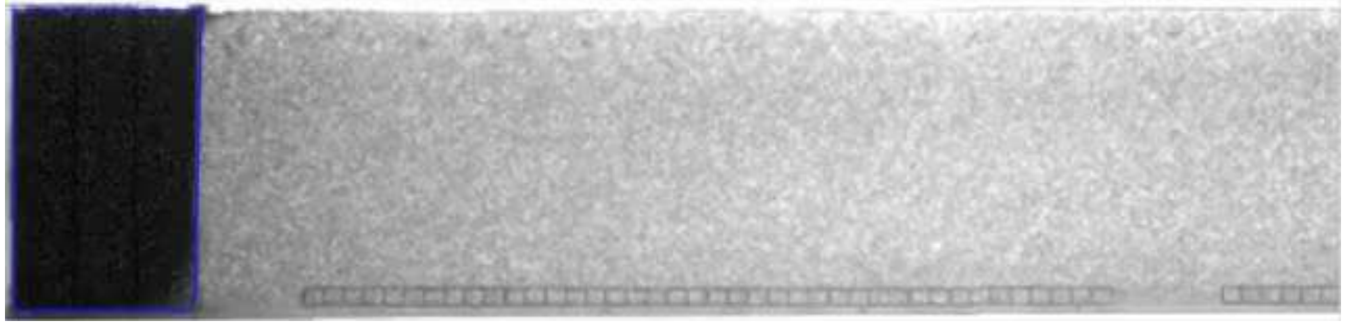
$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

MacMinn, Neufeld, Hesse, and Huppert, *Water Resour. Res.* (2012)

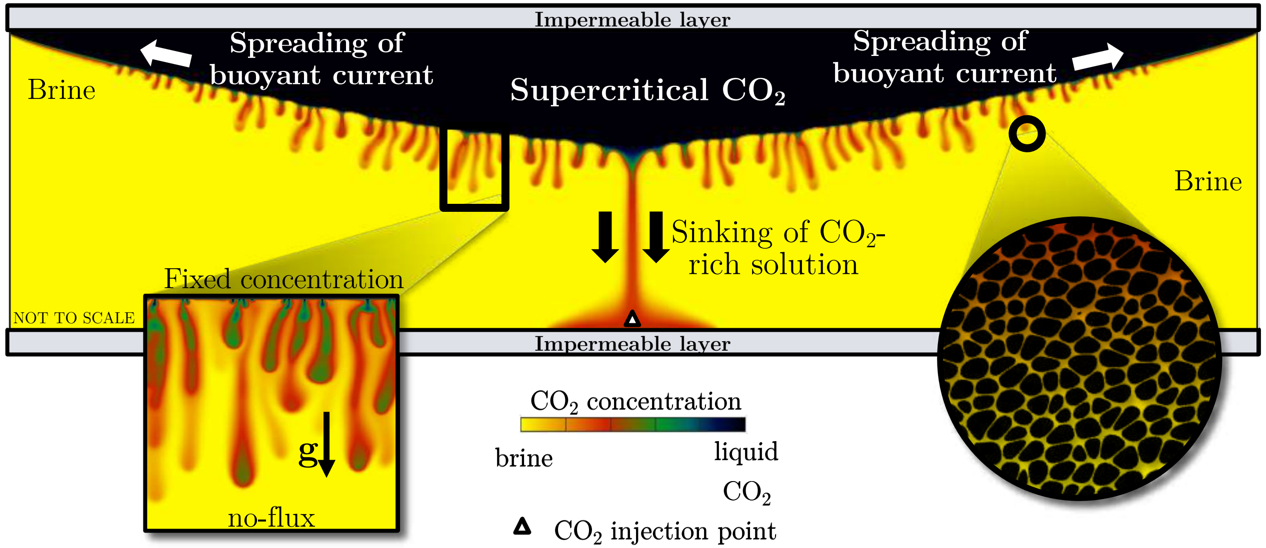
Mobility ratios $M = \mu_w/\mu_c$ and $M_m = \mu_w/\mu_m$

Buoyancy velocity ratio $\delta = W_m^*/W^*$

Volume fraction $X_v = \rho_m X_m/\rho_c$



MacMinn, Neufeld, Hesse, and Huppert, *Water Resour. Res.* (2012)



$$\frac{\partial h}{\partial t} - \frac{\partial}{\partial x}\left[(1-f)h\frac{\partial h}{\partial x} - \delta f h_m \frac{\partial h_m}{\partial x}\right] = -\varepsilon_0,$$

$$\frac{\partial h_m}{\partial t} - \frac{\partial}{\partial x}\left[\delta(1-f_m)h_m\frac{\partial h_m}{\partial x} - f_m h \frac{\partial h}{\partial x}\right] = \frac{\varepsilon_0}{X_v}$$

$$f = \frac{Mh^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

$$\varepsilon_0(x) = \begin{cases} 0 & \text{if } \ h(x) = 0 \text{ or } h(x) + h_m(x) = 1 \\ \varepsilon & \text{else,} \end{cases}$$

$$\varepsilon = \frac{q_m^*}{\phi W^*}\left(\frac{L_0^*}{H^*}\right)^2$$

How to determine the dissolution rate q_m^* ?

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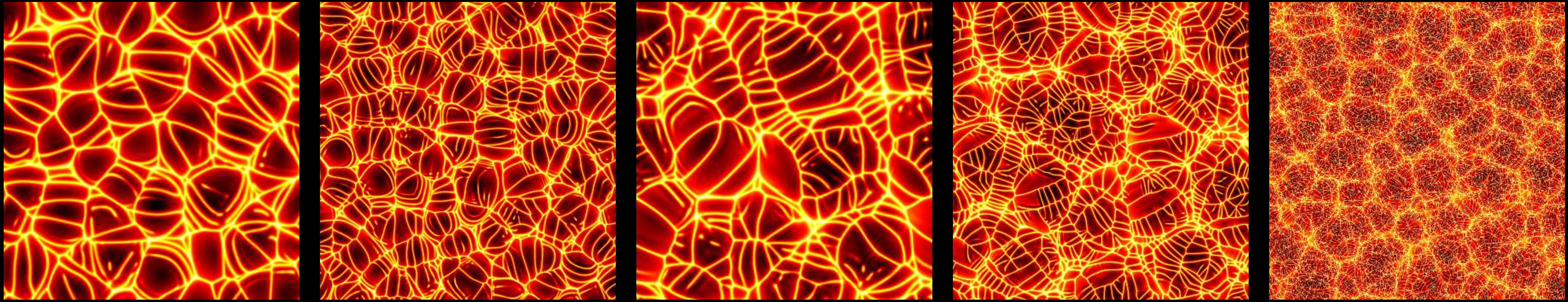
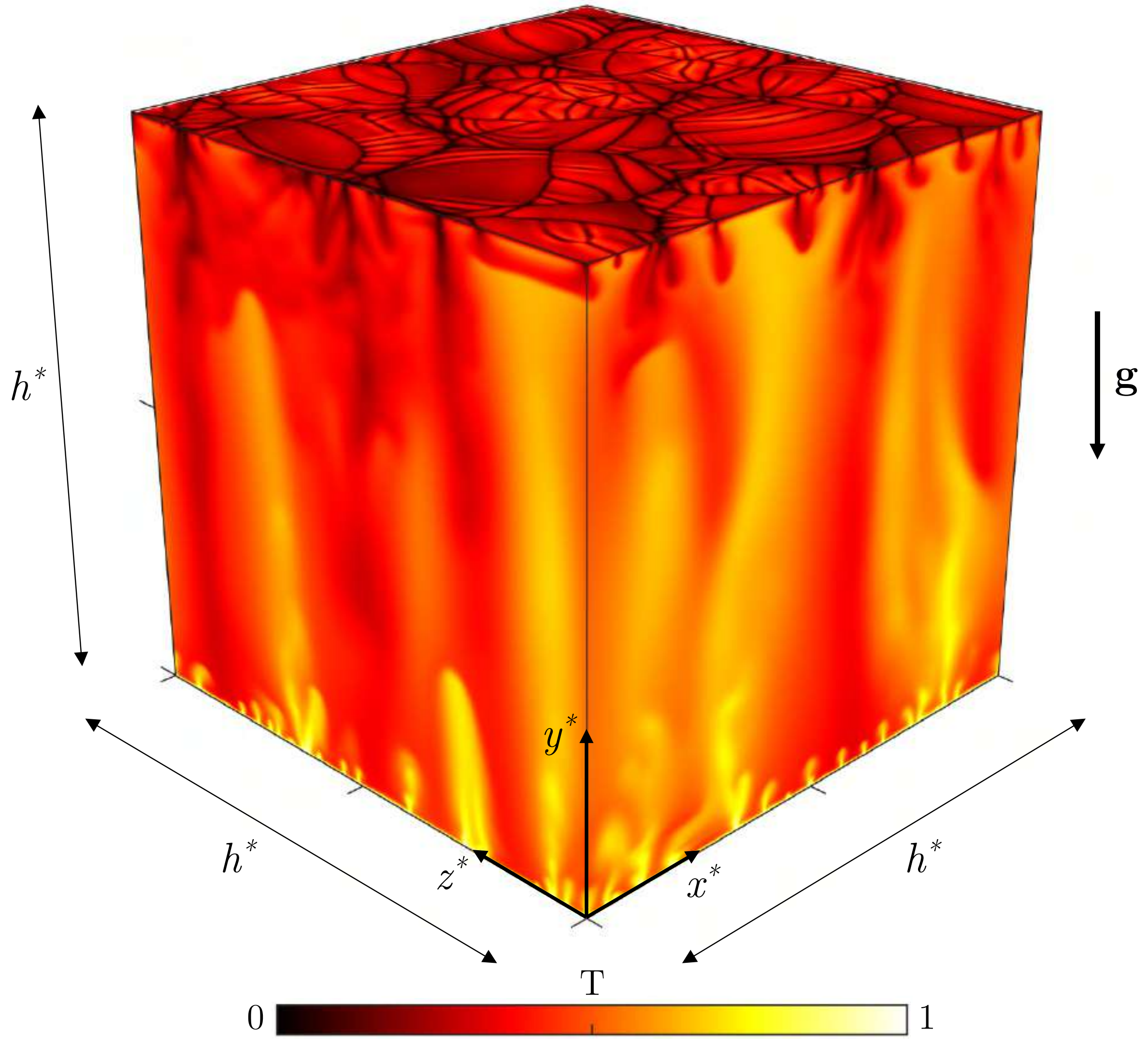




Pirozzoli, De Paoli, Zonta & Soldati, *J. Fluid Mech.* (2021)
De Paoli, Pirozzoli, Zonta & Soldati, *J. Fluid Mech.* (2022)

Governing equations

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

$$\mathbf{u} = -(\nabla p - T\mathbf{k})$$ Darcy

$$\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{Ra}\nabla^2 T$$ advection-diffusion equation

Boundary conditions

$$v(y=0) = 0 \qquad v(y=1) = 0$$ no-penetration

$$T(y=0) = 1 \qquad T(y=1) = 0$$ fixed temperature

How efficient is mixing?
How fast can we dissolve CO2?
How does Nu scale with Ra at high Ra?

Transport scaling in porous media

Governing parameters

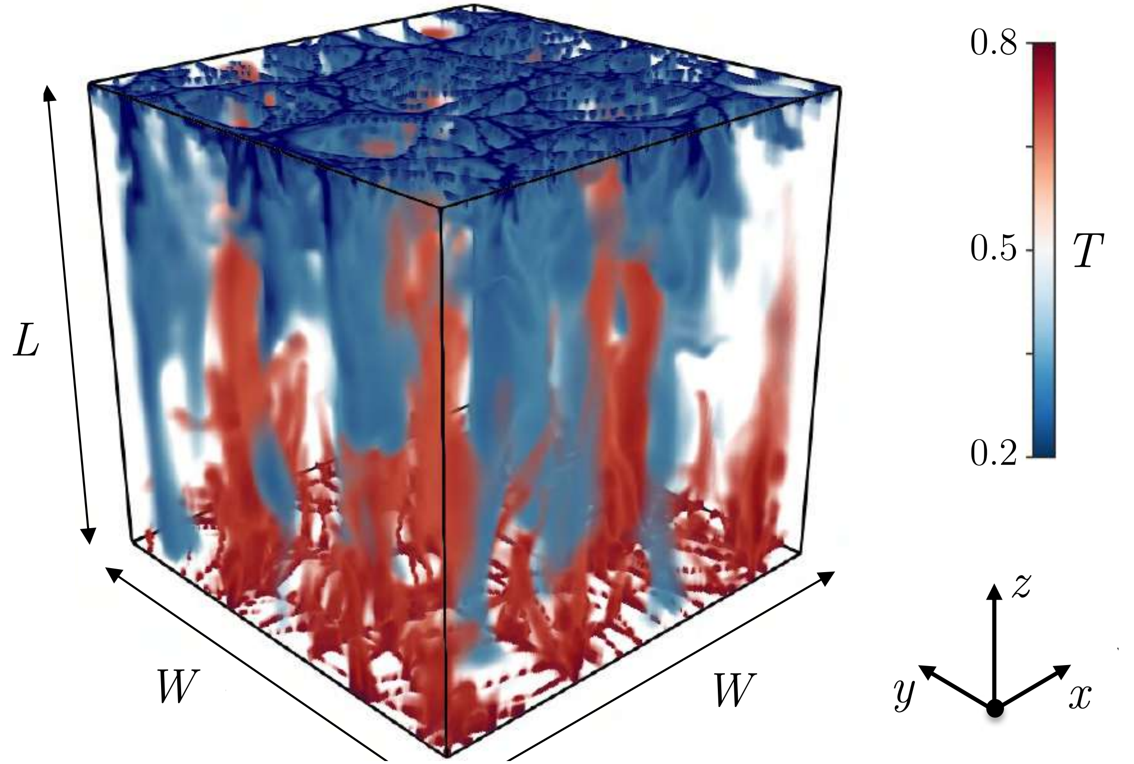
Rayleigh-Darcy number

$$Ra = \frac{\alpha g \Delta K L}{\kappa \nu}$$

Relative strength of advection compared to diffusive

Domain aspect ratio

$$W/L$$



Response parameters

Nusselt number

$$Nu = Ra\,\overline{\langle u_z T \rangle_A} - \overline{\left\langle \frac{\partial T}{\partial z} \right\rangle_A}$$

