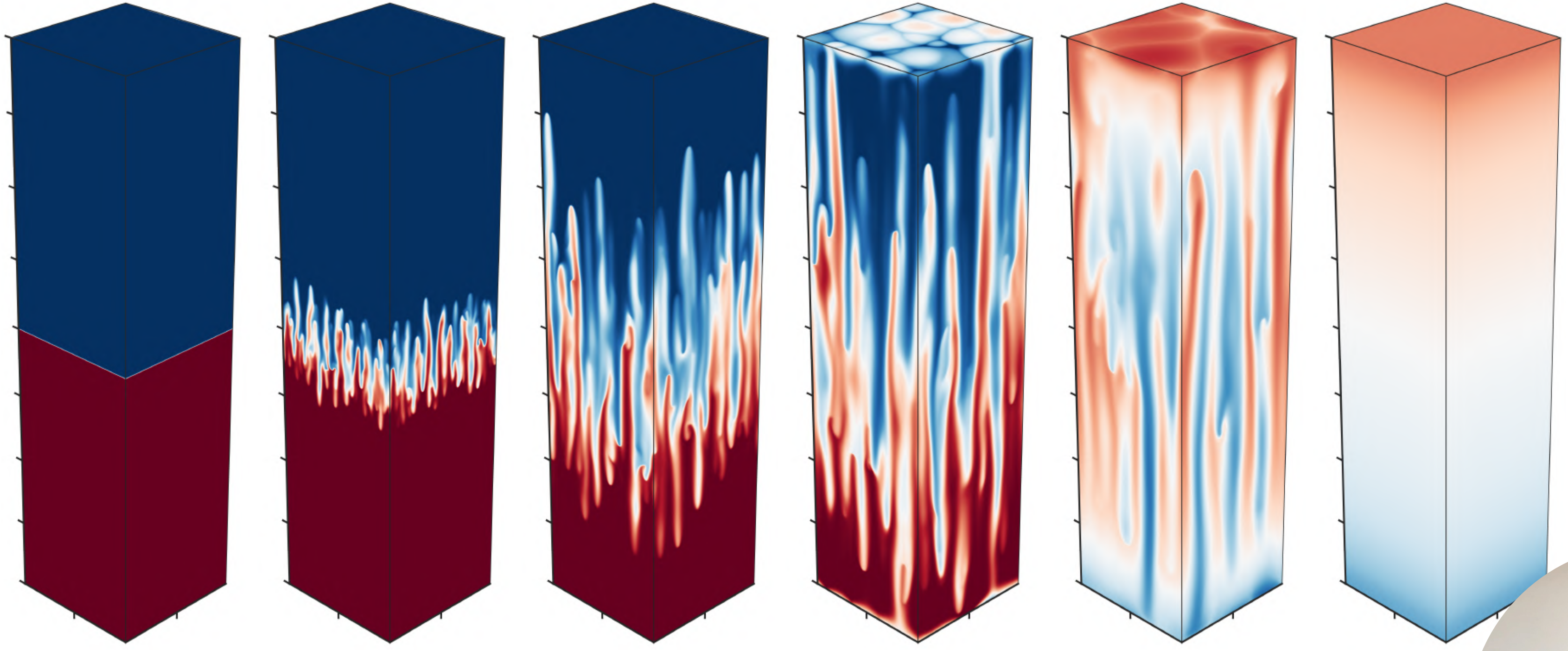
AFiD-Darcy: A finite difference solver for numerical simulations of convective porous media flows



M. De Paoli[1,2], Guru Sreevanshu Yerragolam[1], Detlef Lohse[1] & Roberto Verzicco[1,3,4]

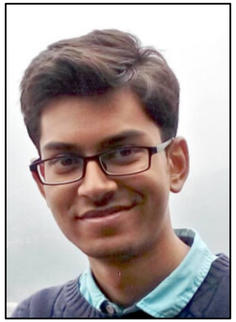
[1]Physics of Fluids Group, University of Twente, Enschede (The Netherlands)
[2]Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna (Austria)
[3]Dipartimento di Ingegneria Industriale, University of Rome “Tor Vergata”, Rome (Italy)
[4]Gran Sasso Science Institute, L’Aquila, (Italy)

De Paoli, M., Yerragolam, G. S., Lohse, D., & Verzicco, R. (2025). *Computer Physics Communications*, 109579. https://doi.org/10.1016/j.cpc.2025.109579

Acknowledgements

D. Lohse

G. S. Yerragolam



R. Verzicco

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Marie Skłodowska-Curie Actions

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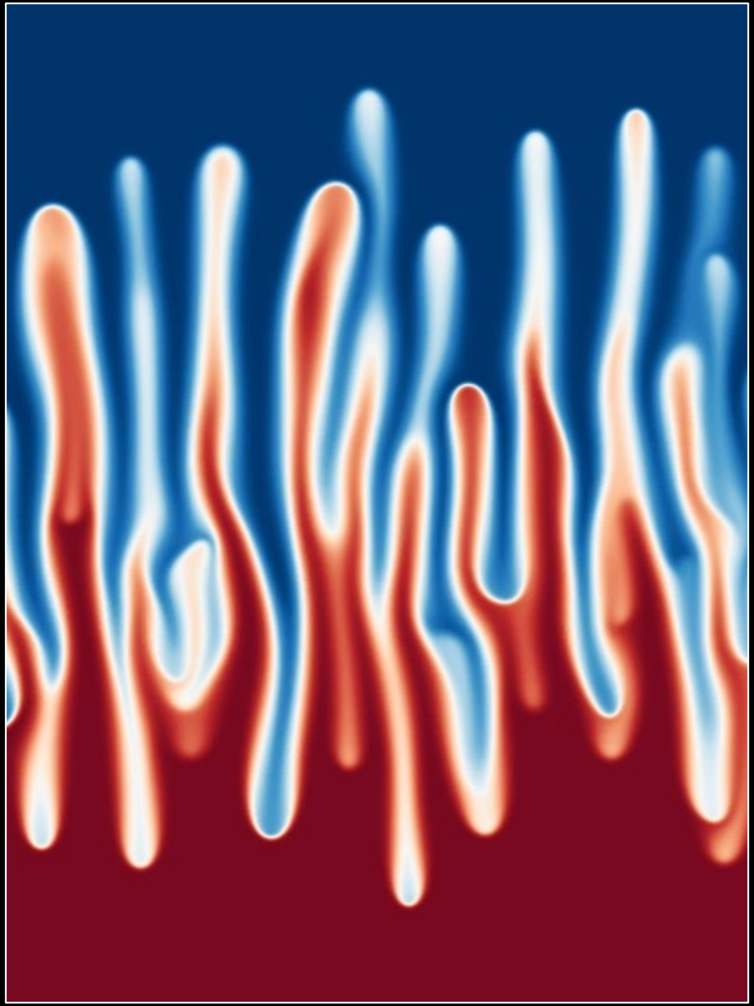
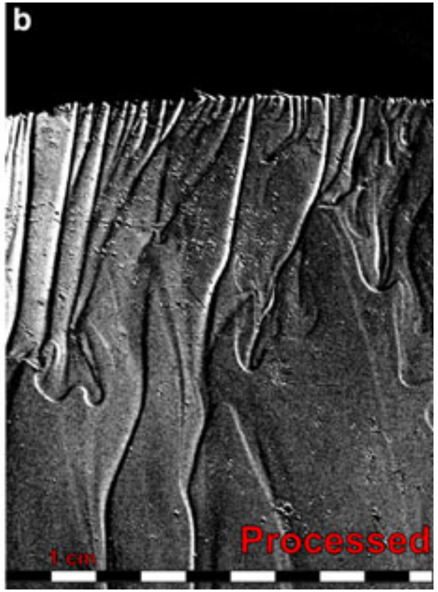
1. Motivation & background
2. Methodology
3. Verification
4. Future developments
5. Conclusions



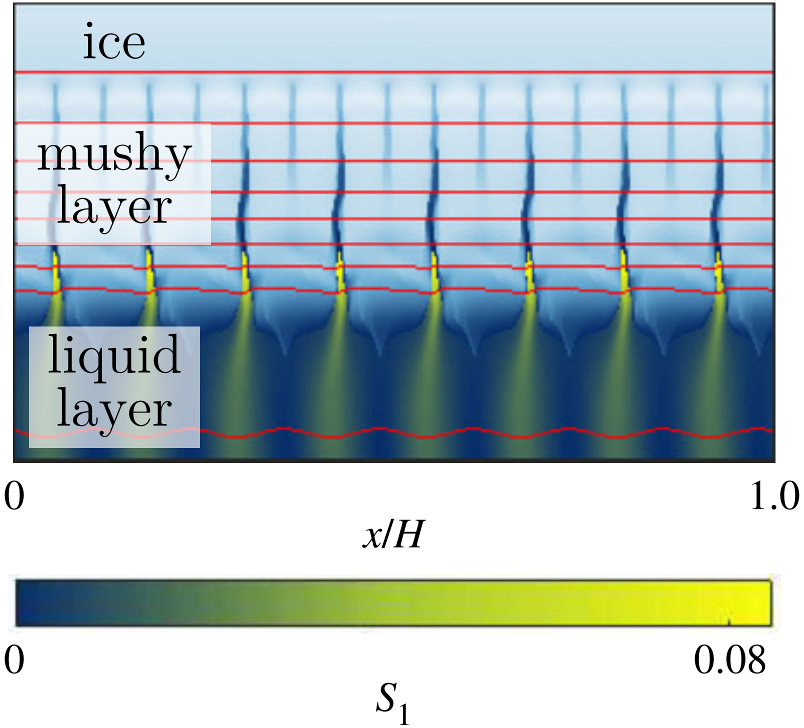
1) Motivation & background

A) Convection in porous media

Sea ice formation



Middleton, C. A., C. Thomas, A. de Wit, And J.-L. Tison. "Visualizing Brine Channel Development and Convective Processes during Artificial Sea-Ice Growth Using Schlieren Optical Methods." *Journal of Glaciology* 62, no. 231 (2016): 1–17. https://doi.org/10.1017/jog.2015.1.



