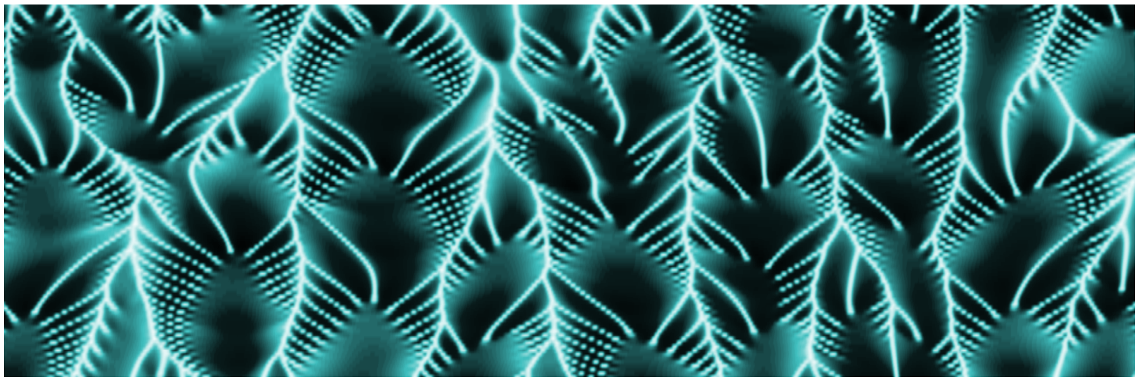
Climate change mitigation
Prediction of CO2 dissolution in geological reservoirs



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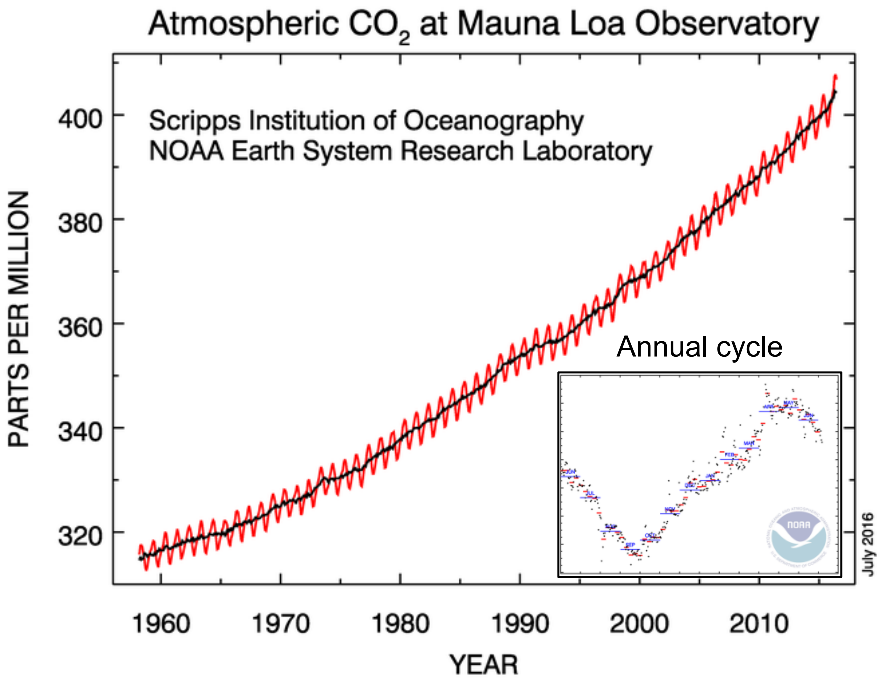
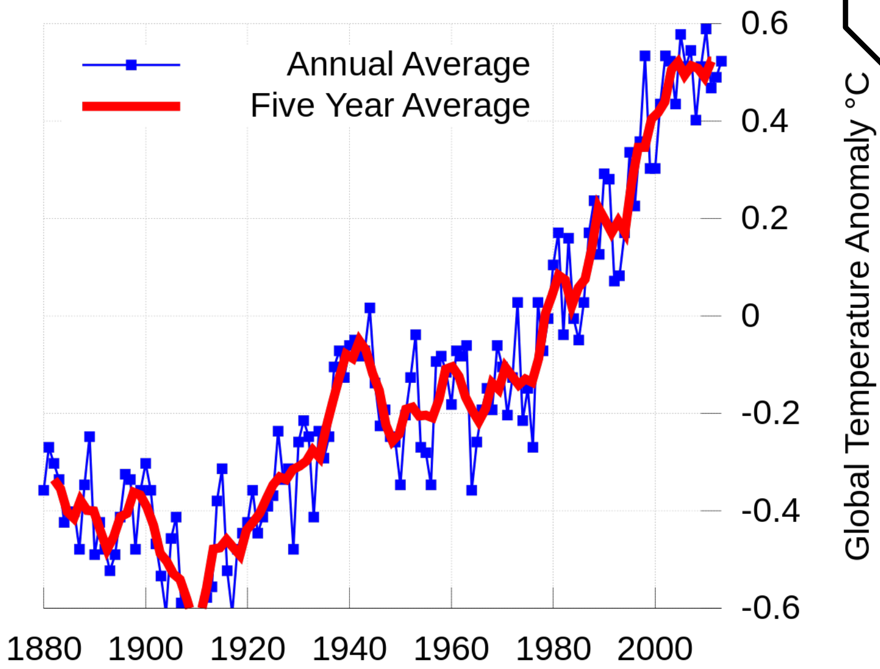
Motivation