Dimensionless heat exchanged

Peclet number

$$Pe = \frac{\mathscr{V} L}{\kappa}$$

Strength of advection compared to diffusion

$$Nu(Ra \rightarrow \infty) = ?$$

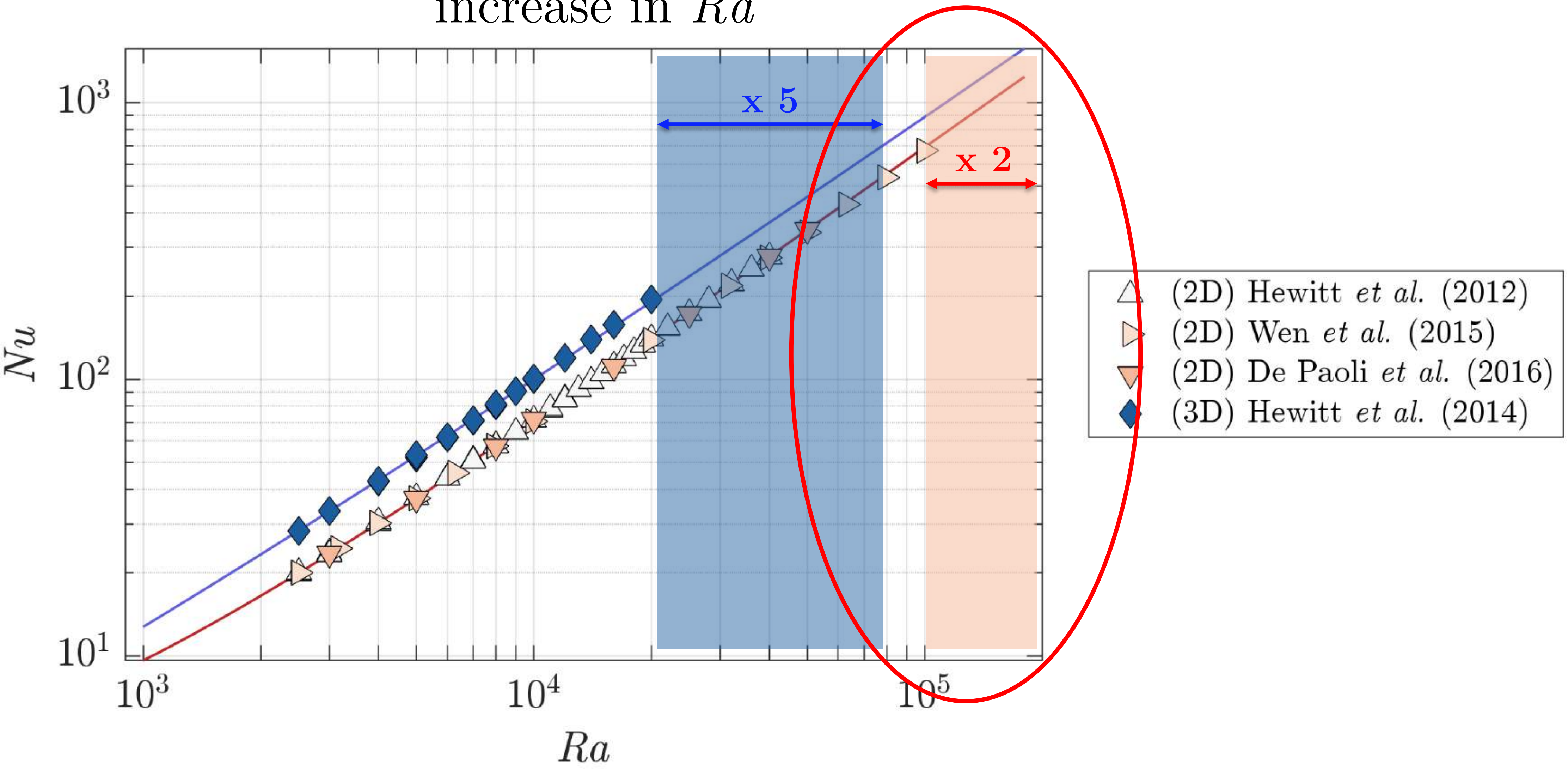
Turbulence

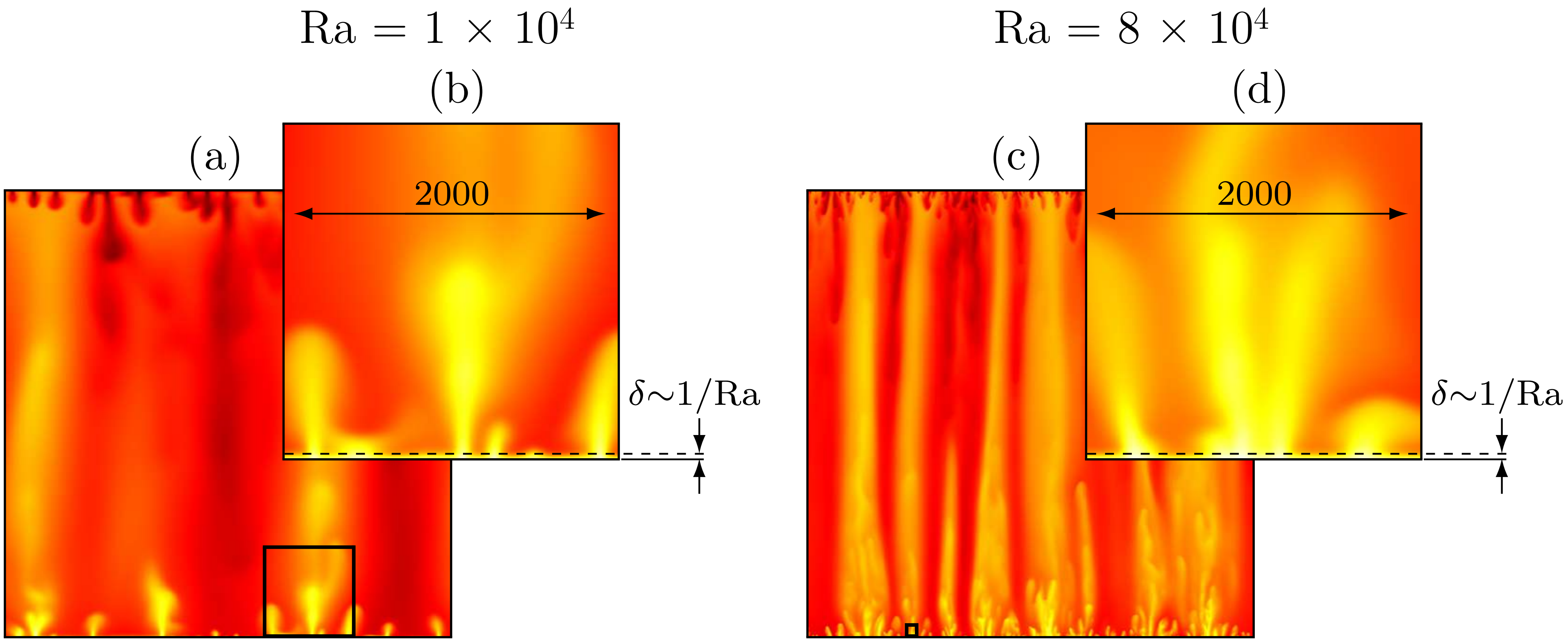
References	hypothesis	scaling
Malkus, M. V. R. 1954, *Proc. R. Soc. Lond. A* 225, 196–212. Priestley, C. H. B. 1954, *Aust. J. Phys.* 7 (1), 176–201. Howard, L. N. 1966, *In Proc. 11th Int. Cong. App. Mech.*, pp. 1109–1115.	Heat transfer is independent of the thickness of the boundary layer. Therefore, the lower and upper b.l.s evolve independently.	$Nu \sim Ra^{1/3}$

Porous media

References	hypothesis	scaling
Doering, CR & Constantin, P 1998, *J. Fluid Mech.* 376, 263–296. Hassanzadeh, P., Chini, G. P. & Doering, C. R. 2014, *J. Fluid Mech.* 751, 627–662.	Such scaling implies that dimensionless flux is independent of thermal diffusivity, and therefore we achieve the so-called ultimate regime.	$Nu \sim Ra$