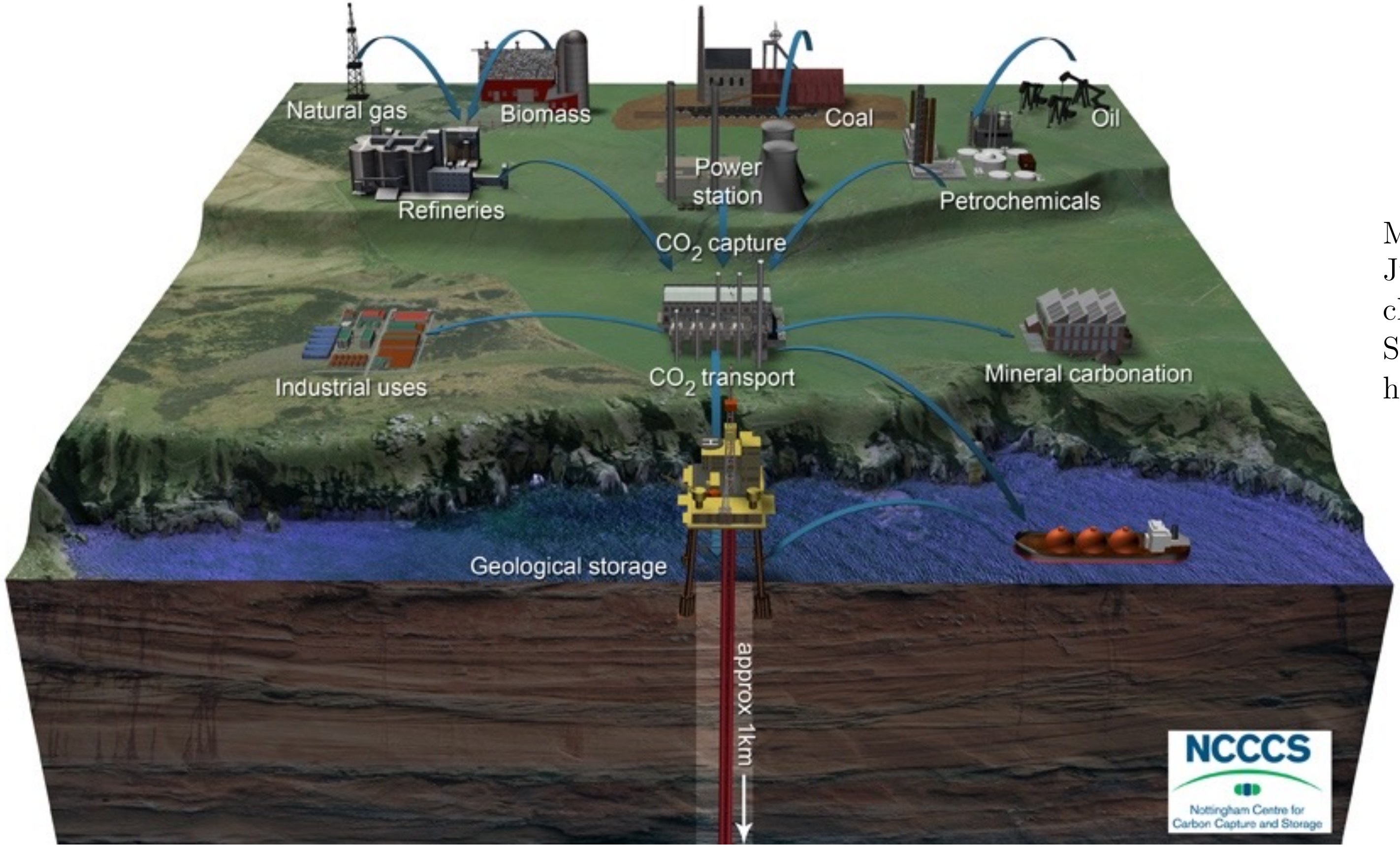
Wells AJ, Hitchen JR, Parkinson JRG. 2019 Mushy-layer growth and convection, with application to sea ice. *Phil. Trans. R. Soc. A* 377: 20180165. http://dx.doi.org/10.1098/rsta.2018.0165

Other applications

Craig T. Simmons, Thomas R. Fenstemaker, John M. Sharp, Variable-density groundwater flow and solute transport in heterogeneous porous media: approaches, resolutions and future challenges, *Journal of Contaminant Hydrology*, 2001, https://doi.org/10.1016/S0169-7722(01)00160-7

De Paoli, M. Convective mixing in porous media: a review of Darcy, pore-scale and Hele-Shaw studies. *Eur. Phys. J. E* 46, 129 (2023). https://doi.org/10.1140/epje/s10189-023-00390-8

https://www.youtube.com/watch?v=RZwjnRfImbo&t=58s&ab_channel=YOUTUBEPEDIA



Injection point

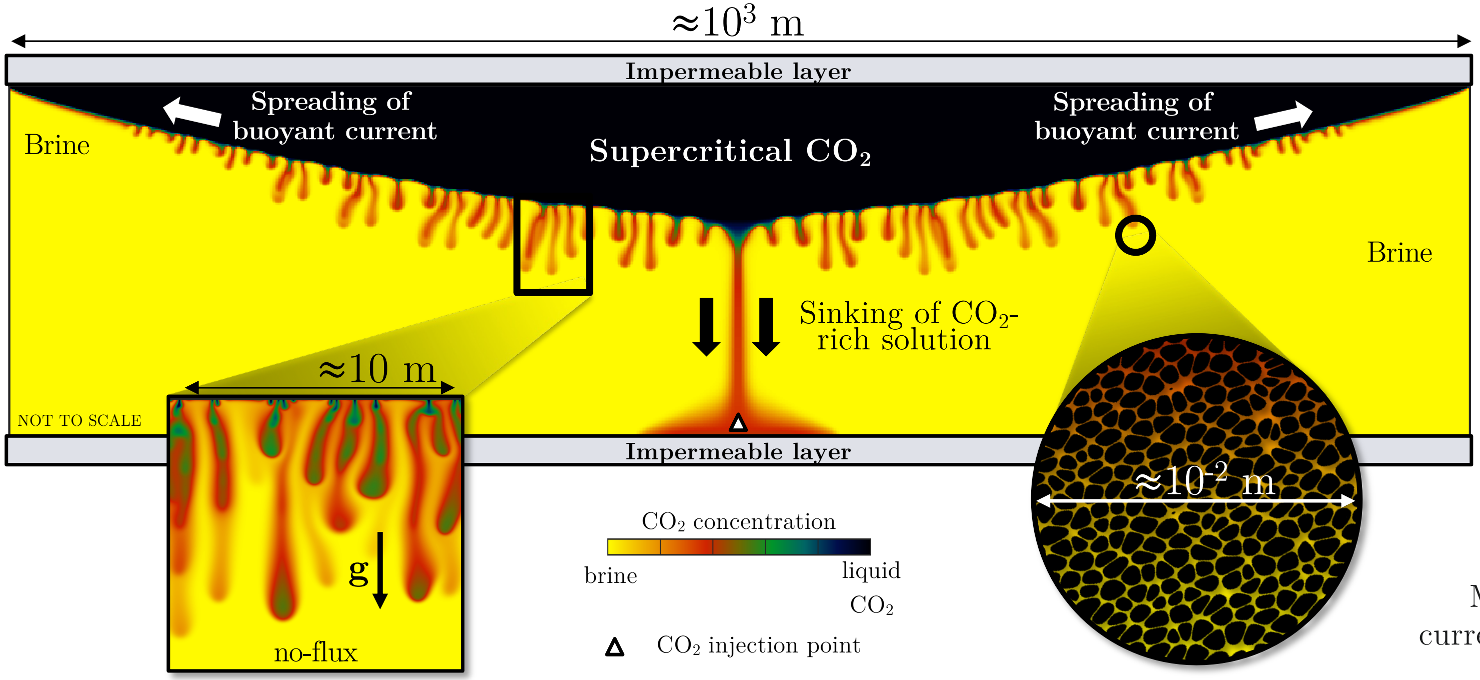
CCS can work as unique climate change mitigation technology for at least 100 years

M.L. Szulczewski, C.W. MacMinn, H.J. Herzog, & R. Juanes, Lifetime of carbon capture and storage as a climate-change mitigation technology, Proc. Natl. Acad. Sci. U.S.A. 109 (14) 5185-5189, https://doi.org/10.1073/pnas.1115347109 (2012)

Physics of Fluids

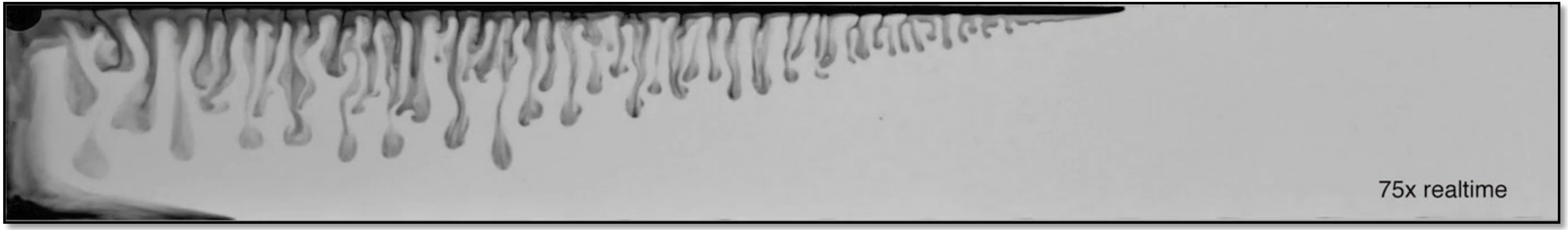
B) Carbon Capture and Storage

COMPUTER PHYSICS COMMUNICATIONS

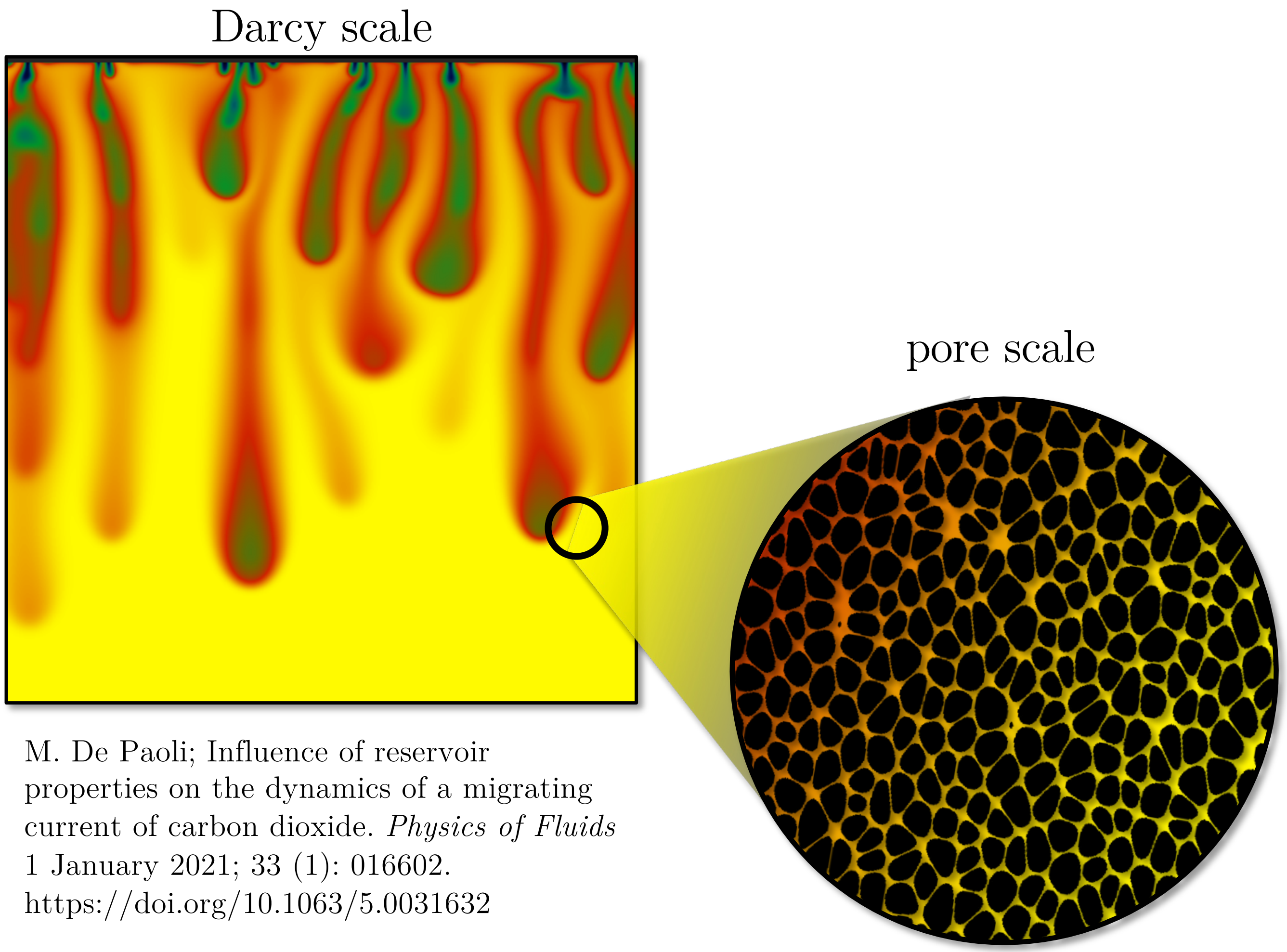


M. De Paoli; Influence of reservoir properties on the dynamics of a migrating current of carbon dioxide. *Physics of Fluids* 1 January 2021; 33 (1): 016602. https://doi.org/10.1063/5.0031632