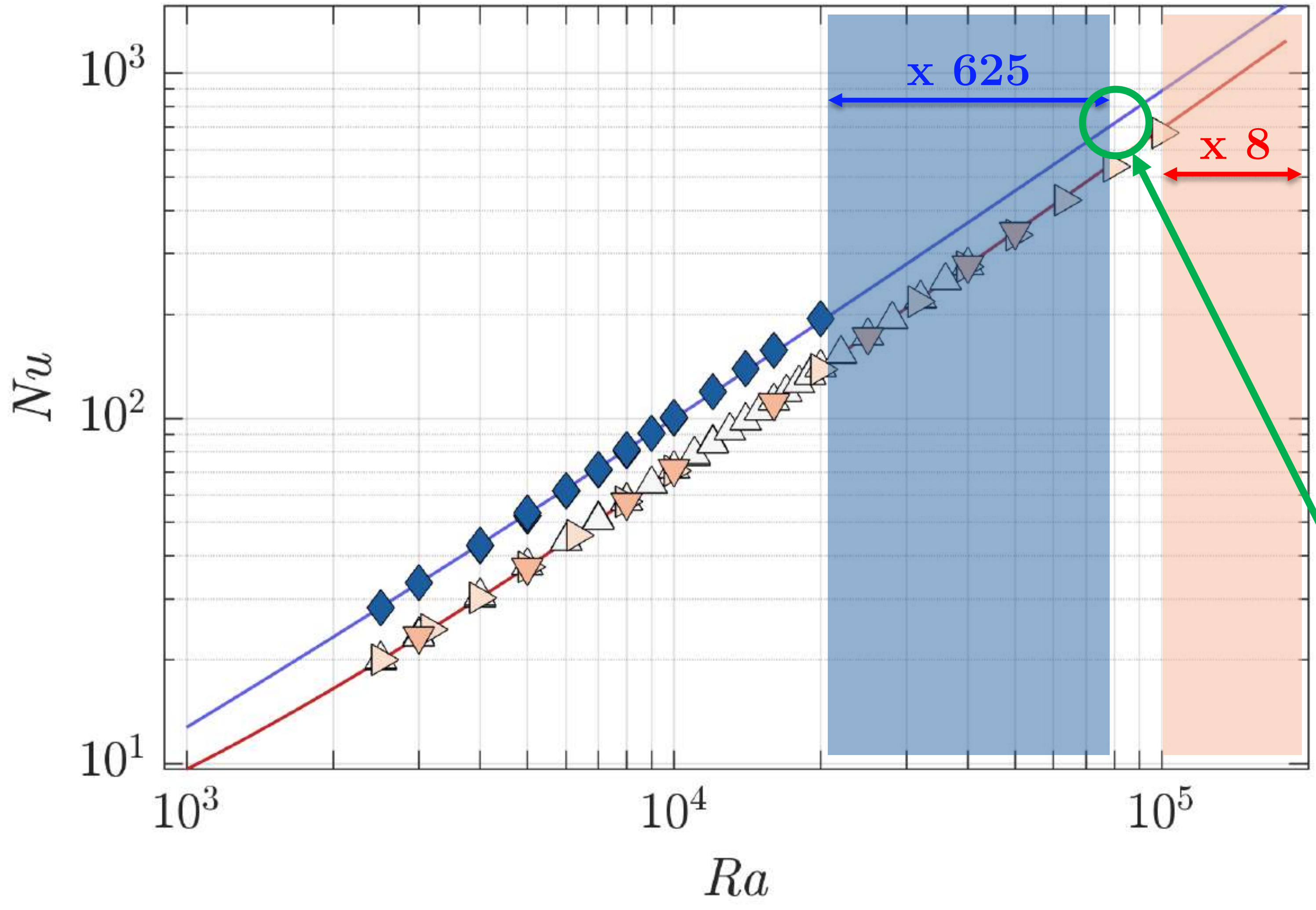
increase in Ra





$$\delta \sim \frac{1}{Nu} \approx \frac{1}{Ra}$$

increase in computational cost



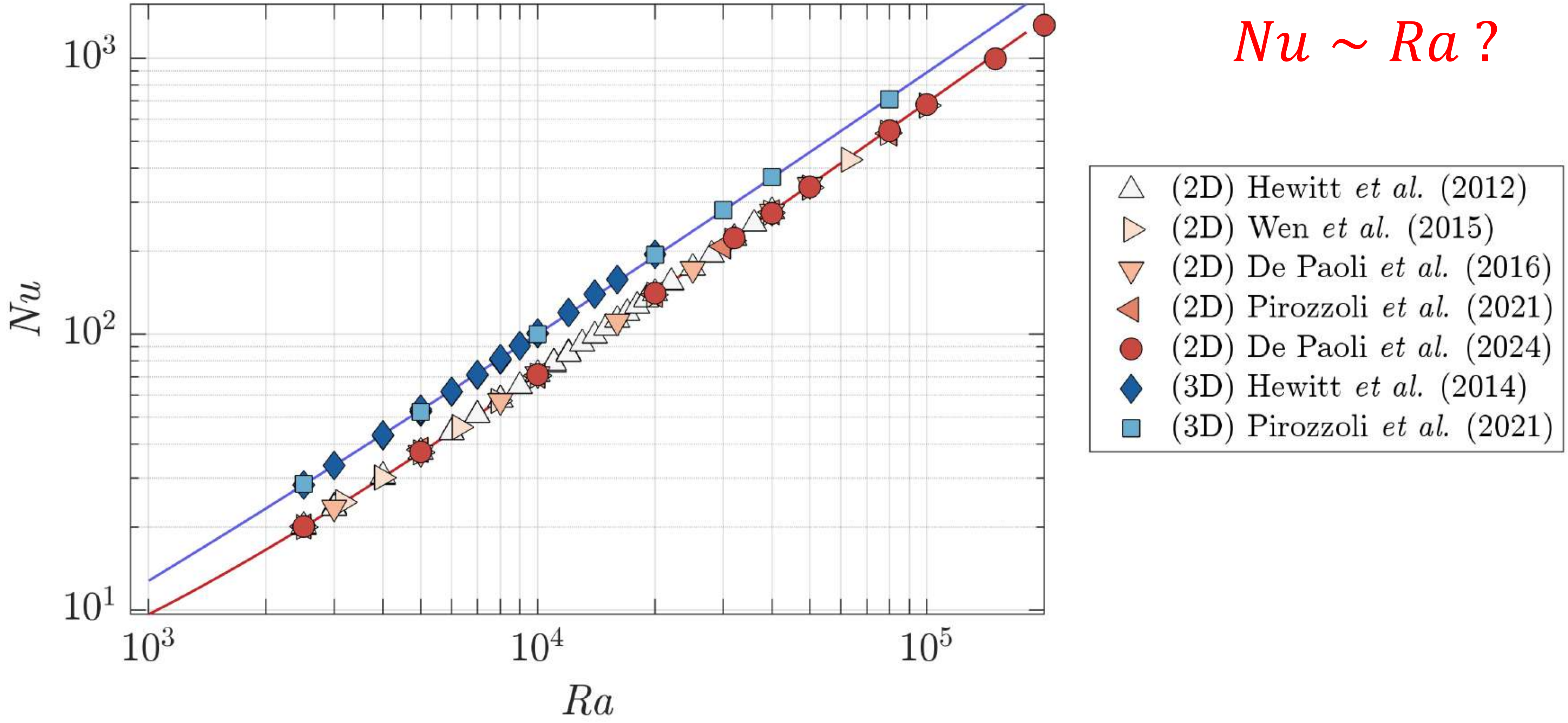
$Nu \approx Ra$

$$\Rightarrow \Delta x \sim \frac{1}{Ra}, \Delta t \sim \frac{1}{Ra}$$

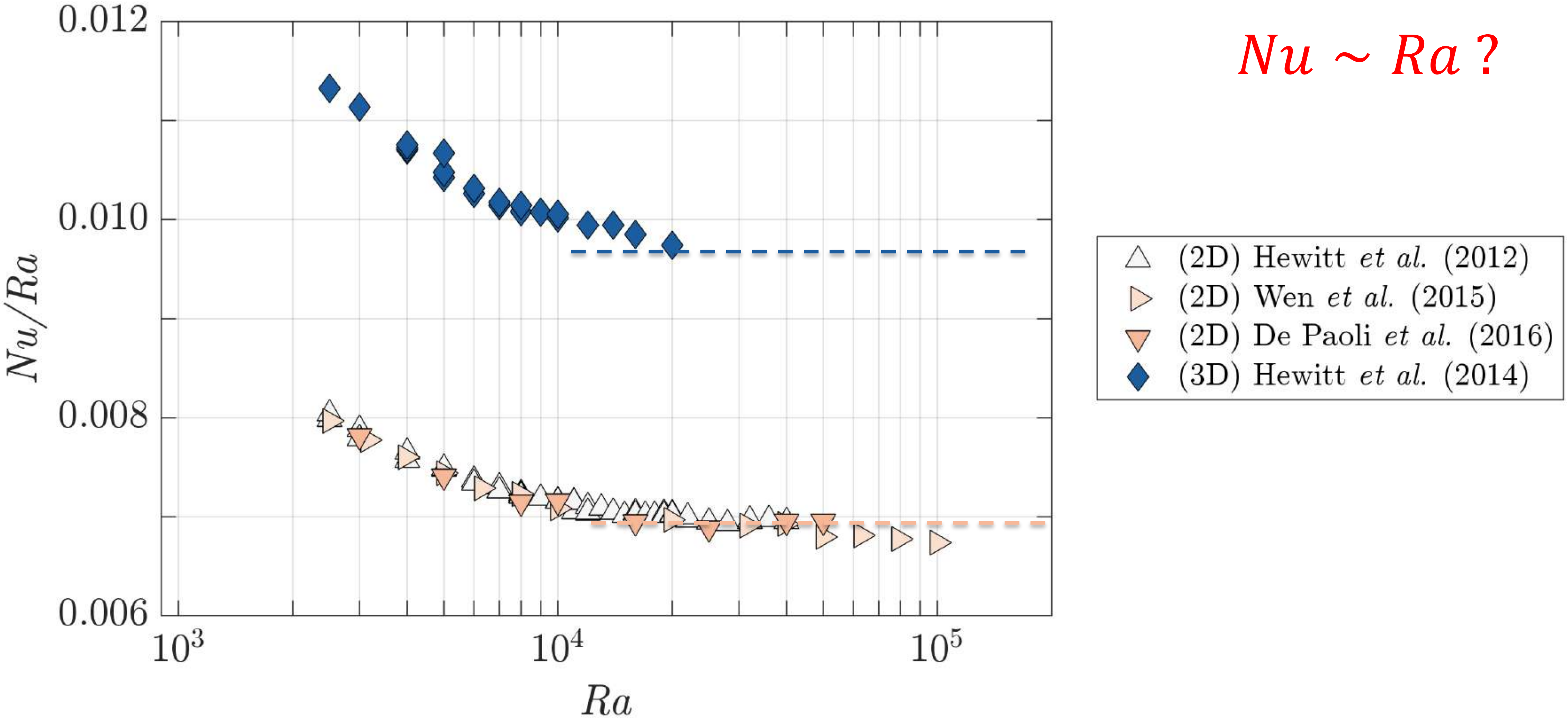
$$\Rightarrow N_x \times N_y \times N_z \times N_T \sim Ra^4 \quad \text{(3D)}$$

$$\Rightarrow N_x \times N_y \times N_T \sim Ra^3 \quad \text{(2D)}$$

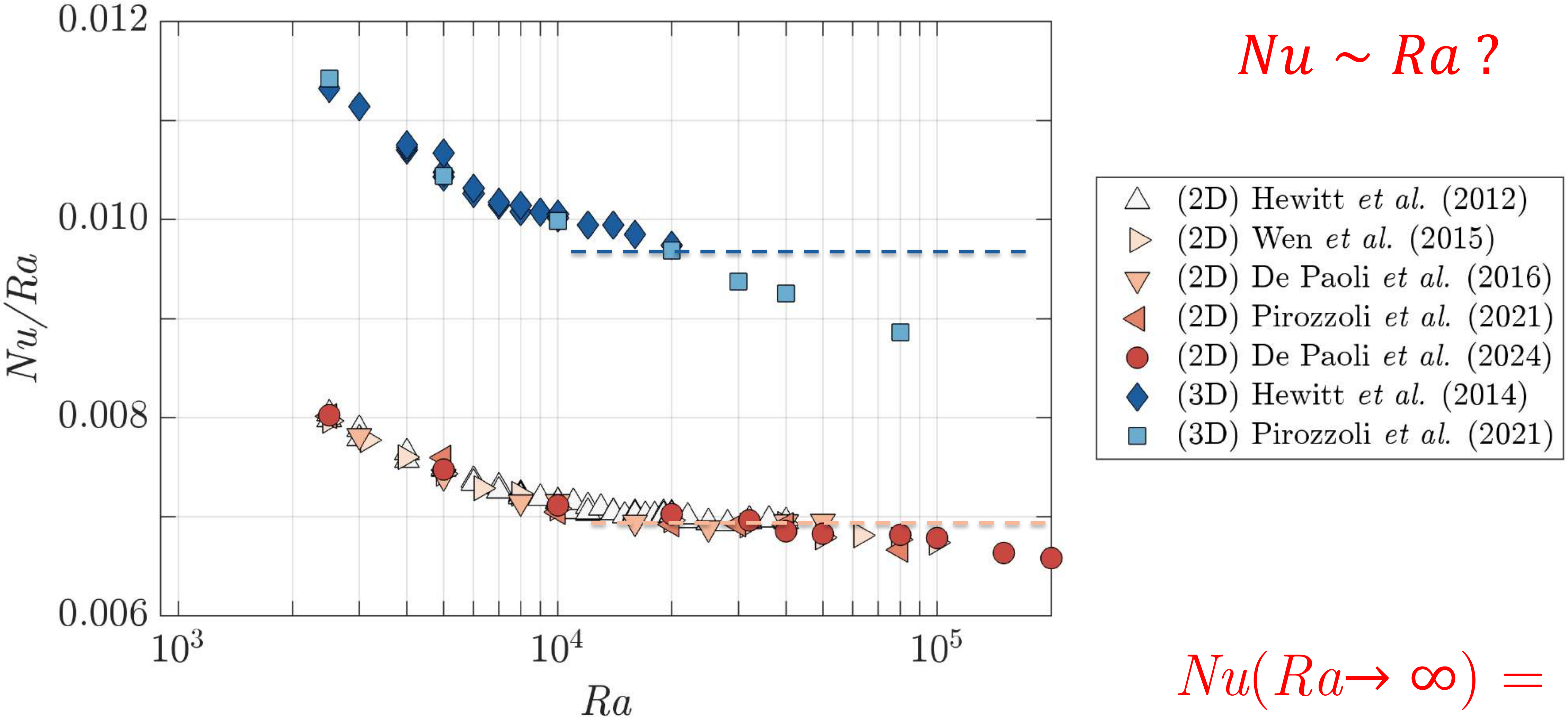
≈ 100B grid points,
≈ 66k cores for 2 months
≈ 100M CPU hours


Nu
10^3
10^2
10^1
10^3
10^4
10^5
Ra
(2D) Hewitt *et al.* (2012)
(2D) Wen *et al.* (2015)
(2D) De Paoli *et al.* (2016)
(2D) Pirozzoli *et al.* (2021)
(2D) De Paoli *et al.* (2024)
(3D) Hewitt *et al.* (2014)
(3D) Pirozzoli *et al.* (2021)

$Nu \sim Ra\,?$

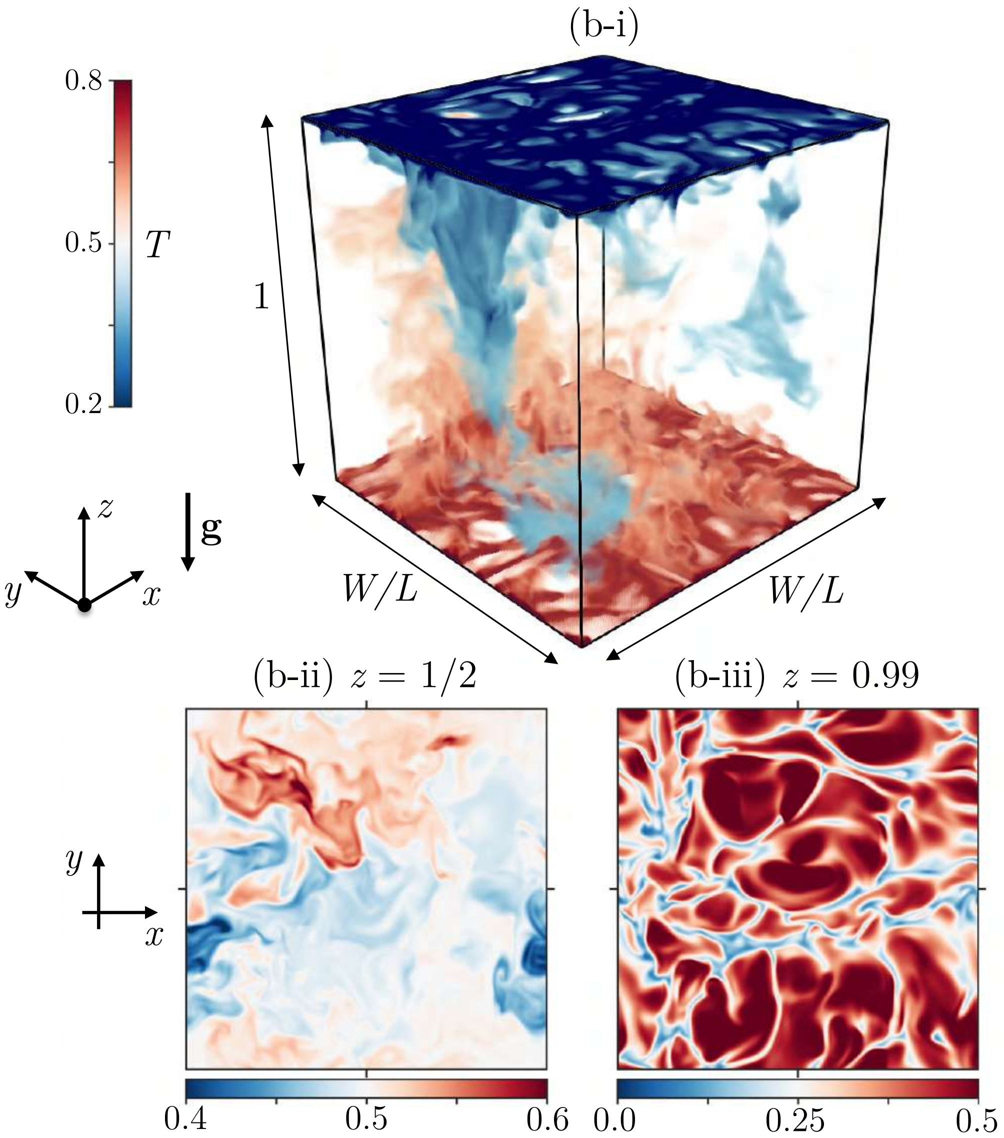

0.012
0.010
0.008
0.006
Nu/Ra
10^3
10^4
10^5
Ra
(2D) Hewitt et al. (2012)
(2D) Wen et al. (2015)
(2D) De Paoli et al. (2016)
(3D) Hewitt et al. (2014)

$Nu \sim Ra\,?$



$Nu \sim Ra\,?$

$Nu(Ra \to \infty) = ?$



Turbulent convection

Turbulence

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Malkus, M. V. R. 1954, *Proc. R. Soc. Lond. A* 225, 196–212. Priestley, C. H. B. 1954, *Aust. J. Phys.* 7 (1), 176–201. Howard, L. N. 1966, *In Proc. 11th Int. Cong. App. Mech.*, pp. 1109–1115.	Heat transfer is independent of the thickness of the boundary layer. Therefore, the lower and upper b.l.s evolve independently.	$Nu \sim Ra^{1/3}$

Porous media

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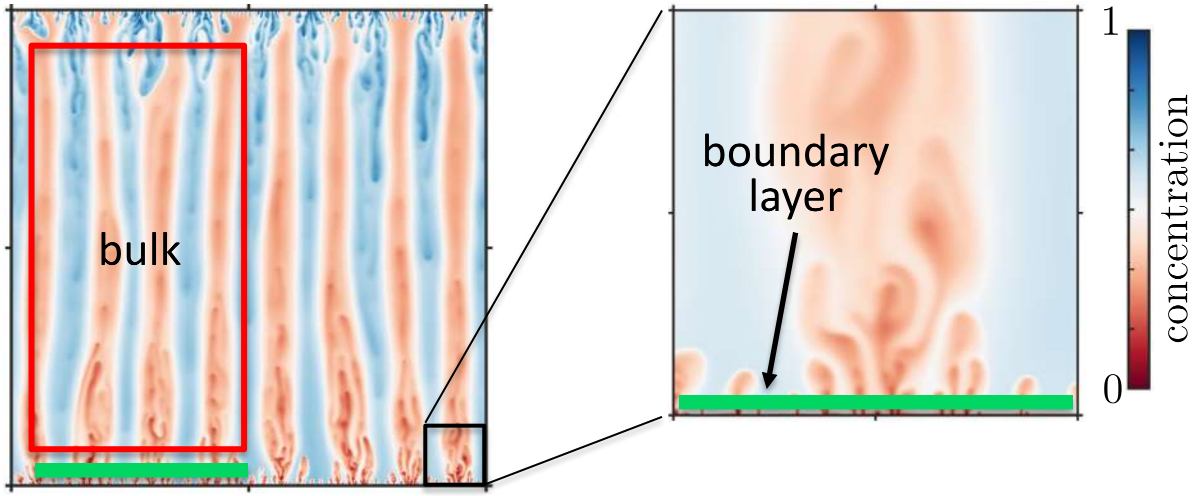
Turbulence – $Ra \to \infty$

References	hypothesis	scaling
Malkus, M. V. R. 1954, *Proc. R. Soc. Lond. A* 225, 196–212. Priestley, C. H. B. 1954, *Aust. J. Phys.* 7 (1), 176–201. Howard, L. N. 1966, *In Proc. 11th Int. Cong. App. Mech.*, pp. 1109–1115.	Heat transfer is independent of the thickness of the boundary layer. Therefore, the lower and upper b.l.s evolve independently.	$Nu \sim Ra^{1/3}$
Shraiman, B. I. & Siggia, E. D. 1990, *Phys. Rev. A* 42, 3650–3653.	Thermal b.l. deeply nested within the turbulent viscous b.l. ($Pr > 1$)	$Nu \sim Ra^{2/7}$
Kraichnan, R. H. 1962, *Phys. Fluids* 5, 1374–1389	Using classical mixing length arguments for turbulent boundary layer, *elusive* asymptotic regime for arbitrary Pr (diffusion-free regime)	$Nu \sim \dfrac{Ra^{1/2}}{(\ln Ra)^{3/2}}$

Verzicco, R. (2012). Boundary layer structure in confined turbulent thermal convection. *Journal of Fluid Mechanics*, *706*, 1-4.

Derive global relations for heat/mass transport



Zhu, Fu & **De Paoli** (in press) *J. Fluid Mech.*

1) Derive global exact relations

2) Split dissipation in BULK and BL contributions

3) Derive scaling laws for Nu

$$\epsilon = \epsilon_{BL} + \epsilon_{bulk}$$

1) Derive global exact relations

Governing equations

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

$$\mathbf{u} = -(\nabla p - T\mathbf{k})$$

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

Governing parameters

$$Ra = \frac{\alpha g \Delta K L}{\kappa \nu} \qquad W/L$$

Response parameters

$$Nu = Ra\,\overline{\langle u_z T\rangle}_A - \overline{\left\langle \frac{\partial T}{\partial z} \right\rangle}_A$$

$$Pe = \frac{\mathscr{V} L}{\kappa} = Ra\,\frac{\mathscr{V}}{\mathscr{U}}$$

$$\mathscr{V} = \mathscr{U}\sqrt{\overline{\langle |\mathbf{u}|^2 \rangle}},$$

Exact global relations

$$\overline{\langle |\nabla T|^2 \rangle} = Nu$$

$$\epsilon = \kappa \frac{\Delta^2}{L^2}\overline{\langle |\nabla T|^2 \rangle} = \kappa \frac{\Delta^2}{L^2} Nu$$

$$Pe^2 = (Nu - 1)\,Ra$$

2) Split dissipation in BULK and BL

Governing equations

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

$$\mathbf{u} = -(\nabla p - T\mathbf{k})$$

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

Governing parameters

$$Ra = \frac{\alpha g \Delta K L}{\kappa \nu} \qquad W/L$$

Response parameters

$$Nu = Ra\,\overline{\langle u_z T\rangle}_A - \overline{\left\langle \frac{\partial T}{\partial z}\right\rangle}_A$$

$$Pe = \frac{\mathscr{V} L}{\kappa} = Ra\,\frac{\mathscr{V}}{\mathscr{U}}$$

$$\mathscr{V} = \mathscr{U}\sqrt{\overline{\langle |\mathbf{u}|^2\rangle}},$$

Split dissipation

$$\epsilon = \epsilon_{BL} + \epsilon_{bulk}$$

$$\epsilon_{BL} \sim \kappa \frac{\Delta^2}{\lambda^2}\frac{\lambda}{L} \sim \kappa \frac{\Delta^2}{L^2} Ra$$

$$\epsilon_{bulk} \sim \kappa \frac{\Delta^2}{L^2} Pe \frac{\ell}{L}$$

$$\ell/L \sim Ra^{-1/2} \quad (3D)$$

$$\ell/L \sim Ra^{-5/14} \quad (2D)$$

$$\sim \kappa \frac{\Delta^2}{L^2} Nu^{1/2} Ra^{1/7} \quad (2D)$$

$$\sim \kappa \frac{\Delta^2}{L^2} Nu^{1/2} \quad (3D)$$

Governing equations

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

$$\mathbf{u} = -(\nabla p - T\mathbf{k})$$

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

Governing parameters

$$Ra = \frac{\alpha g \Delta K L}{\kappa \nu} \qquad W/L$$

Response parameters

$$Nu = Ra\,\overline{\langle u_z T\rangle}_A - \overline{\left\langle \frac{\partial T}{\partial z}\right\rangle}_A$$

$$Pe = \frac{\mathscr{V} L}{\kappa} = Ra\,\frac{\mathscr{V}}{\mathscr{U}}$$

$$\mathscr{V} = \mathscr{U}\sqrt{\overline{\langle |\mathbf{u}|^2\rangle}},$$

Derive scaling laws for Nu(Ra)

$$\epsilon = \epsilon_{BL} + \epsilon_{bulk}$$

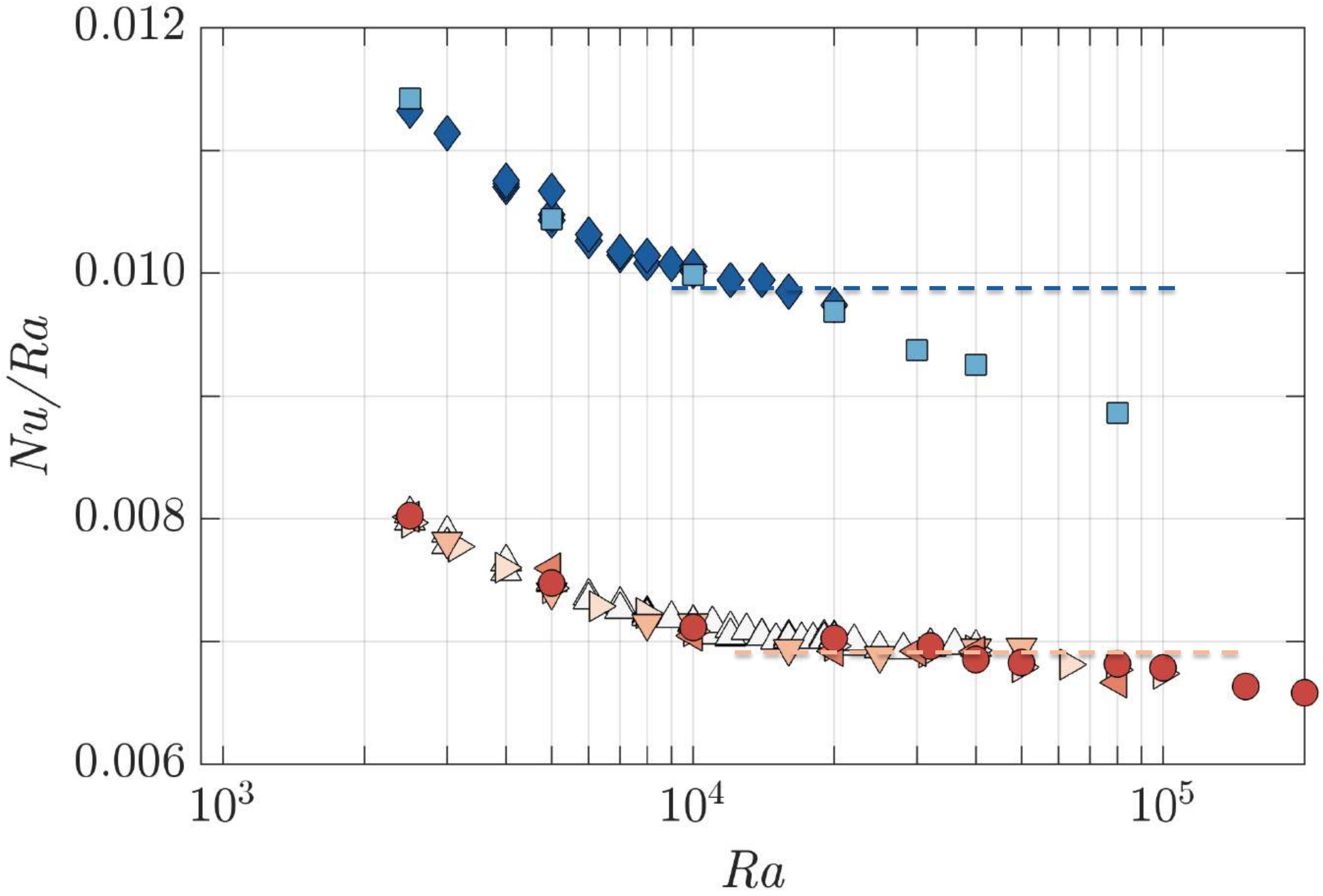
$$\epsilon = \kappa \frac{\Delta^2}{L^2}\overline{\langle |\nabla T|^2\rangle} = \kappa \frac{\Delta^2}{L^2} Nu$$

$$Nu = A_2\, Ra + B_2\, Nu^{1/2}\, Ra^{1/7} \qquad (2D)$$

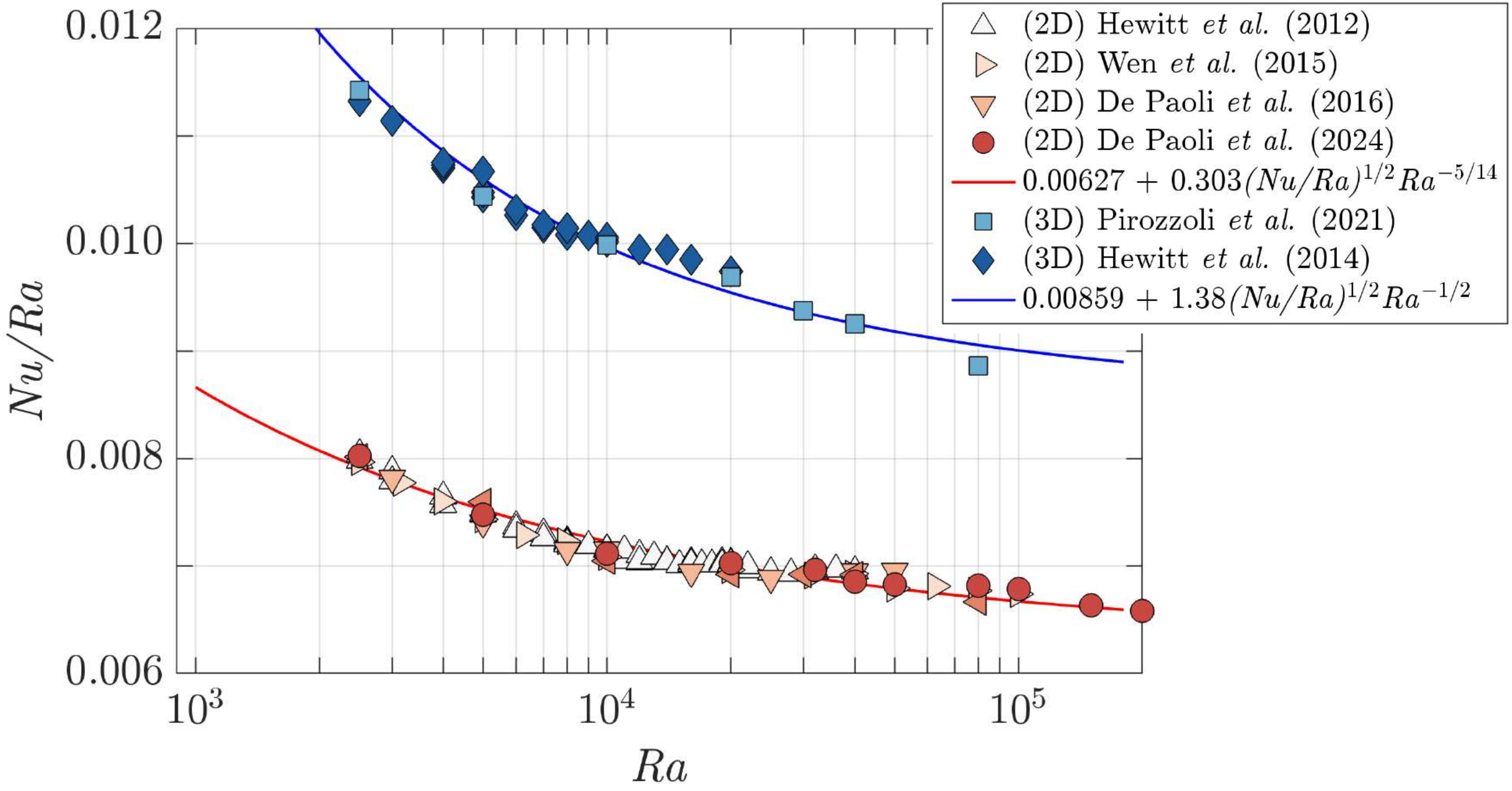
$$Nu = A_3\, Ra + B_3\, Nu^{1/2} \qquad (3D)$$