MacMinn, C. W., and R. Juanes (2013), Buoyant currents arrested by convective dissolution, *Geophys. Res. Lett.*, 40, 2017–2022, doi:10.1002/grl.50473.



B) Carbon Capture and Storage



M. De Paoli; Influence of reservoir properties on the dynamics of a migrating current of carbon dioxide. *Physics of Fluids* 1 January 2021; 33 (1): 016602. https://doi.org/10.1063/5.0031632

Focus on the **Darcy scale**:

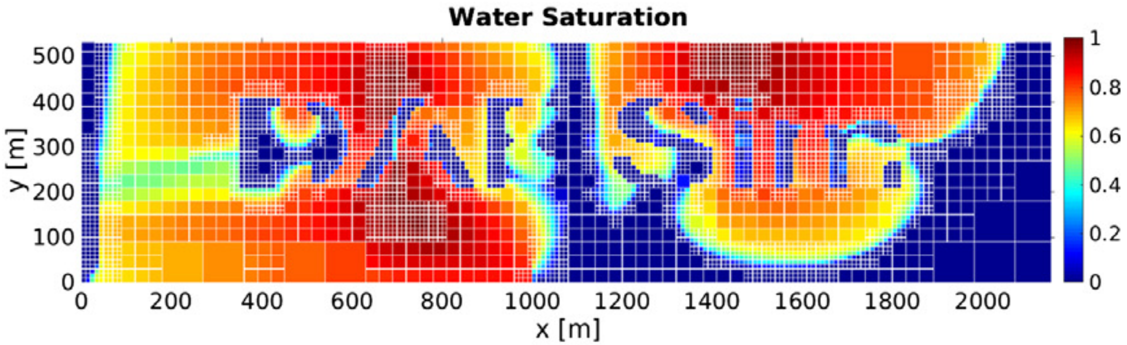
- Flow equation valid for a Reference Elementary Volume (REV)
- Size of flow structures > size of the pores
- Importance of dissipative mechanisms dominate over driving mechanisms quantified by Rayleigh-Darcy number, Ra

How are heat and mass transported in buoyancy-driven porous media flows?

How are heat and mass transported in buoyancy-driven porous media flows?

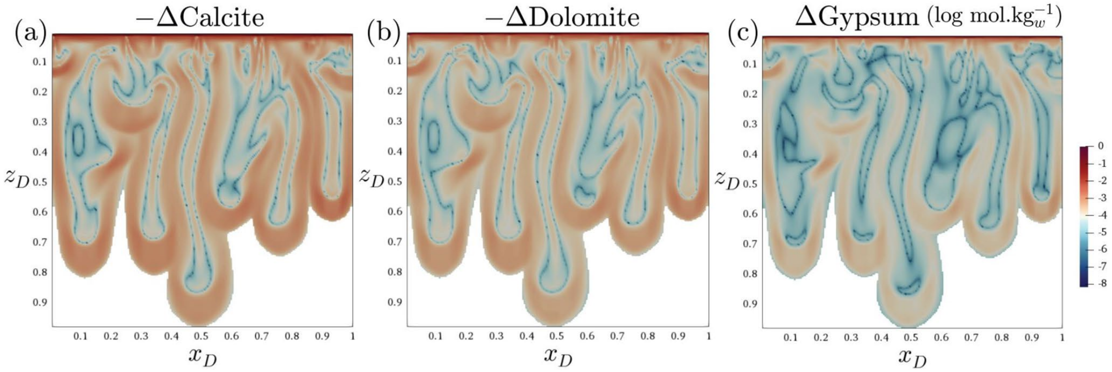
Heterogeneous media

- Cusini, M., van Kruijsdijk, C., & Hajibeygi, H. (2016). Algebraic dynamic multilevel (ADM) method for fully implicit simulations of multiphase flow in porous media. *Journal of Computational Physics*, *314*, 60-79. http://dx.doi.org/10.1016/j.jcp.2016.03.007
- Wang, Y., Vuik, C., & Hajibeygi, H. (2022). Analysis of hydrodynamic trapping interactions during full-cycle injection and migration of CO2 in deep saline aquifers. *Advances in Water Resources*, *159*, 104073. https://doi.org/10.1016/j.advwatres.2021.104073



Geochemistry

- H. Erfani, M. Babaei, V. Niasar, Dynamics of CO2 density-driven flow in carbonate aquifers: effects of dispersion and geochemistry, Water Resour. Res. 57 (4) (2021) e2020WR027829. https://doi.org/10.1029/2020WR027829
- T. Koch, D. Gläser, K. Weishaupt, S. Ackermann, M. Beck, B. Becker, S. Burbulla, H. Class, E. Coltman, S. Emmert, et al., Dumux 3–an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling, Comput. Math. Appl. 81 (2021) 423–443. https://doi.org/10.1016/j.camwa.2020.02.012



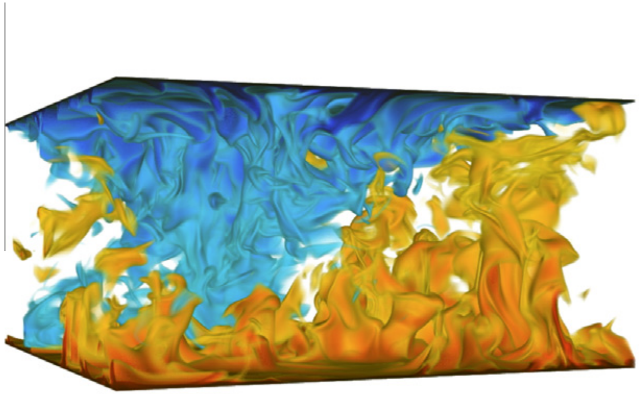
What is missing: highly parallel open-source code for buoyancy-driven wall-bounded flows

Physics of Fluids

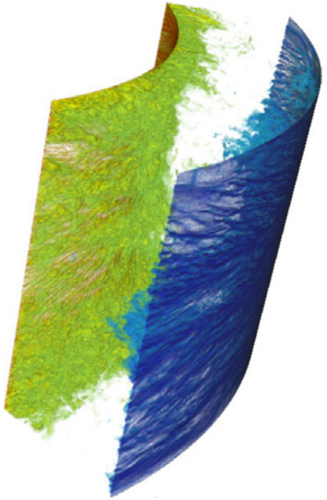
AFiD – Advanced Finite Difference solver for wall-bounded flows