(theoretical) linear scaling + sublinear correction

3) Derive scaling laws for Nu



3) Derive scaling laws for Nu



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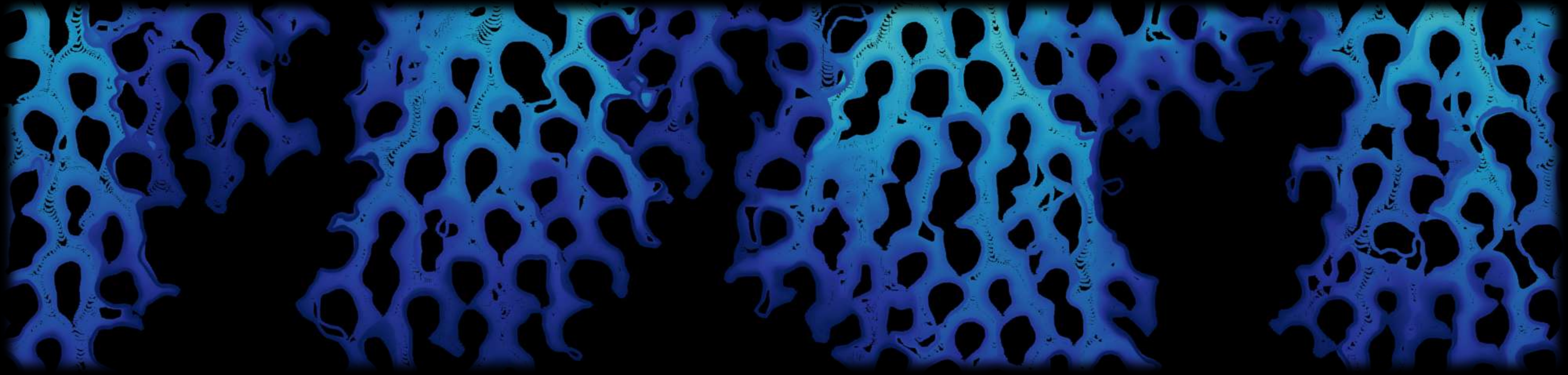
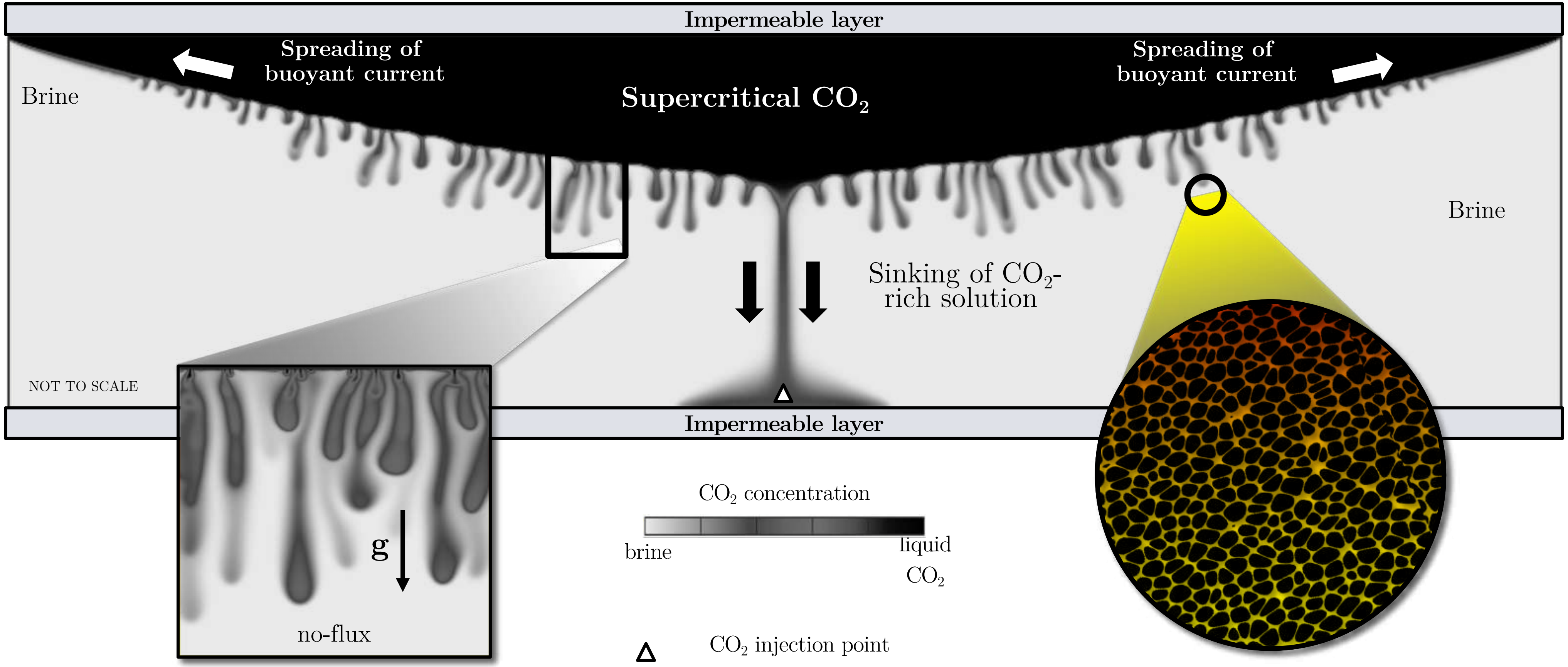
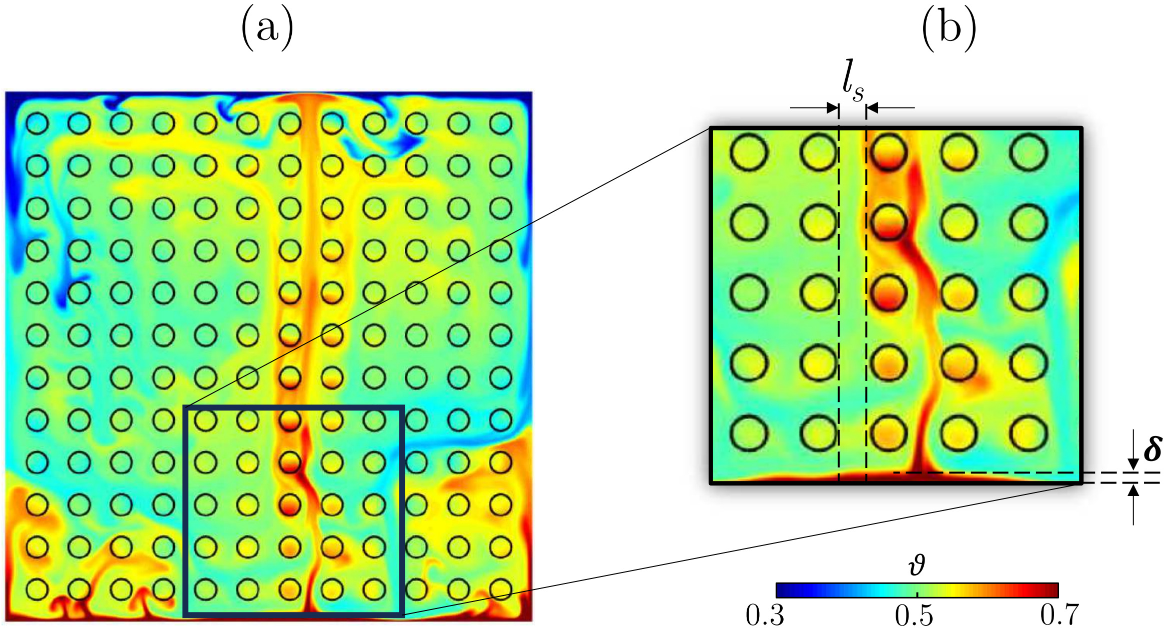
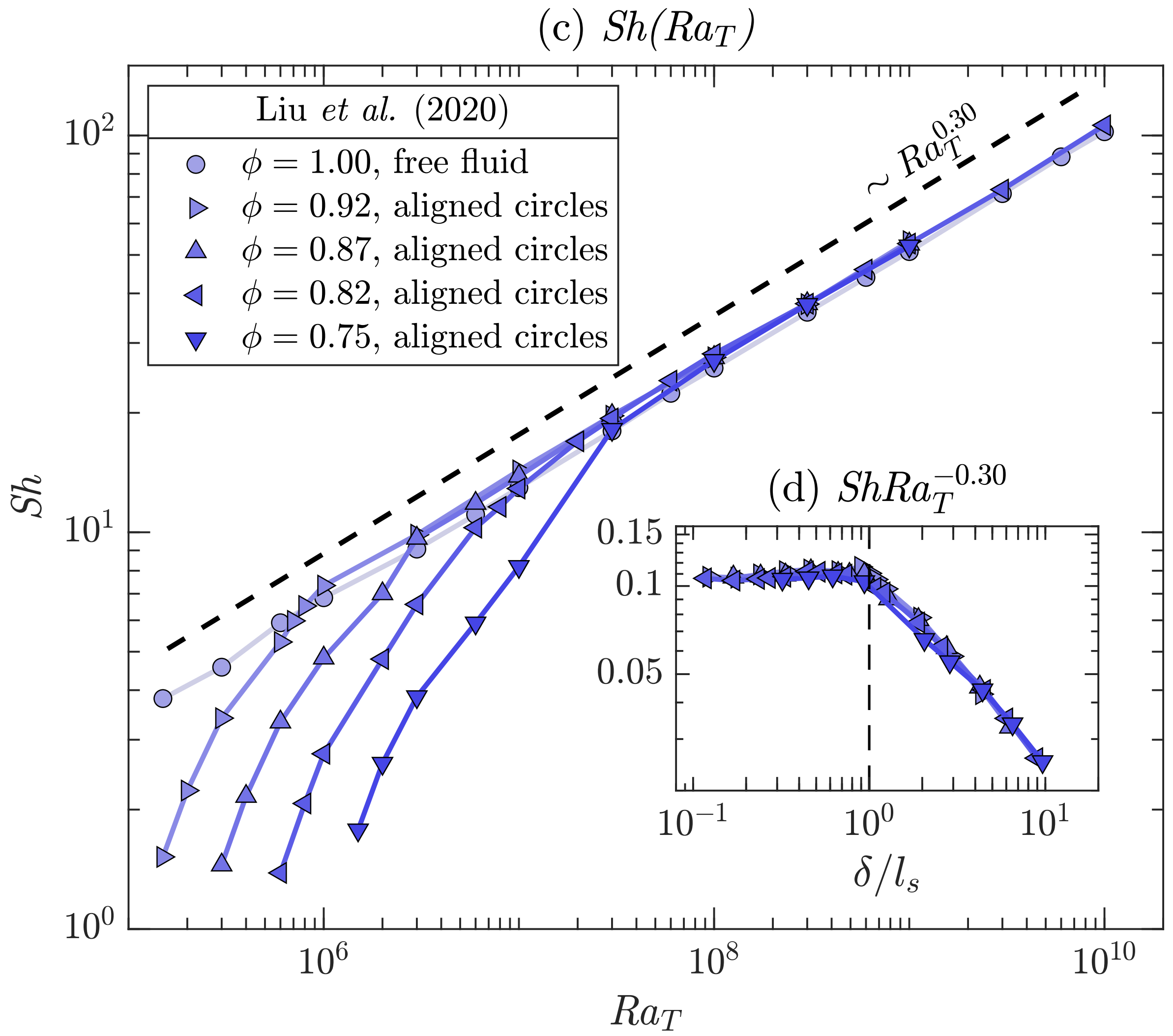




De Paoli, *Phys. Fluids* (2021)

Additional non-Darcy effects:
Relative size of flow structures and pores



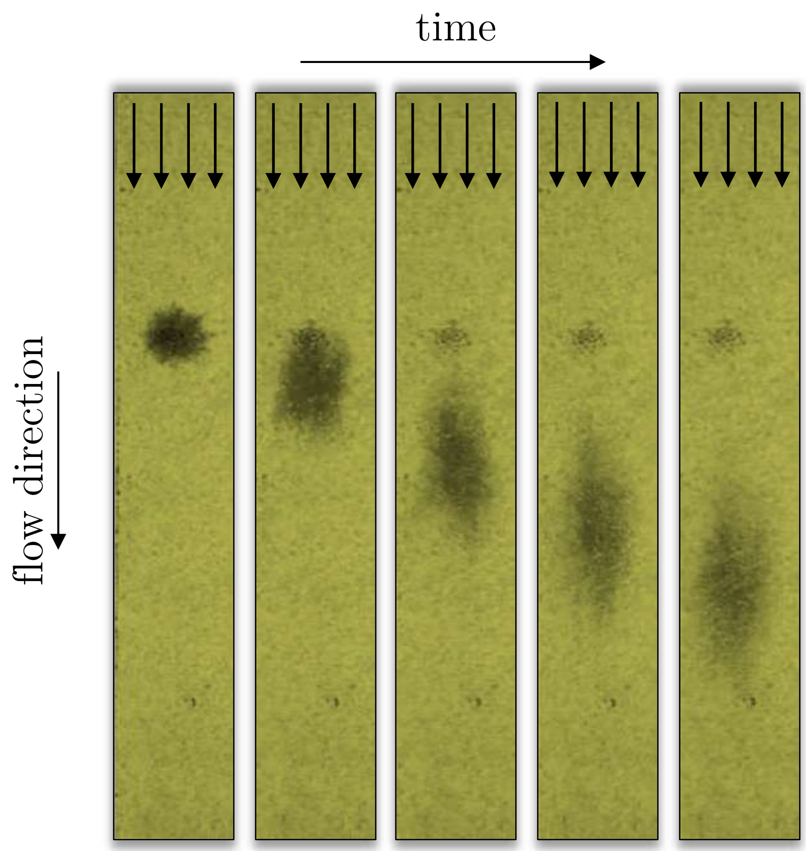


De Paoli, *Eur. Phys. J. E* (2023)

Liu et al., *J. Fluid Mech.* (2020)

Mechanism of dispersion

Patch of dye in a uniform flow through a porous medium



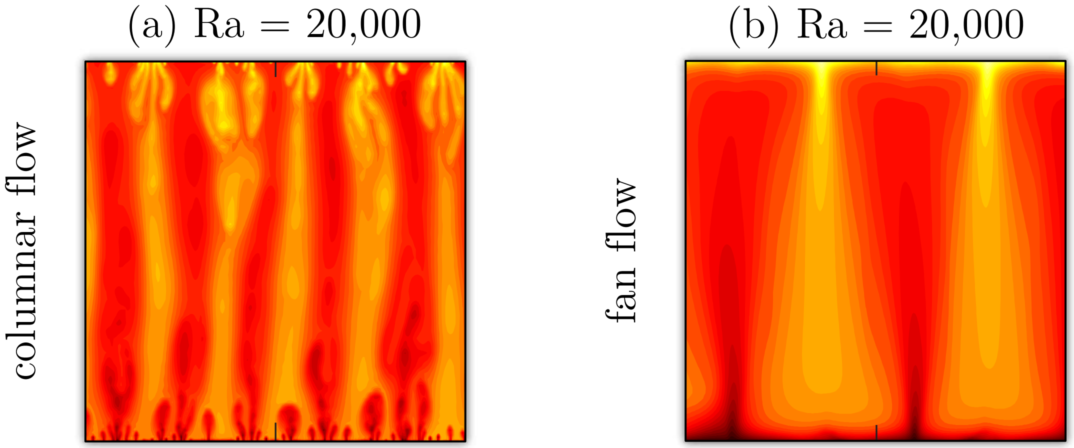
Woods, *Flows in porous rocks* (2015)

Darcy formulation of dispersion

$$\phi \frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C - \phi D \nabla C) = 0$$

Fickian formulation for dispersion

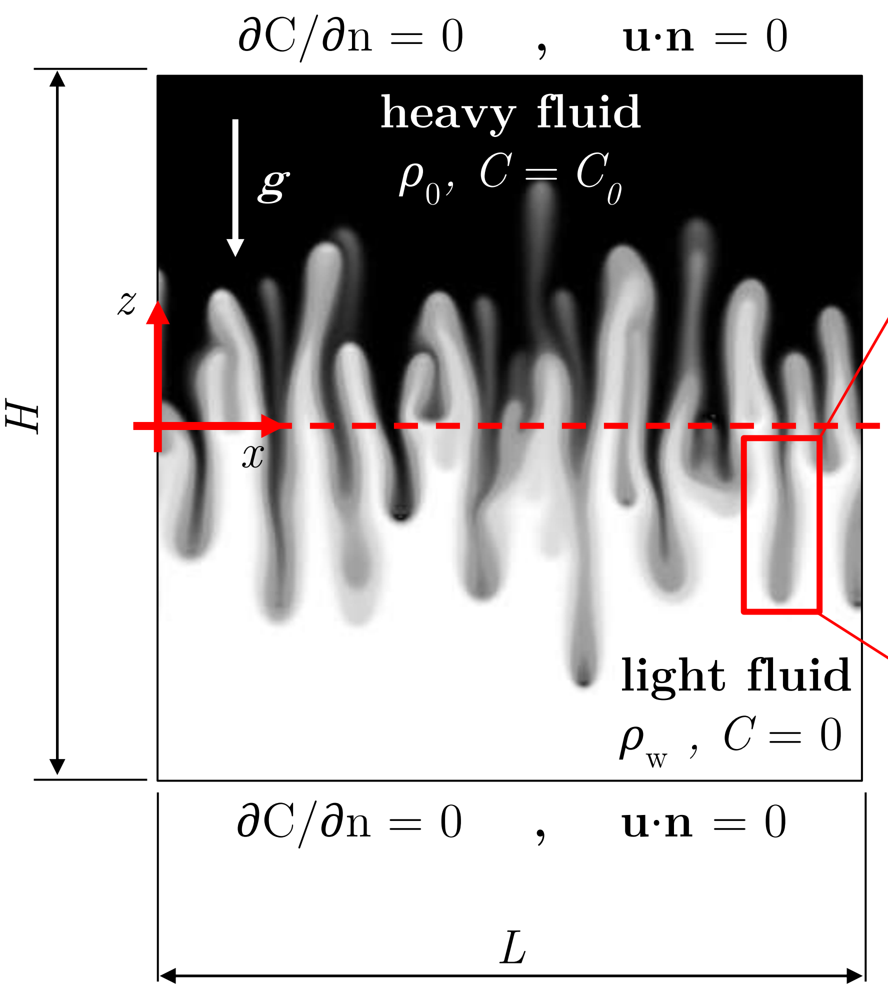
$$\mathbf{D} = D\mathbf{I} + (\alpha_L - \alpha_T)\frac{\mathbf{uu}}{|\mathbf{u}|} + \alpha_T \mathbf{uI},$$



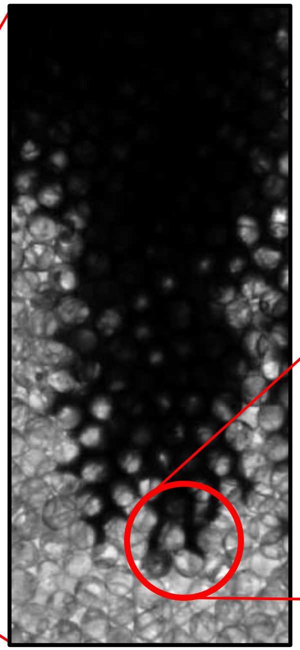
Liang et al., *Geophys. Res. Lett.* (2018)
Chang et al., *Phys. Rev. Fluids* (2018)

These models required validation: Experiments and simulations in porous media

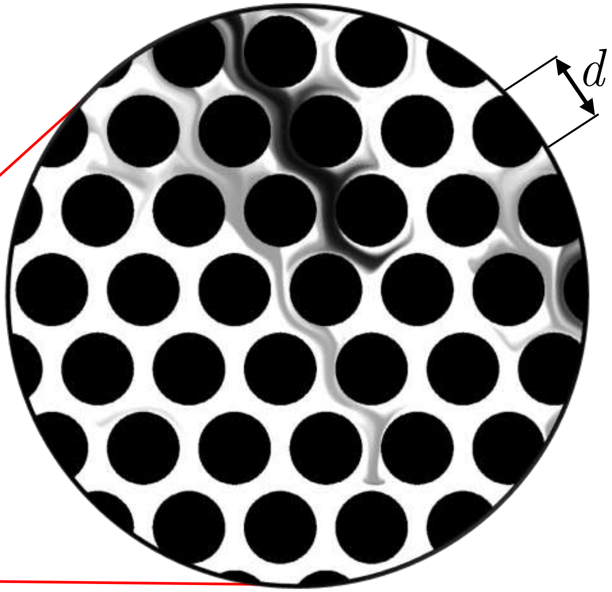
Flow configuration



experiments



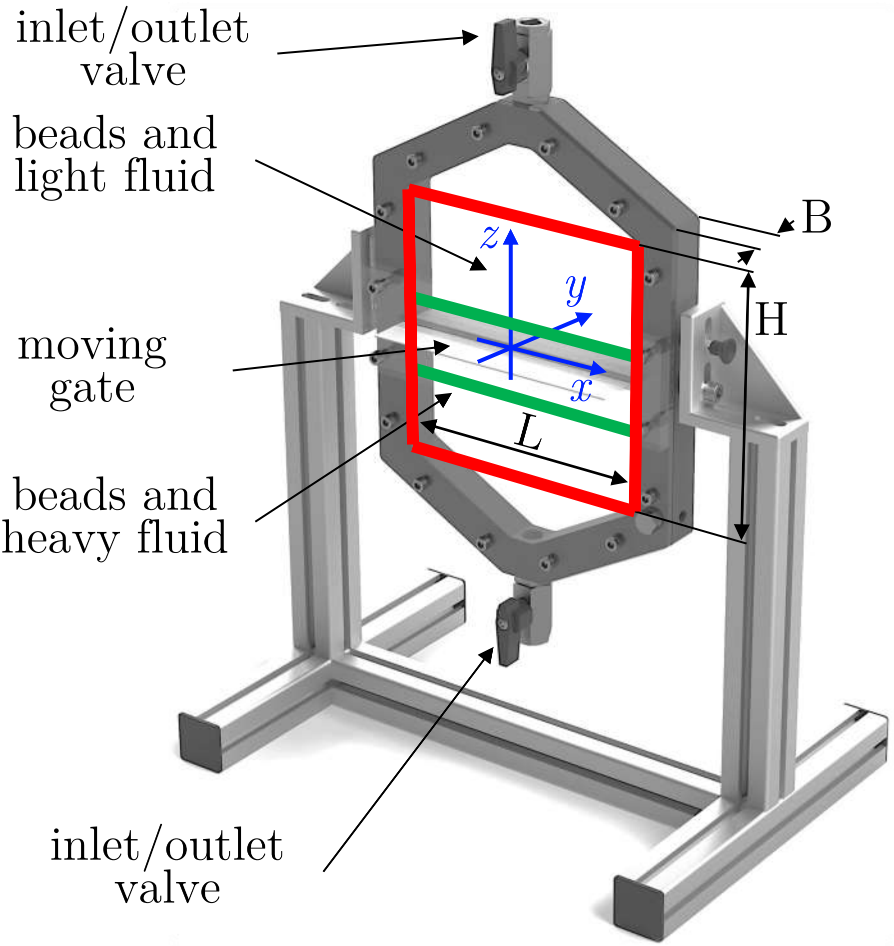
simulations



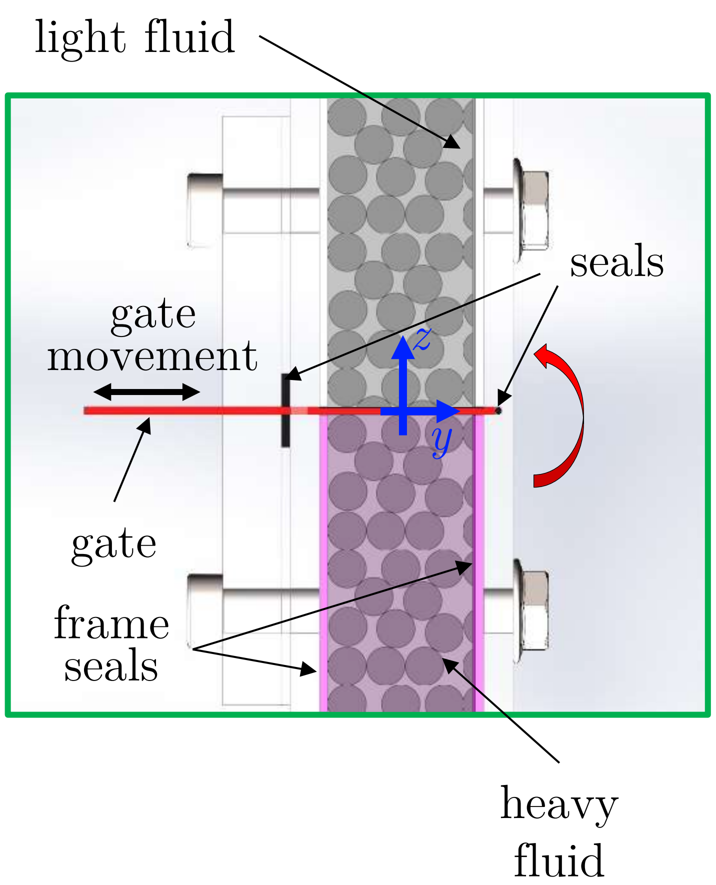
- High Schmidt number
- Porosity matched $\phi = 0.37$
- Solid impermeable to solute
- Linear dependency $\rho(C)$

Experimental setup

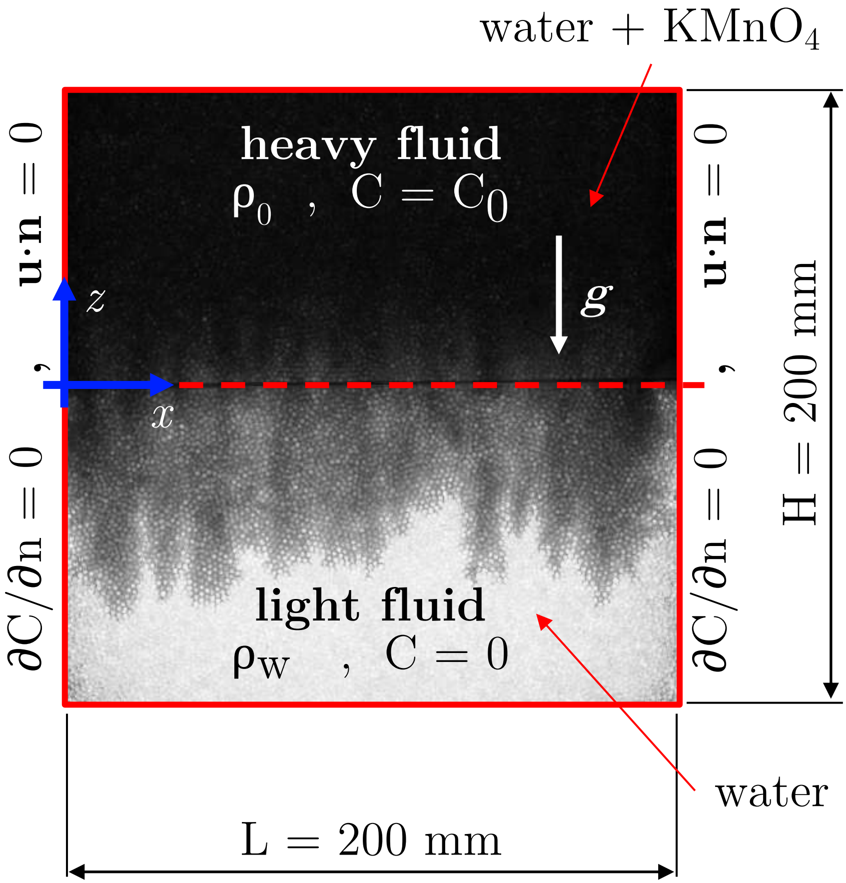
(a) Hele-Shaw cell



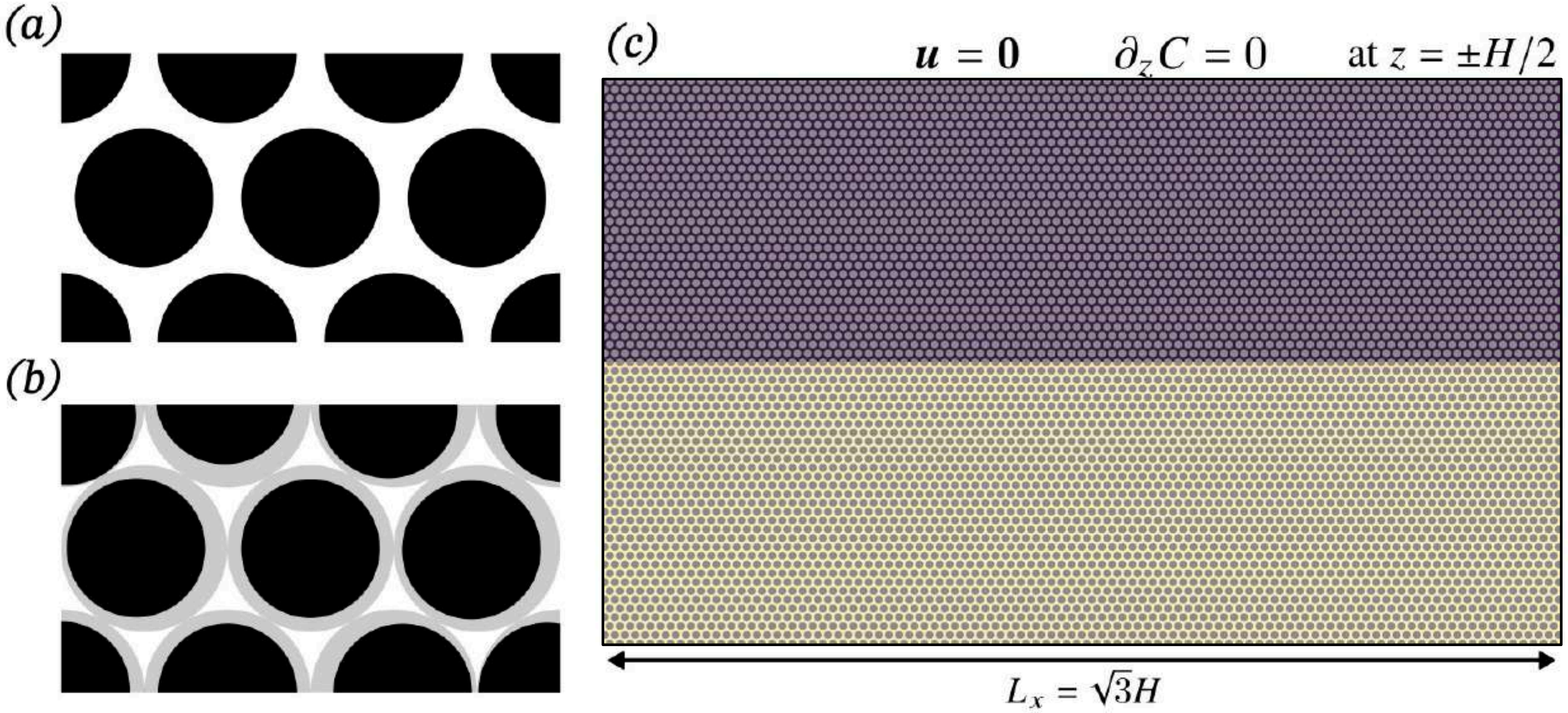
(b) gate (side view)



(c) measurement region



Numerical method



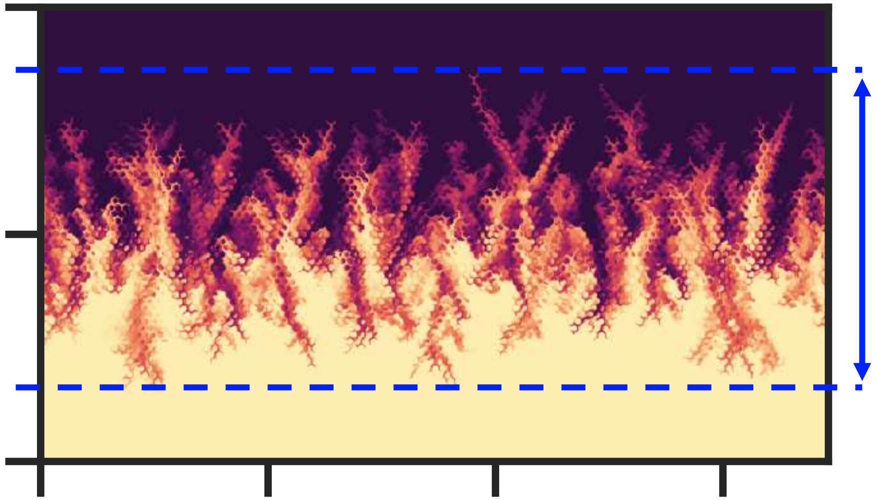
$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \boldsymbol{\nabla})\boldsymbol{u} = -\rho_0^{-1}\boldsymbol{\nabla} p + \nu \nabla^2 \boldsymbol{u} - g\beta C \hat{\boldsymbol{z}},$$