Geometry

Cartesian



Cylindrical



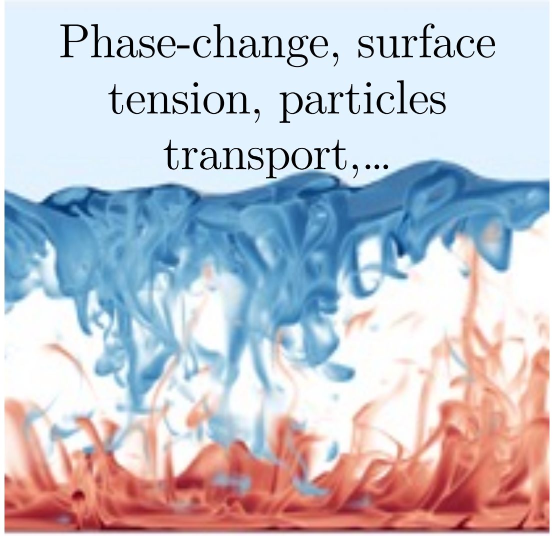
Language & libraries

FORTRAN 90
FFTW3
HDF5

Parallelization

MPI
OpenMP
CUDA

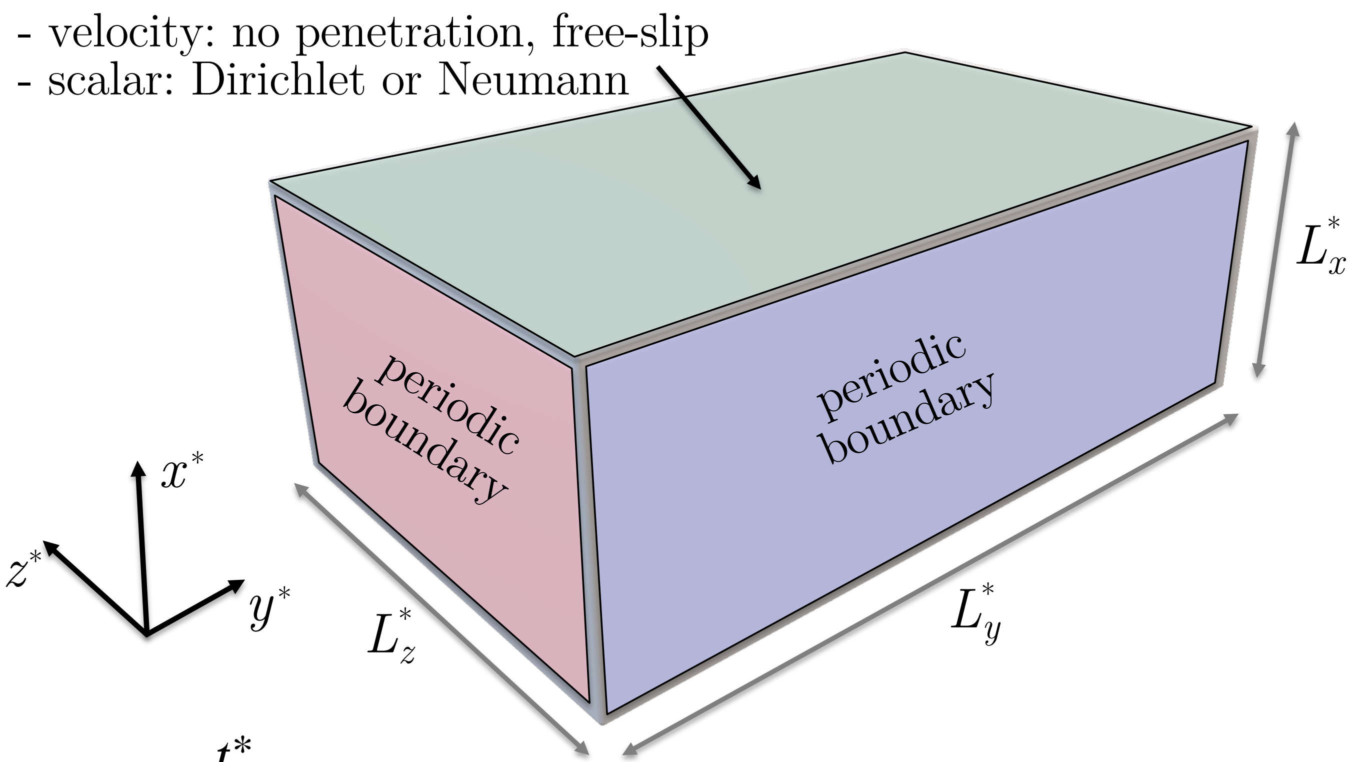
Fluid and flow models



E.P. Van Der Poel, R. Ostilla-Mónico, J. Donners, R. Verzicco, A pencil distributed finite difference code for strongly turbulent wall-bounded flows. Comput. Fluids, 116 (2015), pp. 10-16. https://doi.org/10.1016/j.compfluid.2015.04.007
Yang, Rui, Christopher J. Howland, Hao-Ran Liu, Roberto Verzicco, and Detlef Lohse. “Morphology Evolution of a Melting Solid Layer above Its Melt Heated from Below.” Journal of Fluid Mechanics 956 (2023): A23. https://doi.org/10.1017/jfm.2023.15.

2) Methodology

A) Flow configuration



$$x = \frac{x^*}{L_x^*} \qquad t = \frac{t^*}{\phi L_x^* / \mathcal{U}^*}$$

$$\mathcal{U}^* = g \Delta \rho^* \kappa / \mu$$

Equations obtained scaling the flow variables with respect to convective scales

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(\mathbf{u}C - \frac{1}{Ra} \nabla C \right) = 0$$

Advection-diffusion equation

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

Continuity

$$\mathbf{u} = -\left(\nabla p + C \mathbf{i} \right),$$

Darcy law + linear dependence of density and concentration

$$Ra = \frac{g \Delta \rho^* \kappa L_x^*}{\phi D \mu} = \frac{\mathcal{U}^* L_x^*}{\phi D}$$

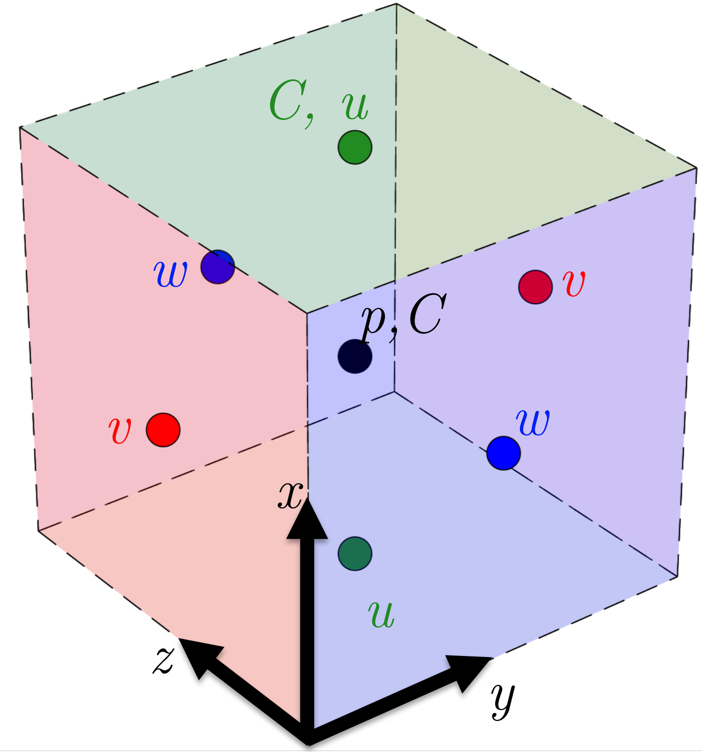
Governing parameter
Rayleigh-Darcy number

C) Numerical details

Discretization	Finite-differences, 2-nd order centered

Discretization	Finite-differences, 2-nd order centered
Grid	Staggered (energy conserving for $\Delta t \to 0$)

Variables arrangement on the grid



C) Numerical details

Discretization	Finite-differences, 2-nd order centered
Grid	Staggered (energy conserving for $\Delta t \to 0$)
Spacing	Uniform in periodic direction, non-uniform or uniform in vertical direction

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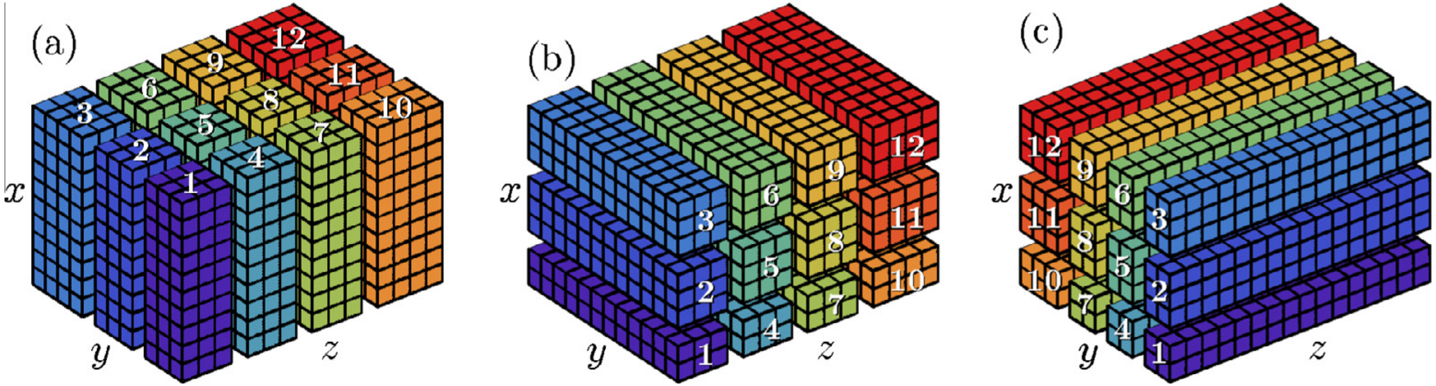
Grid	Staggered (energy conserving for $\Delta t \to 0$)
Spacing	Uniform in periodic direction, non-uniform or uniform in vertical direction
Parallelization	MPI, 2D pencil-like domain decomposition



2DECOMP library

E.P. Van Der Poel, R. Ostilla-Mónico, J. Donners, R. Verzicco, A pencil distributed finite difference code for strongly turbulent wall-bounded flows. Comput. Fluids, 116 (2015), pp. 10-16. https://doi.org/10.1016/j.compfluid.2015.04.007

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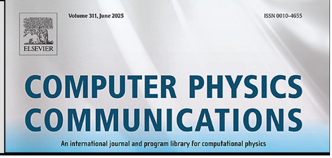

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Spacing	Uniform in periodic direction, non-uniform or uniform in vertical direction
Parallelization	MPI, 2D pencil-like domain decomposition
Time advancement	3rd-order Runge–Kutta (RK3) + Crank-Nicolson

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(\mathbf{u} C - \frac{1}{Ra} \nabla C \right) = 0$$

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

$$\mathbf{u} = -\left(\nabla p + C \mathbf{i} \right),$$

$$\mathbf{u}^* = -\mathcal{G} p^j - C^{j+1} \mathbf{i}$$

1) preliminary non-solenoidal velocity field

$$\mathcal{D}\mathcal{G}\psi = \mathcal{D}\mathbf{u}^*$$

2) pressure correction field ψ is determined solving the Poisson equation

$$\mathbf{u}^{j+1} = \mathbf{u}^* - \mathcal{G}\psi$$

$$p^{j+1} = p^j + \psi$$

3) updated velocity and pressure fields, such that the updated velocity field is solenoidal by construction.

C) Numerical details

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Discretization	Finite-differences, 2-nd order centered
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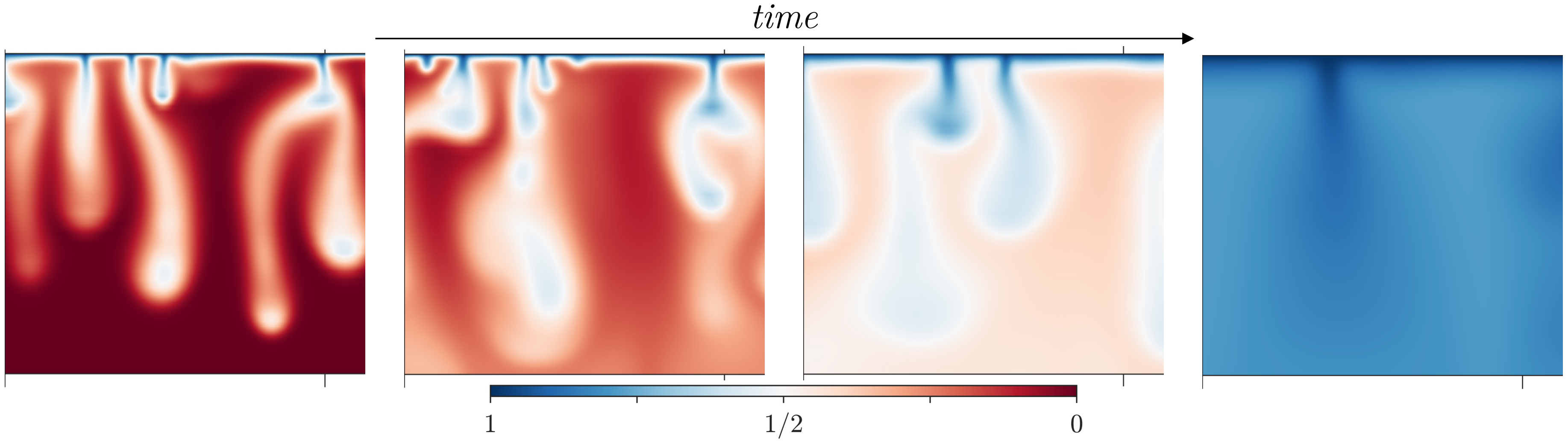
Discretization diffusive term	Fully-implicit or semi-implicit formulations

$$\frac{\partial C}{\partial t} + \nabla \cdot \left(\mathbf{u}C - \frac{1}{Ra} \nabla C \right) = 0$$

Also at large Rayleigh-Darcy numbers, when the problem is transient and the system saturates in solute, the driving force may reduce considerably pointing to the need of an **implicit solver**.