$$\partial_t C + (\boldsymbol{u} \cdot \boldsymbol{\nabla})C = D\nabla^2 C,$$

$$\rho = \rho_0 \left[1 + \frac{\Delta\rho}{\rho_0 C_0}(C - C_0) \right]$$

Finite difference (AFiD, open source)
+
Immersed Boundaries Method

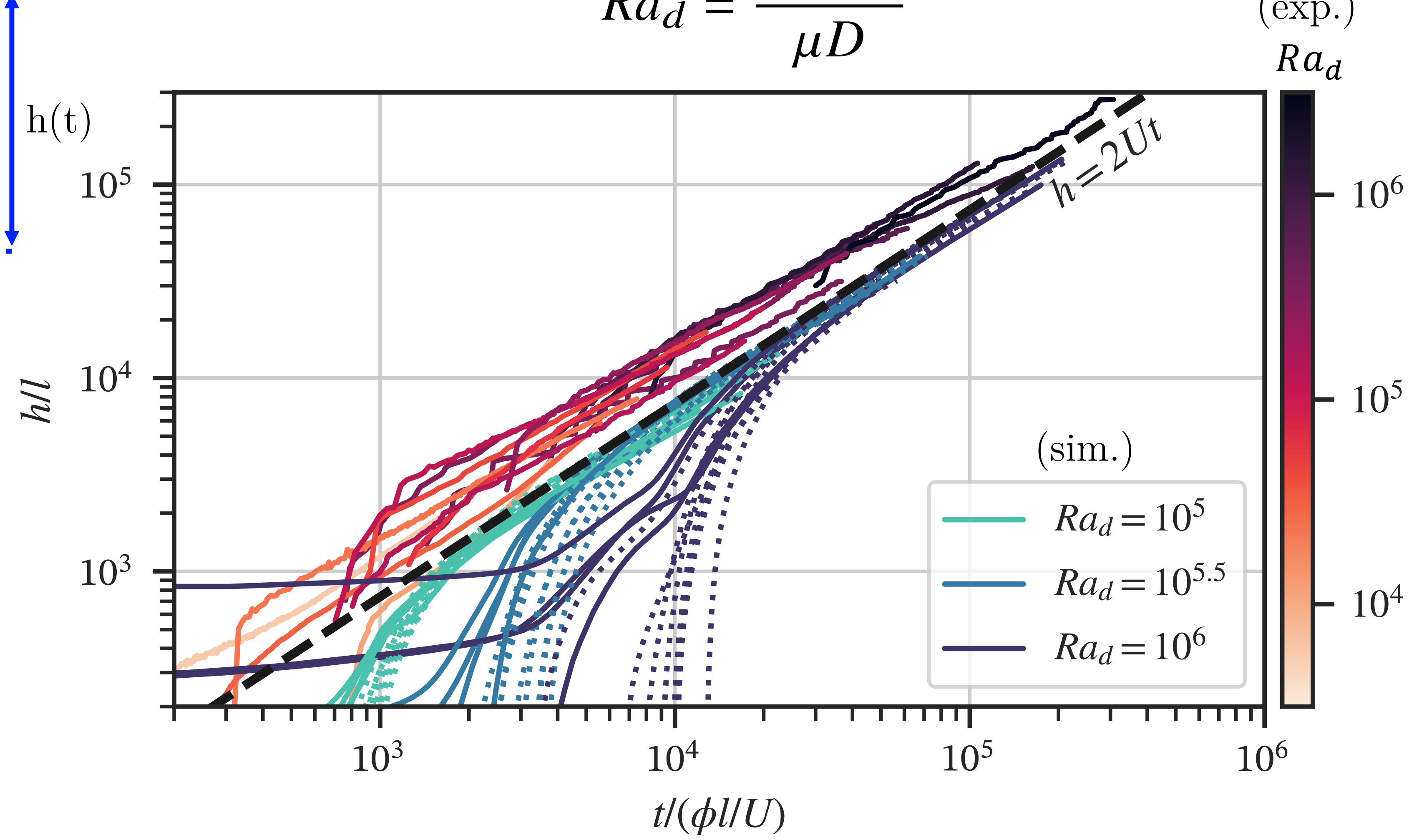
Resolution:
- velocity: ≥ 32 points per diameter
- conc. : ≥ 128 points per diameter



$$U = \frac{g \Delta \rho k}{\mu}$$

$$\ell = \frac{\phi D}{U}$$

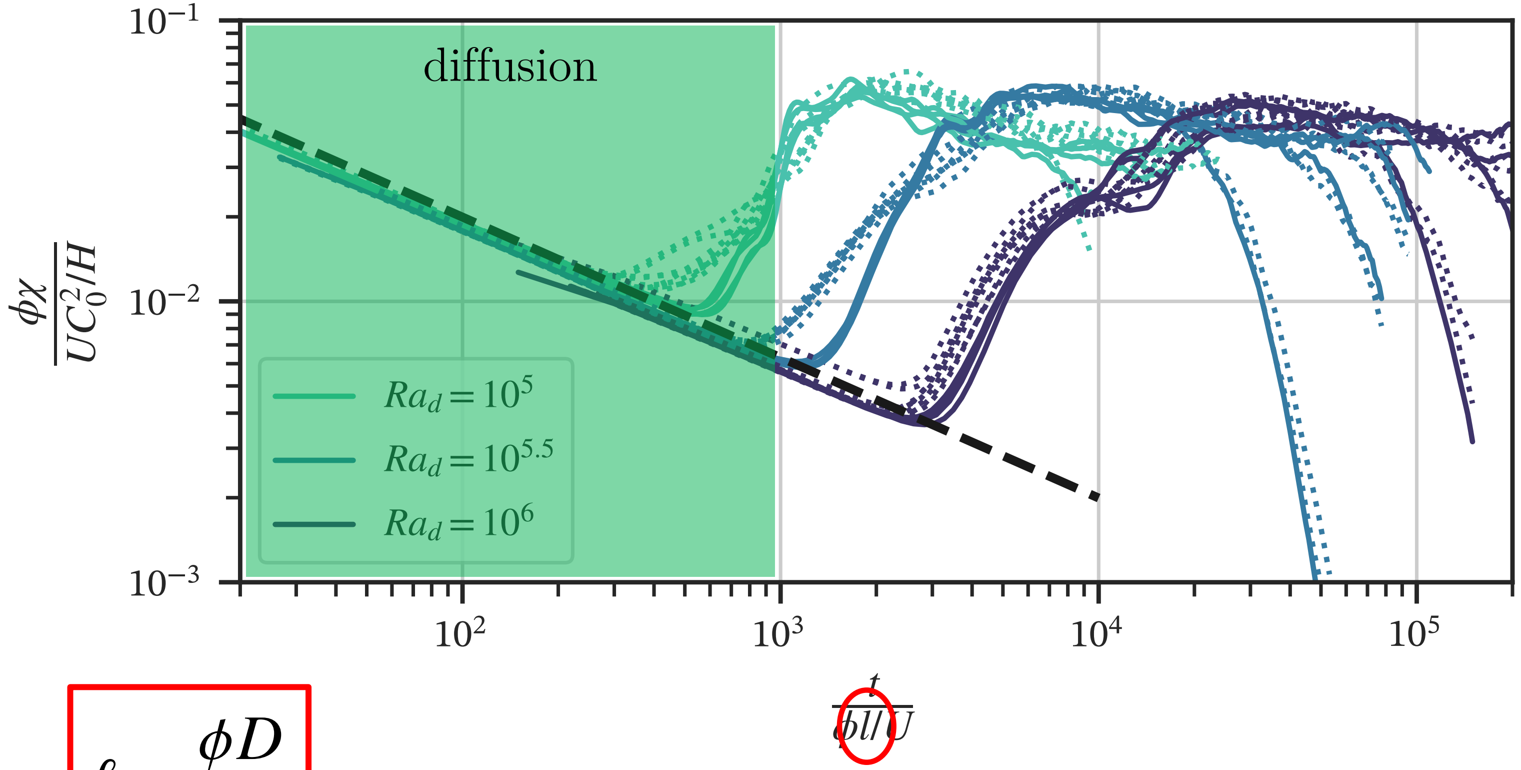
$$Ra_d = \frac{g \Delta \rho d^3}{\mu D}$$



Modelling scalar dissipation

$$\chi = D\langle|\nabla C|^2\rangle_f = \frac{D}{V_f}\int_{V_f}|\nabla C|^2\, dV$$

Can we model this mixing/dissolution process?



$$\ell = \frac{\phi D}{U}$$

Diffusion:

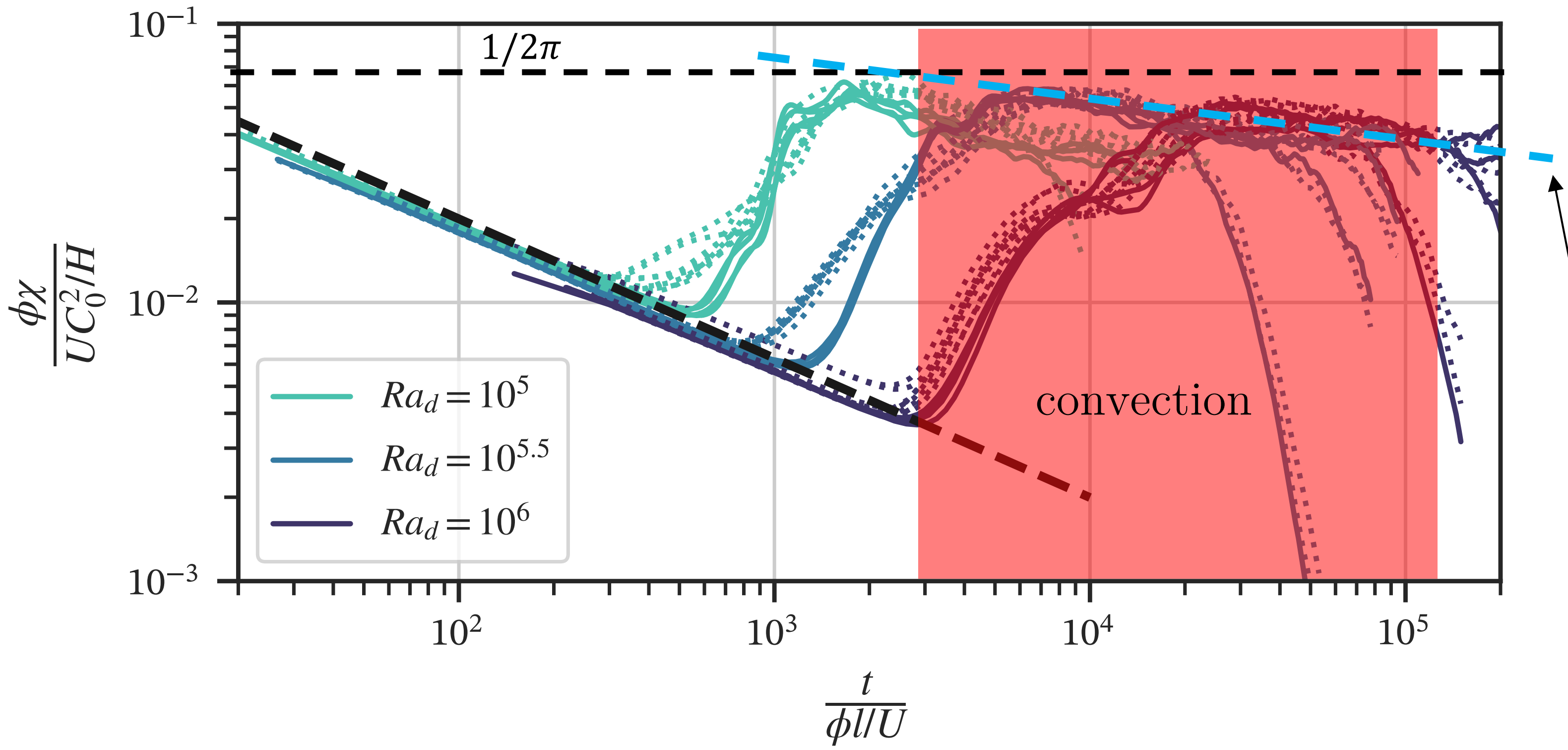
$$C = C_0 + \frac{\Delta C}{2}\text{erf}\left(\frac{z}{\sqrt{2\kappa t}}\right)$$

$$\partial_z C = \frac{\Delta C}{2\sqrt{\pi\kappa t}}\exp\left(-\frac{z^2}{2\kappa t}\right)$$

$$\chi = \kappa\langle|\nabla C|^2\rangle = \frac{\kappa}{H}\int_{-\infty}^{\infty}|\partial_z C|^2 \mathrm{d}z$$

$$= \sqrt{\frac{\kappa}{8\pi t}}\frac{(\Delta C)^2}{H}$$

$$\chi = D\langle|\nabla C|^2\rangle_f = \frac{D}{V_f}\int_{V_f} |\nabla C|^2 \, dV$$



Convection

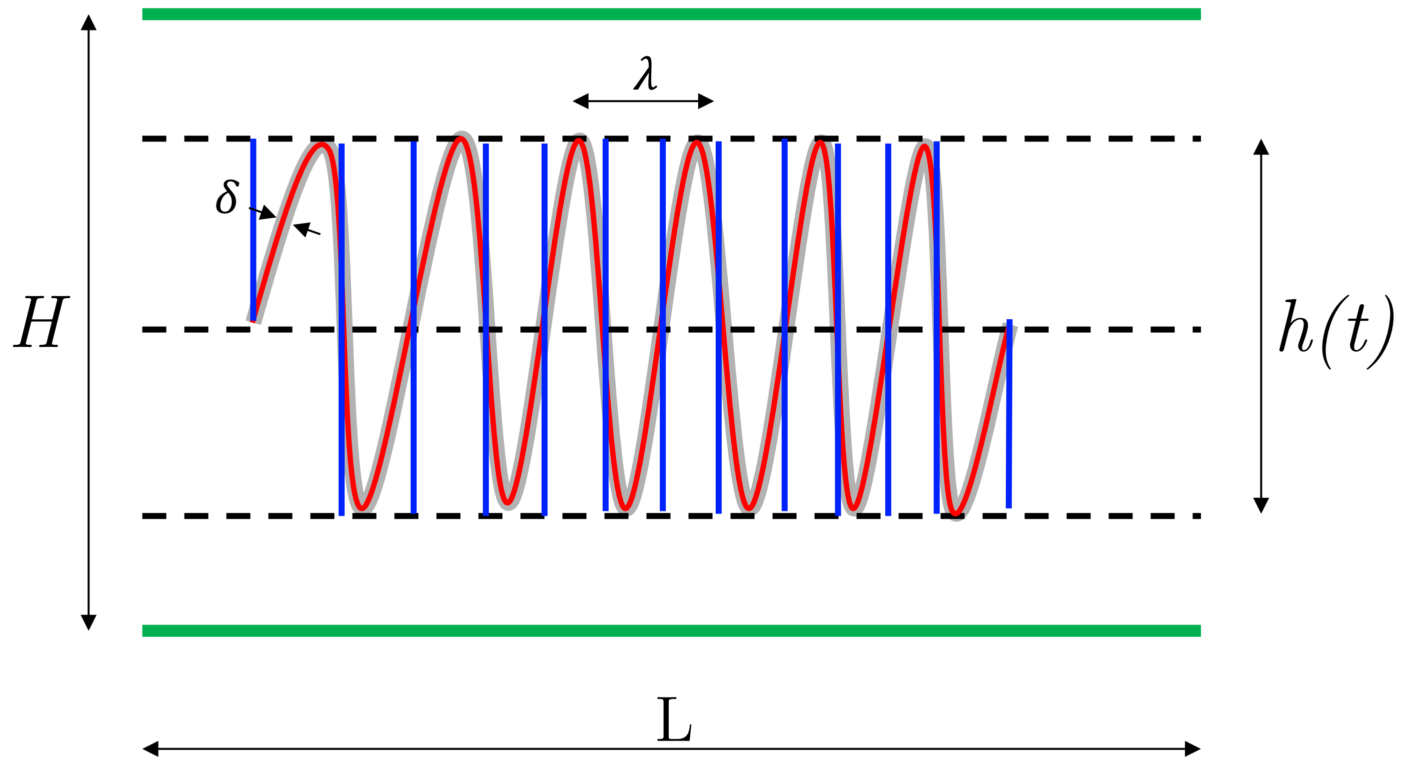
$$\chi = \kappa\langle|\nabla C|^2\rangle = \kappa\frac{L_m}{H}\langle|\nabla C|^2\rangle_{ML},$$

$$|\nabla C| \approx \frac{\Delta C}{2\sqrt{\pi\kappa t}}.$$

$$L_m \approx 2Ut,$$

$$\chi \approx \kappa\frac{2Ut}{H}\frac{(\Delta C)^2}{4\pi\kappa t} = \frac{1}{2\pi}\frac{U_d(\Delta C)^2}{H}.$$