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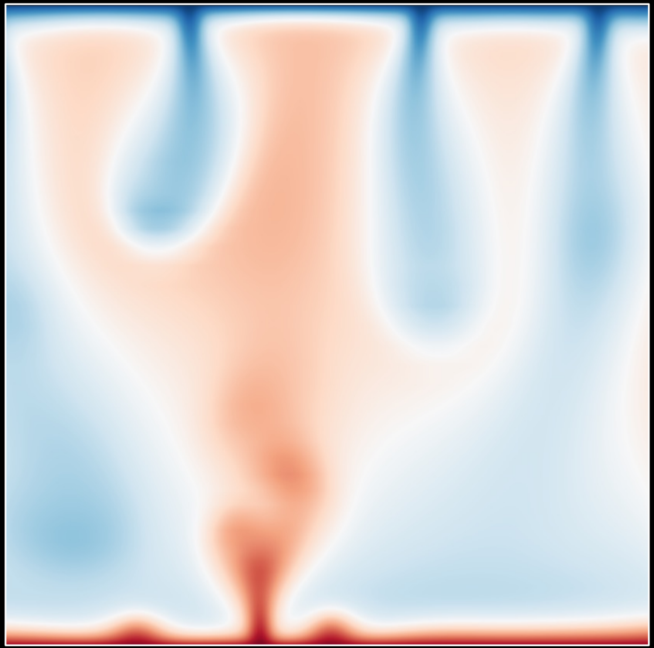
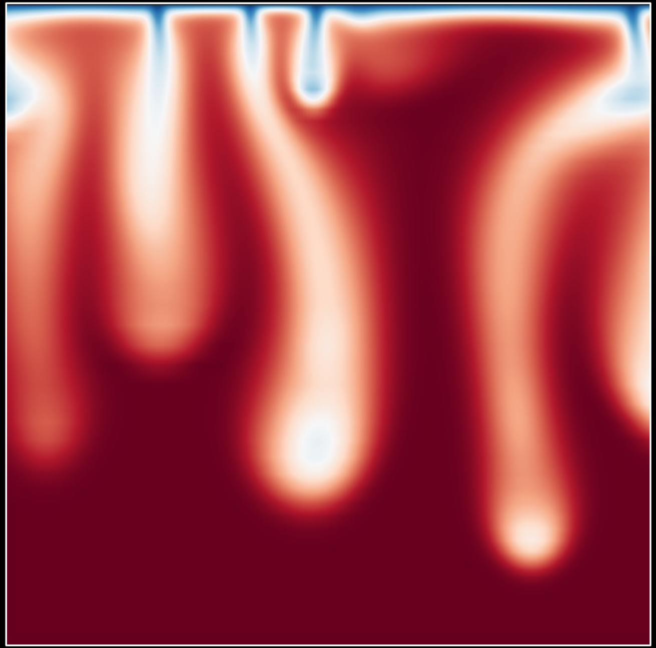
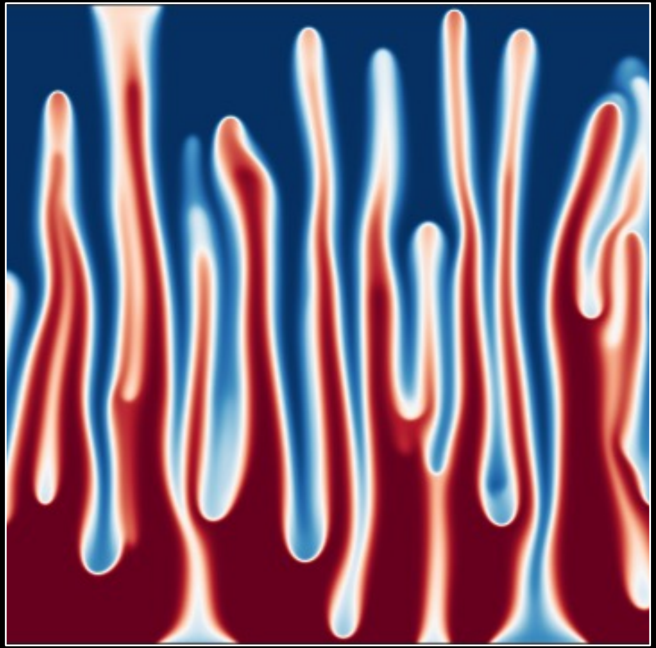
Scheme	**properties**
Semi-implicit: High driving (high values of Ra): only the wall-normal component of $\nabla^2 C$ is solved implicitly, avoiding communications of non-local information for the computation of the implicit derivatives in the wall-parallel directions.	Small Δt Few communications
Fully implicit: All the components of the scalar diffusive term are treated with a Crank–Nicolson scheme.	Large Δt More communications Computationally more intensive

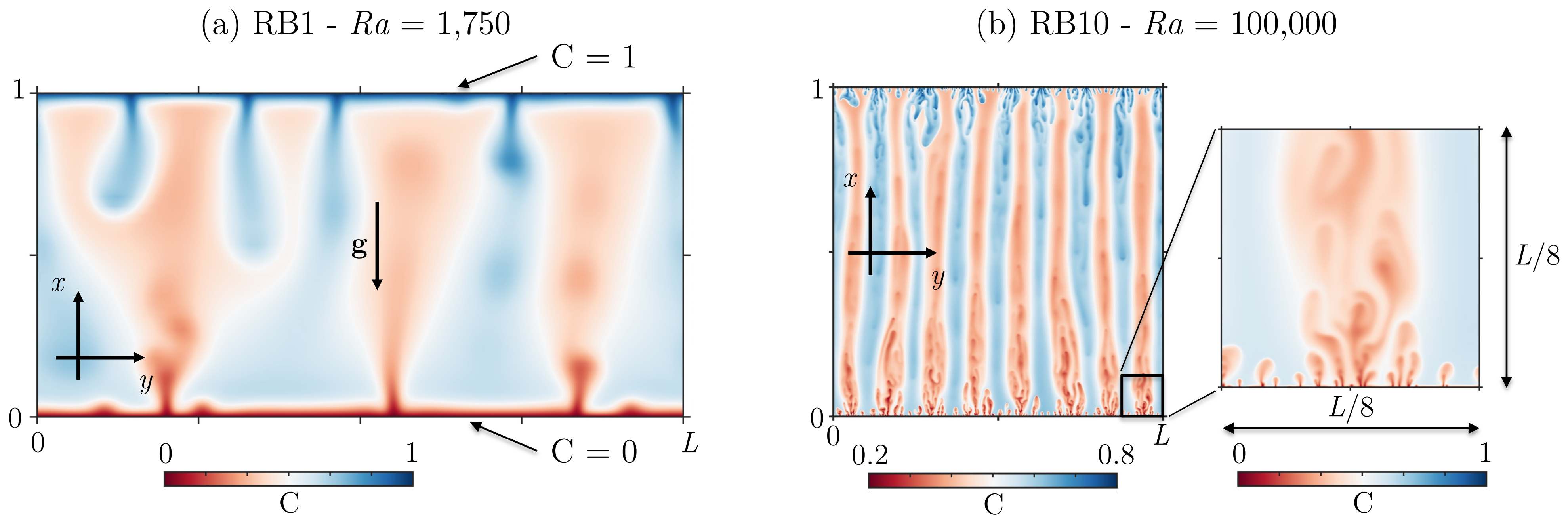
3) Verification

3) Verification

Case I Rayleigh-Bénard	Case II One-sided	Case III Rayleigh-Taylor
$C = 1$	$C = 1$	$\partial_z C = 0$
		
$C = 0$	$\partial_z C = 0$	$\partial_z C = 0$

We double *Ra* with respect to current state-of-art simulations

Case I – Rayleigh-Bénard convection

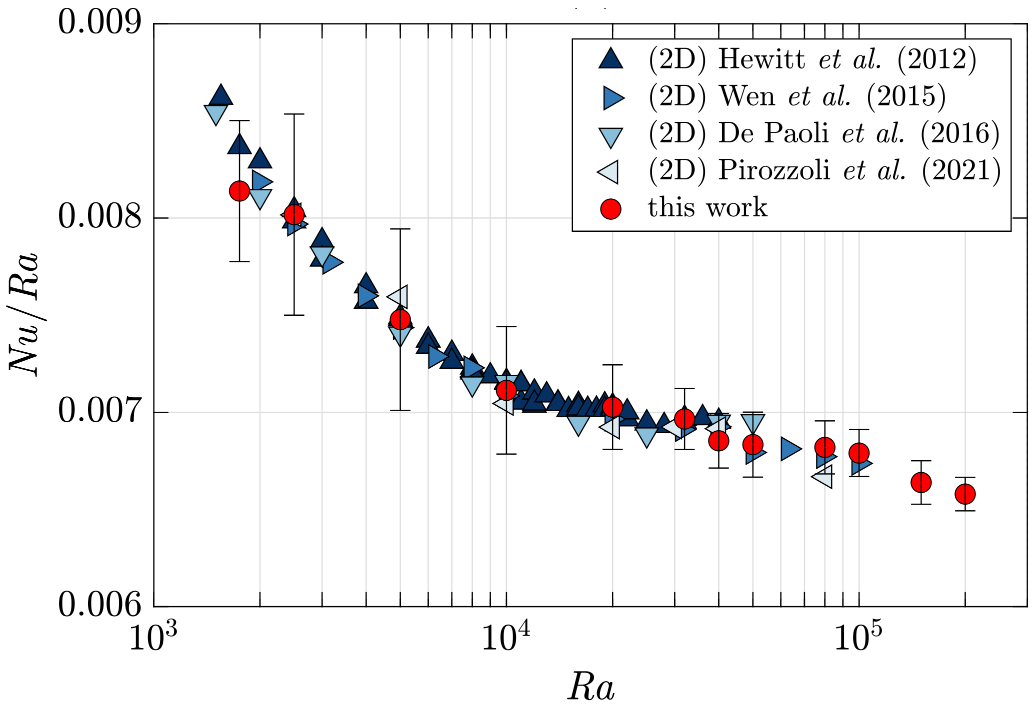


$Nu \sim Ra \quad \Rightarrow \quad N_x \times N_y \times N_z \sim Ra^3$

$\Delta t \sim Ra^{-1}$

Computational costs ~ Ra^3 (2D) or Ra^4 (3D)

Ra	L	$N_x \times N_y \times N_z$
8.00×10^4	1.0	$2048 \times 6144 \times 1$
1.00×10^5	1.0	$2560 \times 7680 \times 1$
1.50×10^5	1.0	$4096 \times 12288 \times 1$
2.00×10^5	1.0	$5120 \times 15360 \times 1$



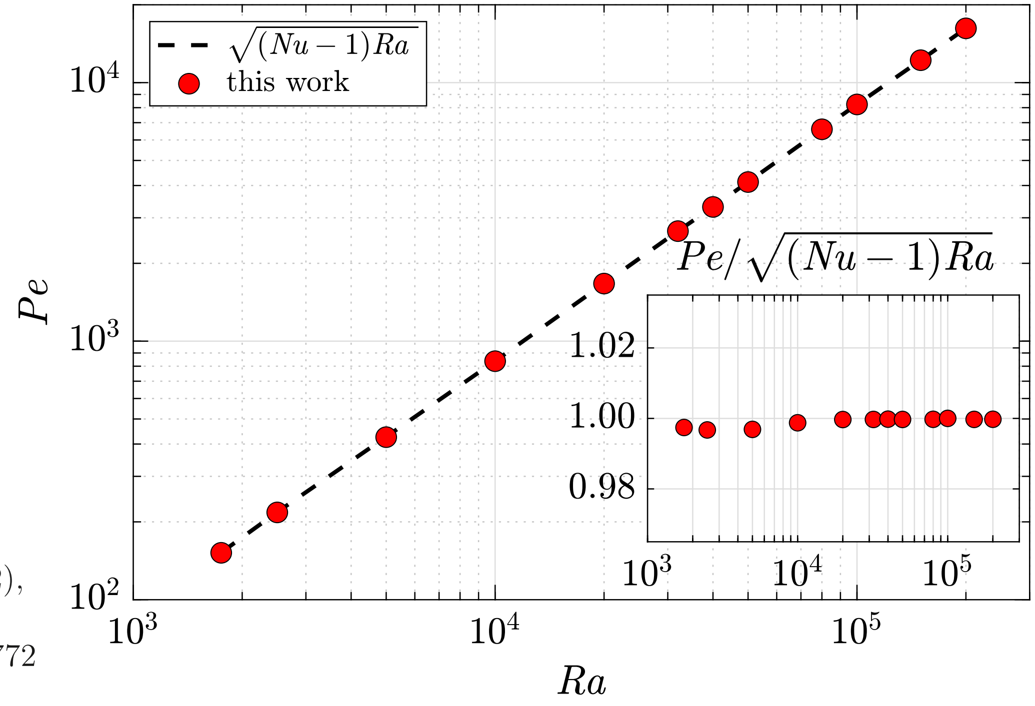
Hewitt, D. R., Neufeld, J. A., & Lister, J. R. (2012). *Physical Review Letters, 108*(22), 224503. https://doi.org/10.1103/PhysRevLett.108.224503

Wen, Baole, Lindsey T. Corson, and Gregory P. Chini, *Journal of Fluid Mechanics* 772 (2015): 197–224. https://doi.org/10.1017/jfm.2015.205

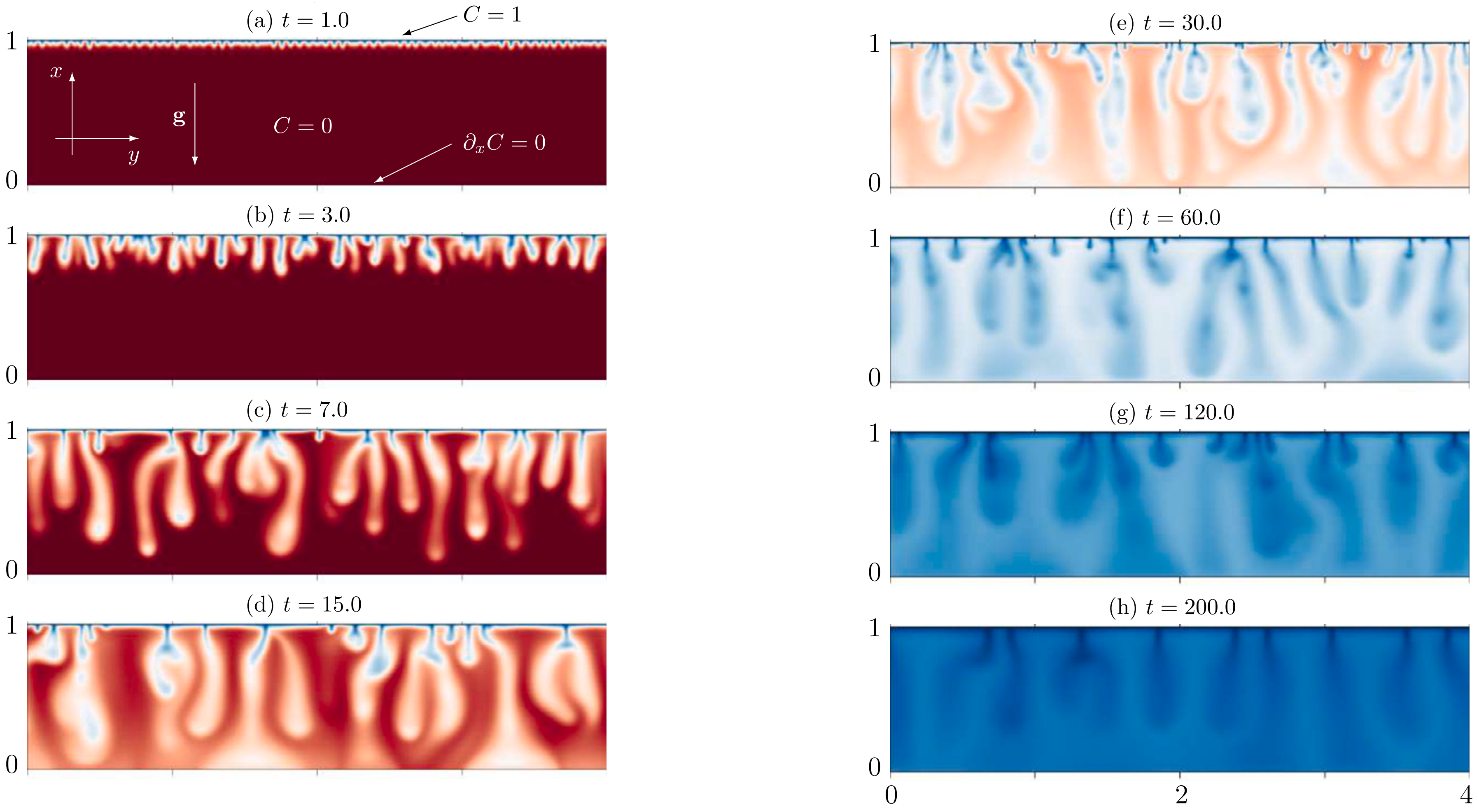
De Paoli, M. Zonta, F. and Soldati, A., Physics of Fluids 1 May 2016; 28 (5): 056601. https://doi.org/10.1063/1.4947425

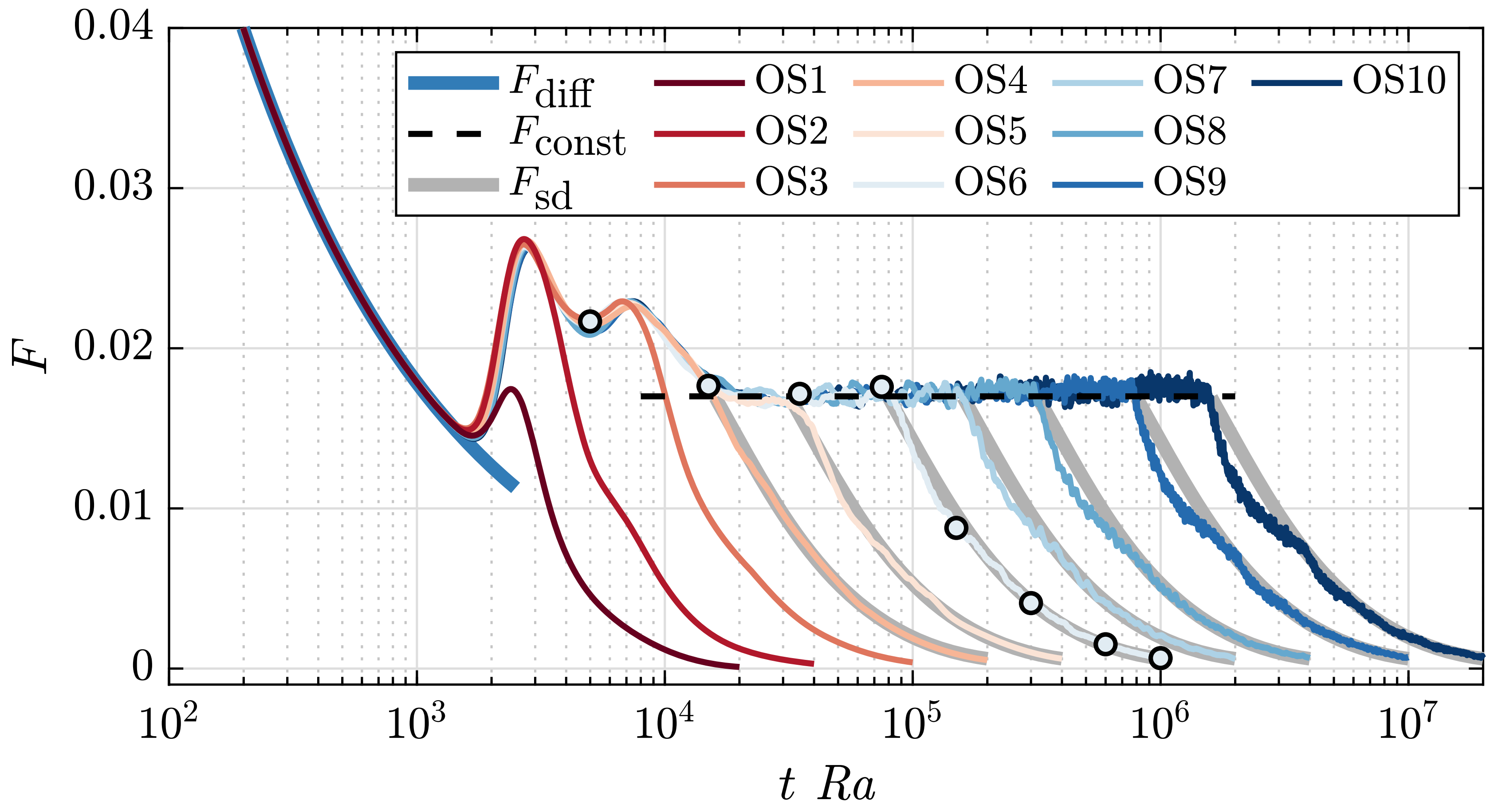
Pirozzoli, Sergio, Marco De Paoli, Francesco Zonta, and Alfredo Soldati. *Journal of Fluid Mechanics* 911 (2021): R4. https://doi.org/10.1017/jfm.2020.1178

Zhu, Xiaojue, Yifeng Fu, and Marco De Paoli. "Transport Scaling in Porous Media Convection." *Journal of Fluid Mechanics* 991 (2024): A4. https://doi.org/10.1017/jfm.2024.528.