$1/2\pi$ is the maximum value of dissipation. Practically, χ decreases with time

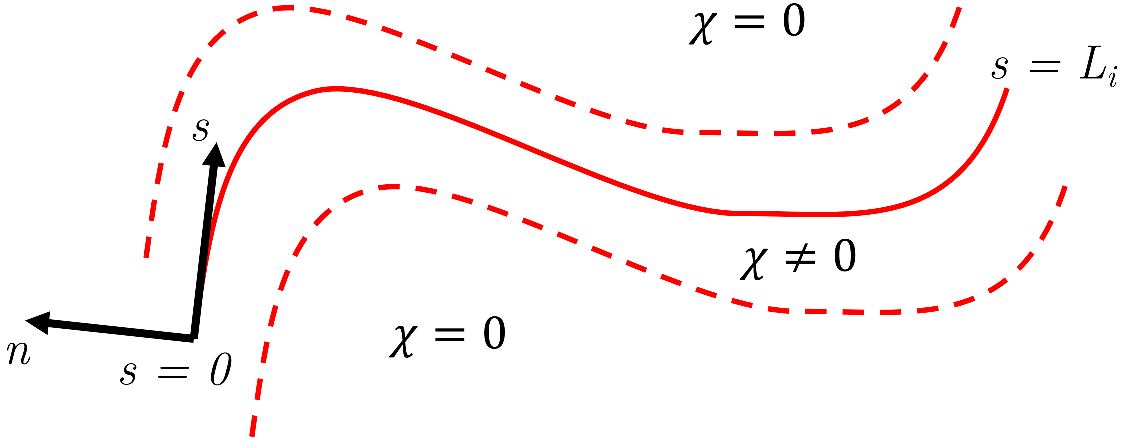


Assume:

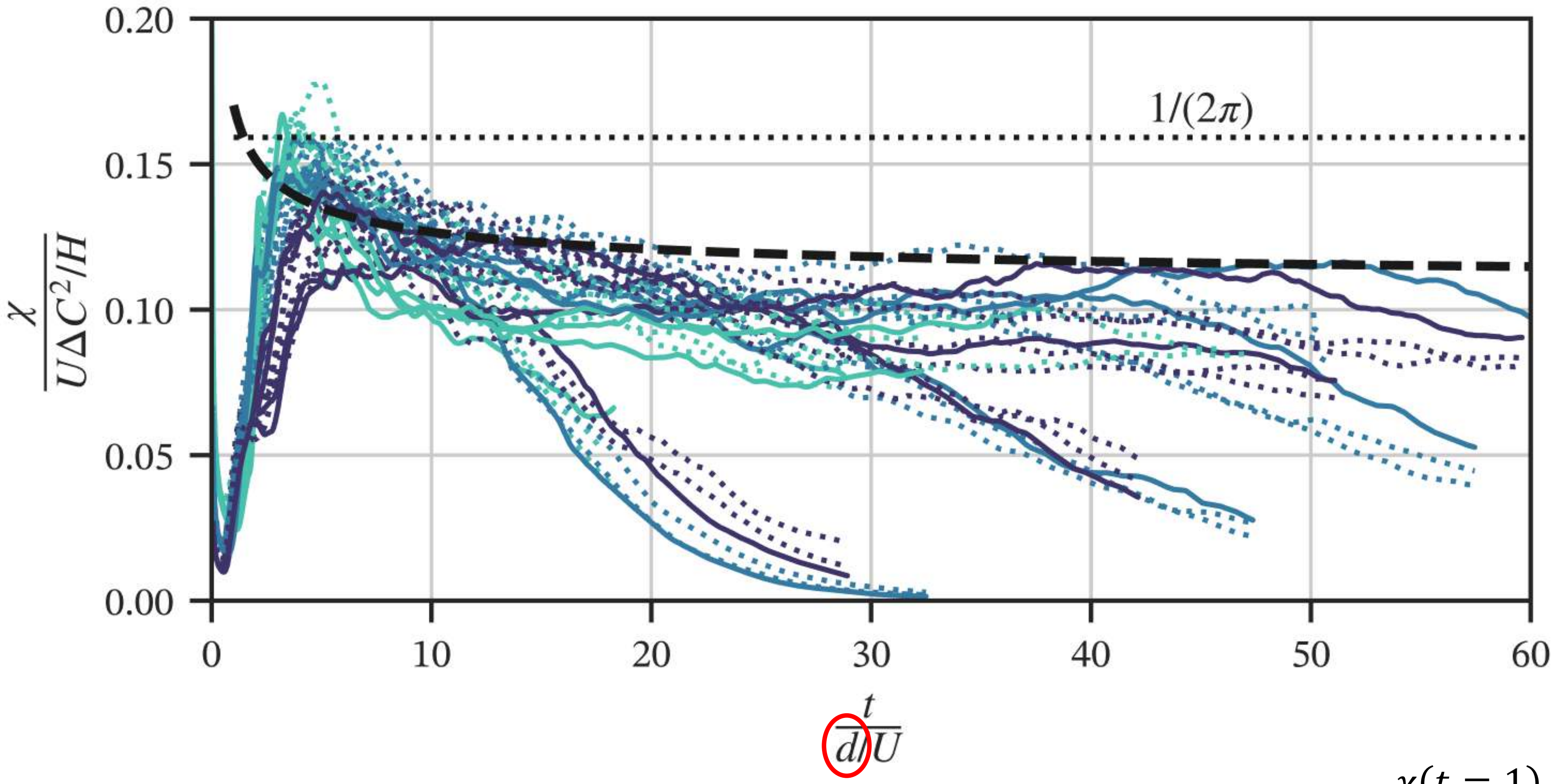
1) Interface grows as:

$$L_i = L + 2\,N_{finger}\,h = L + 2\frac{L}{\lambda}h$$

2) Gradient across the interface evolves according to the diffusive solution



$$\chi = D\langle|\nabla C|^2\rangle = \frac{D L_i}{HL}\int_{-\delta/2}^{+\delta/2}|\partial_n C|^2\,dn$$



$1/2\pi$ is the maximum value of dissipation.

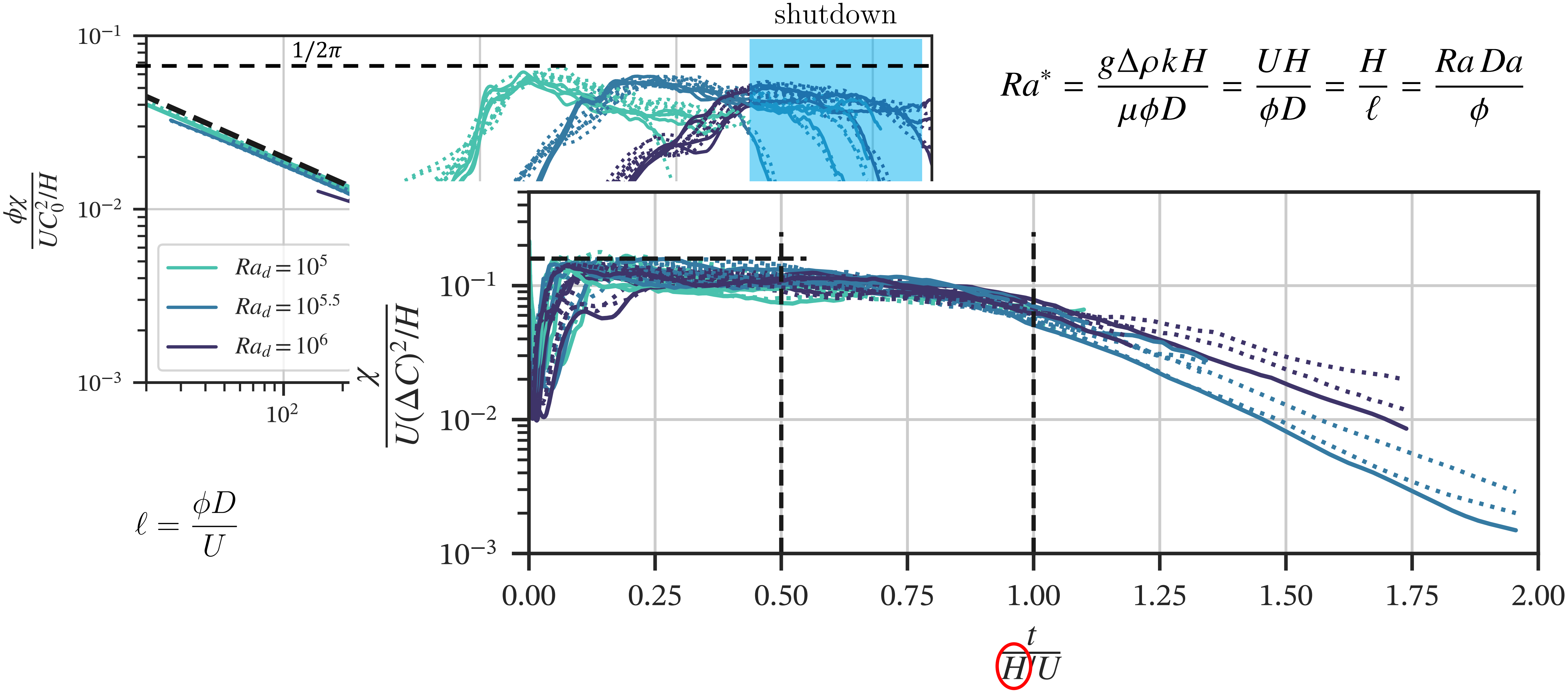
Model shown starting from $t/(d/U)$ =1. Time is also increased by d/U to account for initial condition.

$$\frac{\chi(t=1)}{(\Delta C)^2 U/H} = \frac{\beta}{\alpha\pi}\left(1+\frac{\alpha}{4}\right) \approx \frac{1}{1.92\pi} \approx \frac{1}{2\pi}$$

Modelling scalar dissipation

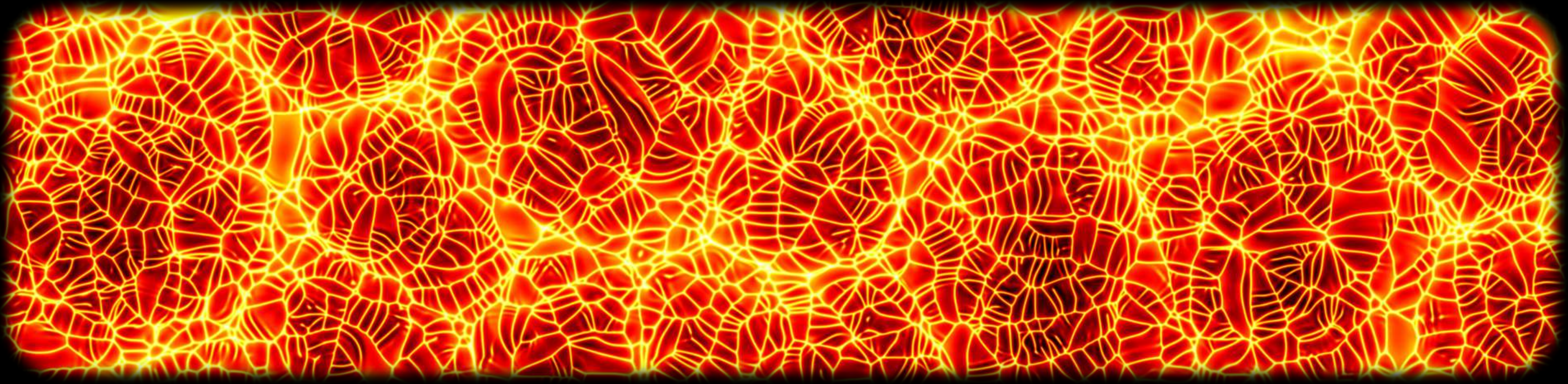
$$Ra^* = \frac{g\Delta\rho k H}{\mu\phi D} = \frac{UH}{\phi D} = \frac{H}{\ell} = \frac{Ra\,Da}{\phi}$$

$$\ell = \frac{\phi D}{U}$$



Presentation outline

1. Motivation
2. Reservoir-scale: multiphase gravity currents
3. Darcy-scale: simulations, experiments and finite-size effects
4. Pore-scale modelling and dispersion
5. **Conclusions and outlook**

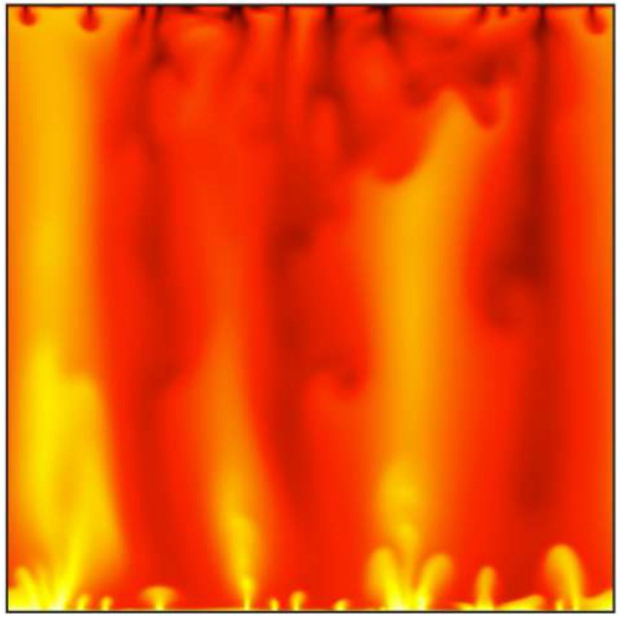


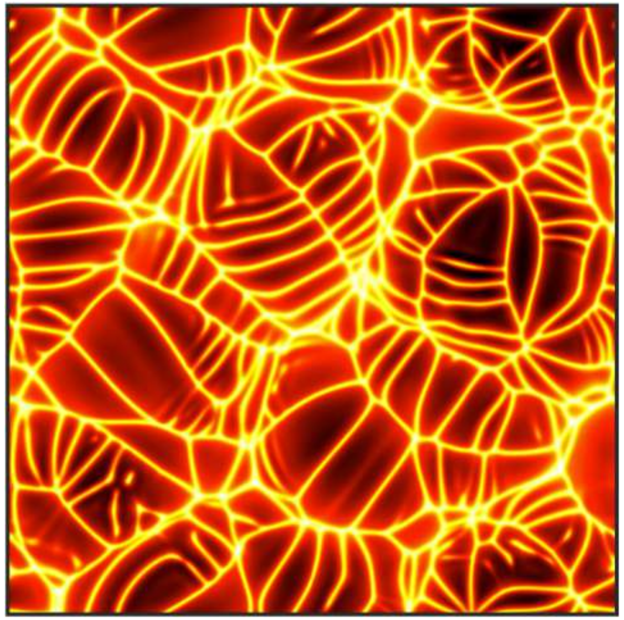
Conclusions and outlook

Convection in porous media is a **multiscale** and **multiphase** process

A **combination of experiments, simulations and theory** is required to model the flow dynamics

Recent developments in numerical and experimental capabilities enable measurements at unprecedented level of detail, but the parameters space is huge!





References

- De Paoli, M., Howland, C. J., Verzicco, R., & Lohse, D. (2024). *Journal of Fluid Mechanics*, *987*, A1.
- Zhu, X., Fu, Y., & De Paoli, M. (2024). *Journal of Fluid Mechanics* (in press).
- De Paoli, M., Yerragolam, G. S., Lohse, D. & Verzicco, R., (2024). AFiD-Darcy: A finite difference solver for numerical simulations of convective porous media flows (under review).

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Conclusions and outlook

Thank you for your attention! Questions?

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High-resolution images, movies and slides are available upon request to m.depaoli@utwente.nl