Case II – one-sided convection



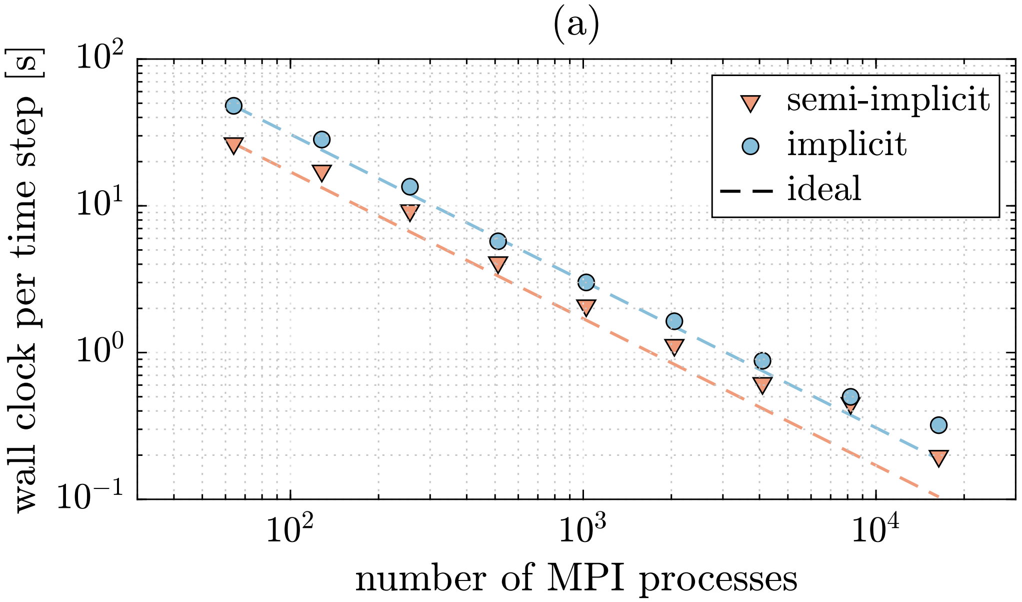


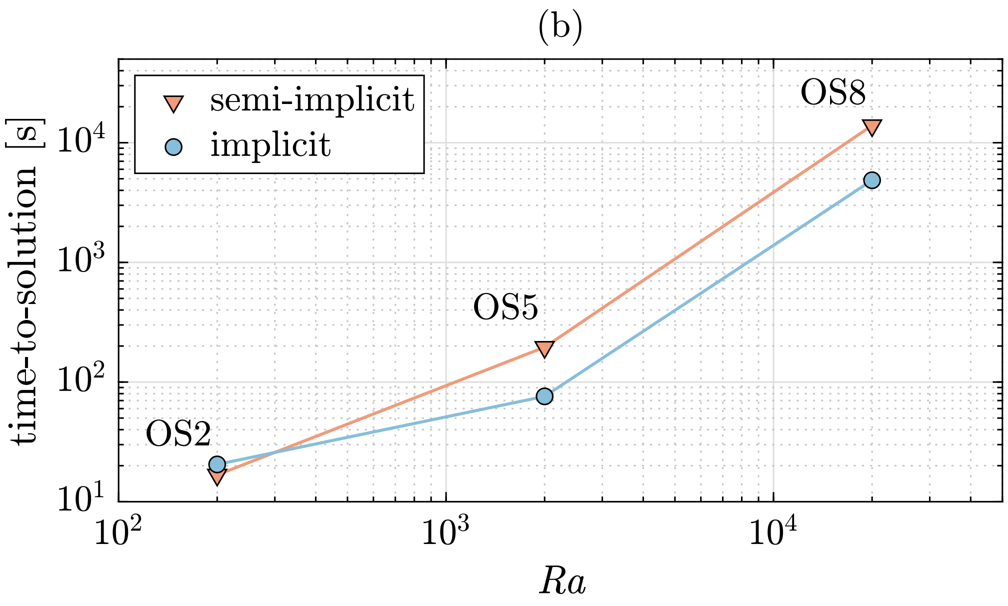
See also for the purpose of verification: Slim, Anja C. "Solutal-Convection Regimes in a Two-Dimensional Porous Medium." *Journal of Fluid Mechanics* 741 (2014): 461–91. https://doi.org/10.1017/jfm.2013.673.

Case II – one-sided convection

Implicit solver: each time step is computationally more expensive

Implicit solver allows larger time steps

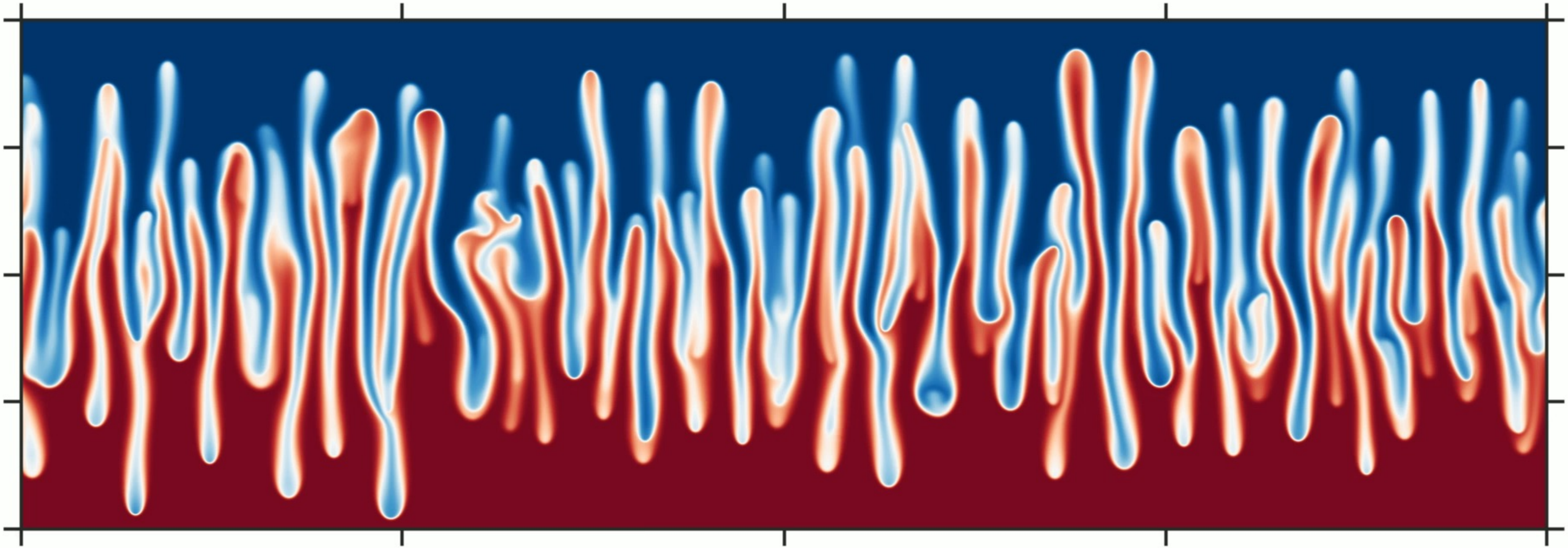




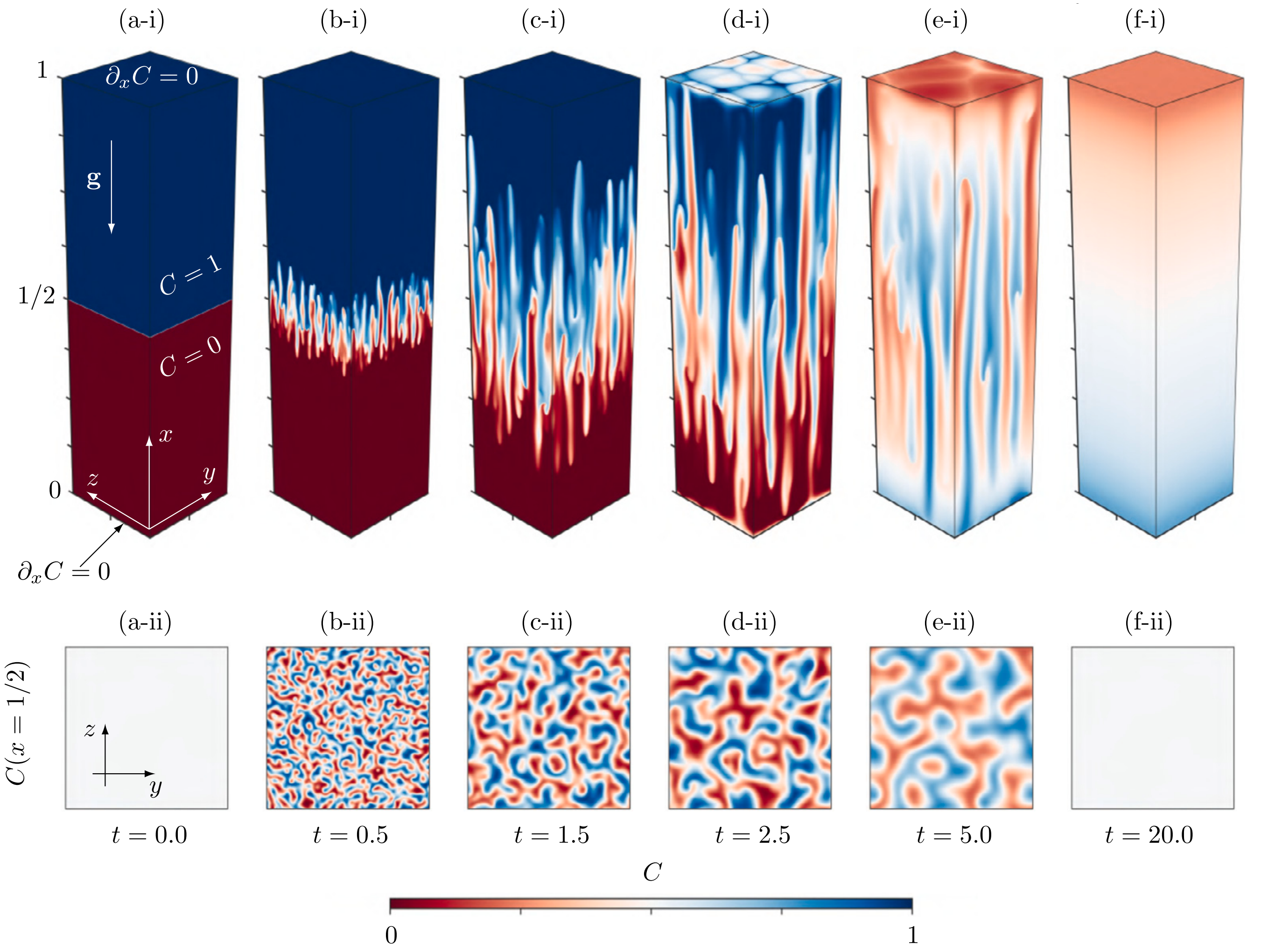
Larger wall-clock per time/step

Smaller time to solution

Case III – Rayleigh-Taylor flow



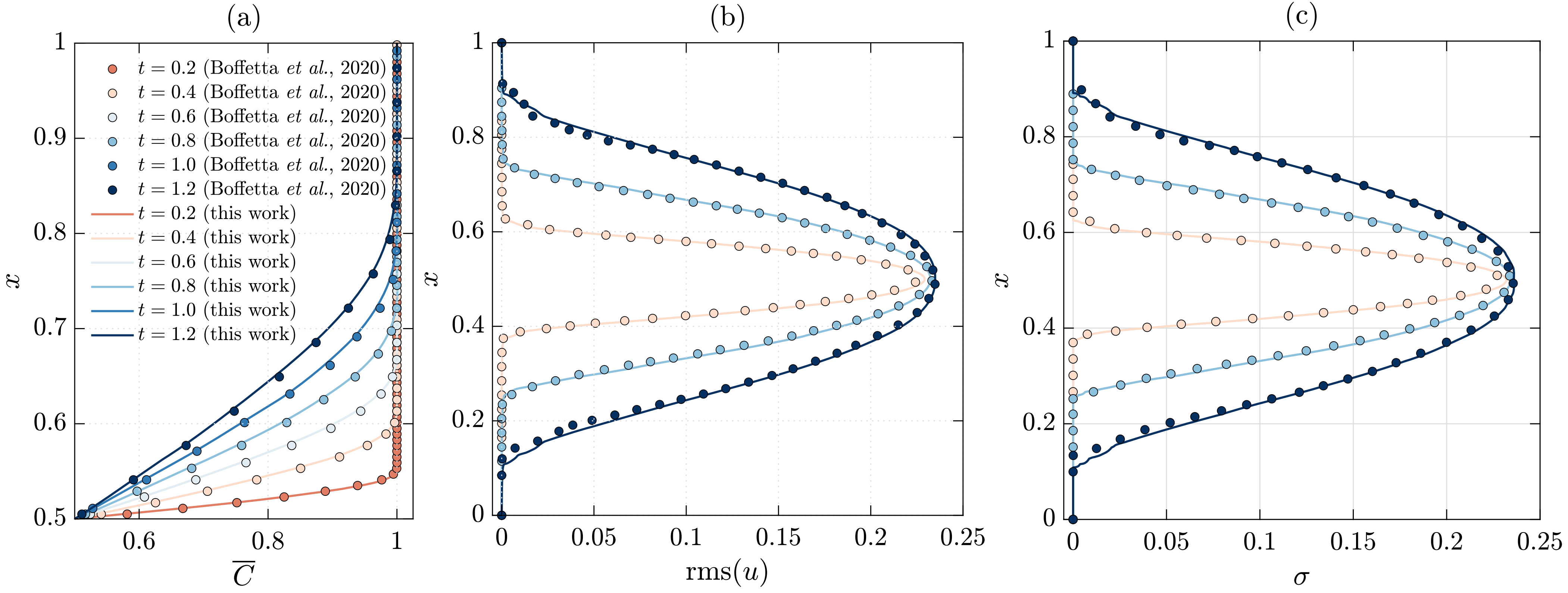
Case III – Rayleigh-Taylor flow



Ra	L	$N_x \times N_y \times N_z$
3.20×10^4	1/4	$2048 \times 512 \times 512$
6.40×10^4	1/4	$4096 \times 1024 \times 1024$
1.28×10^5	1/4	$8192 \times 2048 \times 2048$
2.56×10^5	1/8	$16384 \times 2048 \times 2048$

- Up to 70 Billion grid points
- Up to 64k MPI processes
- Essential to optimize communications

Case III – Rayleigh-Taylor flow

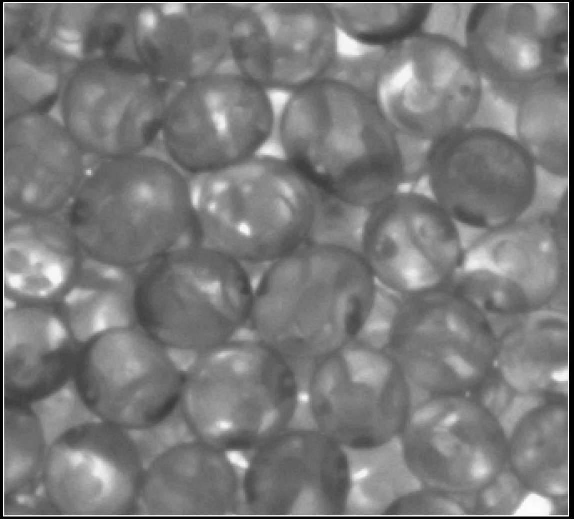


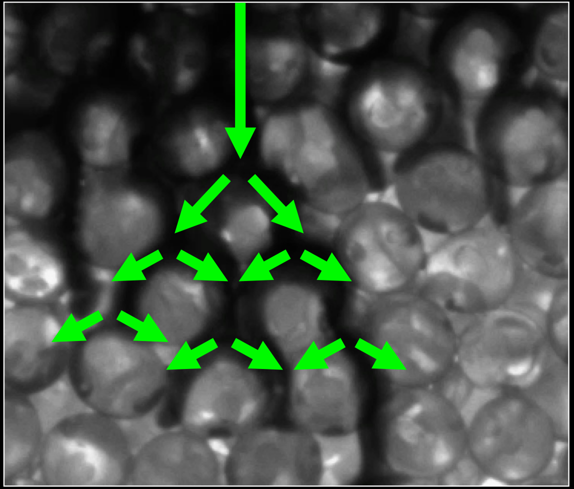
Verified against: Boffetta, G., Borgnino, M., & Musacchio, S. (2020). Scaling of Rayleigh-Taylor mixing in porous media. *Physical Review Fluids*, *5*(6), 062501. https://doi.org/10.1103/PhysRevFluids.5.062501

4) Future developments

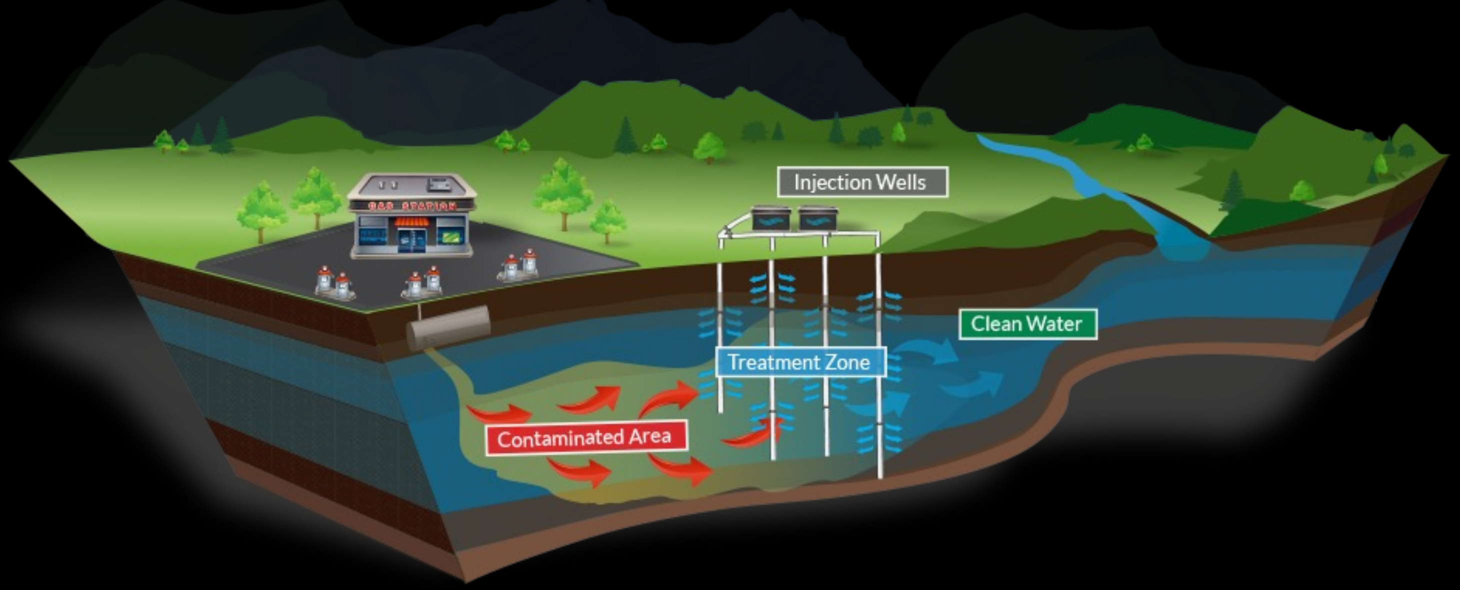
4) Future developments

De Paoli, M., Howland, C.J., Verzicco, R., & Lohse, D. *J. Fluid Mechanics* 987 (2024): A1. https://doi.org/10.1017/jfm.2024.328.





https://envirosouth.com/services/soil-groundwater-remediation/



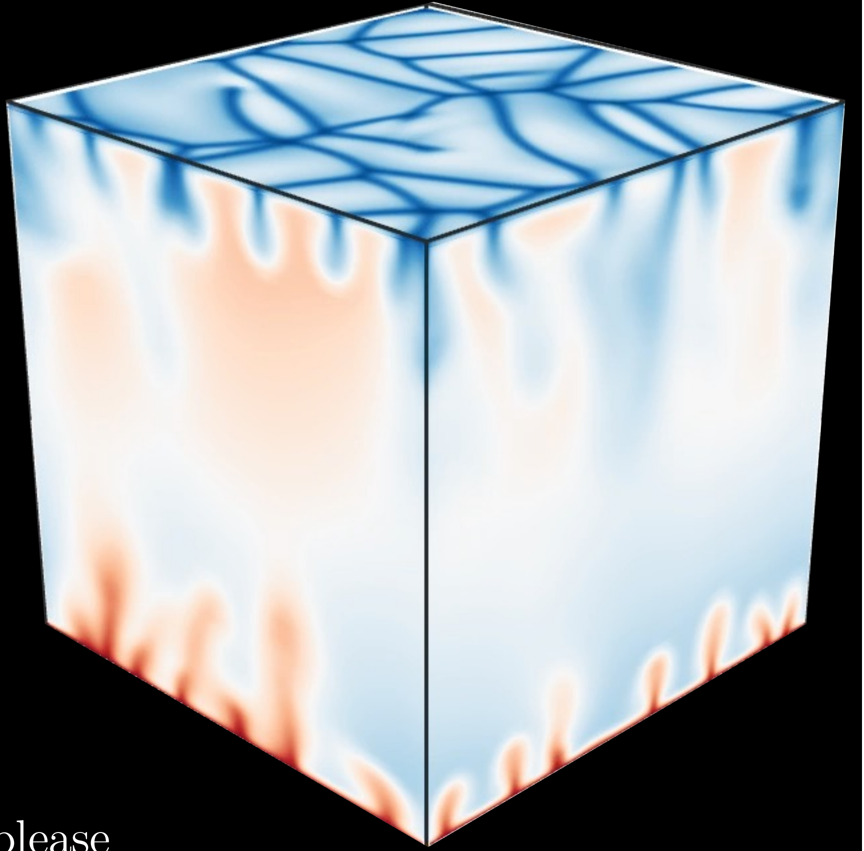
Include the effects of mechanical dispersion (anisotropic Fickian **dispersion** formulation)

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = \nabla \cdot (\mathbf{D} \nabla C) \qquad \mathbf{D} = \mathbf{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + |\mathbf{u}|\mathbf{I}\right]$$

5) Conclusions

5) Conclusions

- We developed a code for numerical simulations of buoyancy-driven Darcy flows: **AFiD-Darcy**
- Massively parallelized and designed for extreme Ra
- Versatile and suitable also at low Ra due to the implicit version
- Open source:
  - Computer Physics Communications Library:
    - https://doi.org/10.17632/xhx3gzpj6n.1
  - GitHub
    - https://github.com/depaolimarco/AFiD-Darcy



Documentation still in development, please contact me for any question:
m.depaoli@utwente.nl ; marco.de.paoli@tuwien.ac.at