80 % of energy is produced from combustion of fossil fuels, and consequent production of Carbon Dioxide (CO_2)

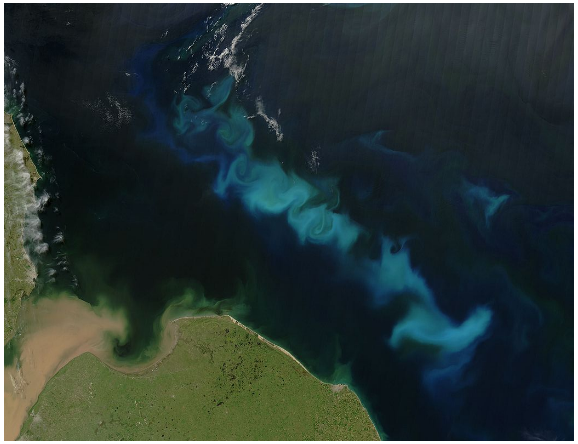




Global average temperatures rise over the last 130 years [Hansen, J., et al., Proc. Natl. Acad. Sci. (2006)]

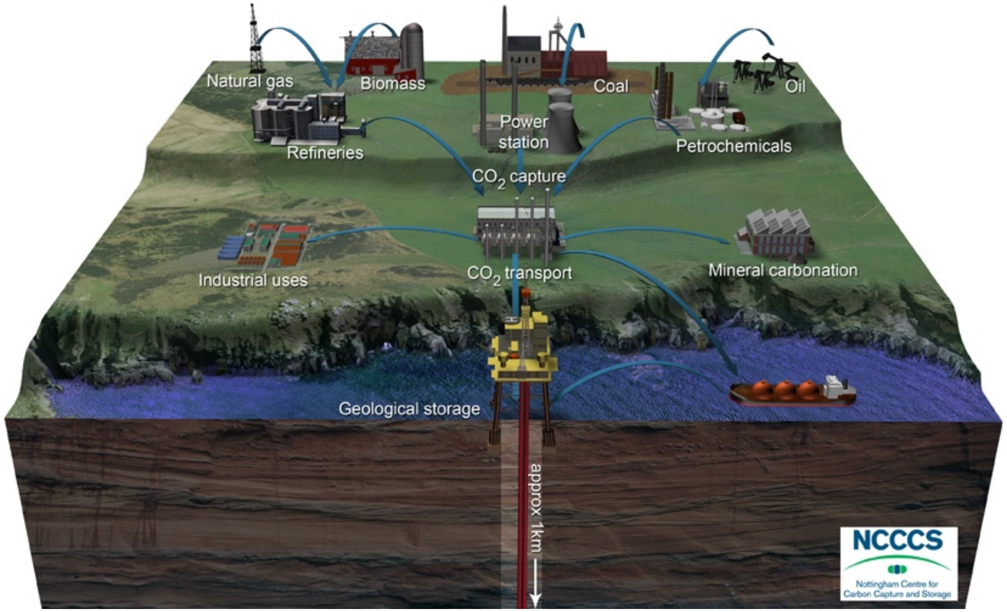
Carbon Sequestration

Iron fertilization of **phytoplankton**



Chemical scrubbers

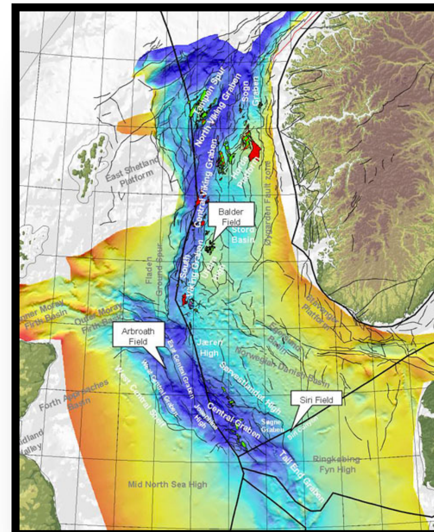
Carbon Capture and **Storage** (CCS) has been identified as a possible solution to the greenhouse effect [Intergovernmental panel on Climate Change, (IPCC) 2005]

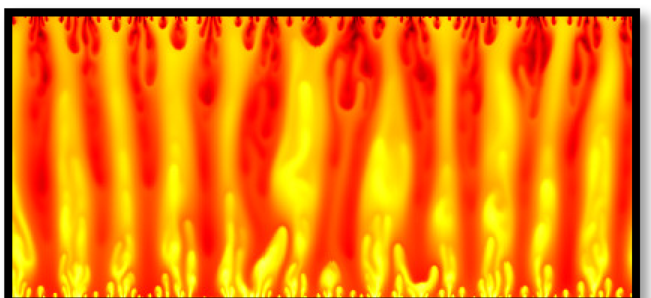


Injection point

Presentation outline

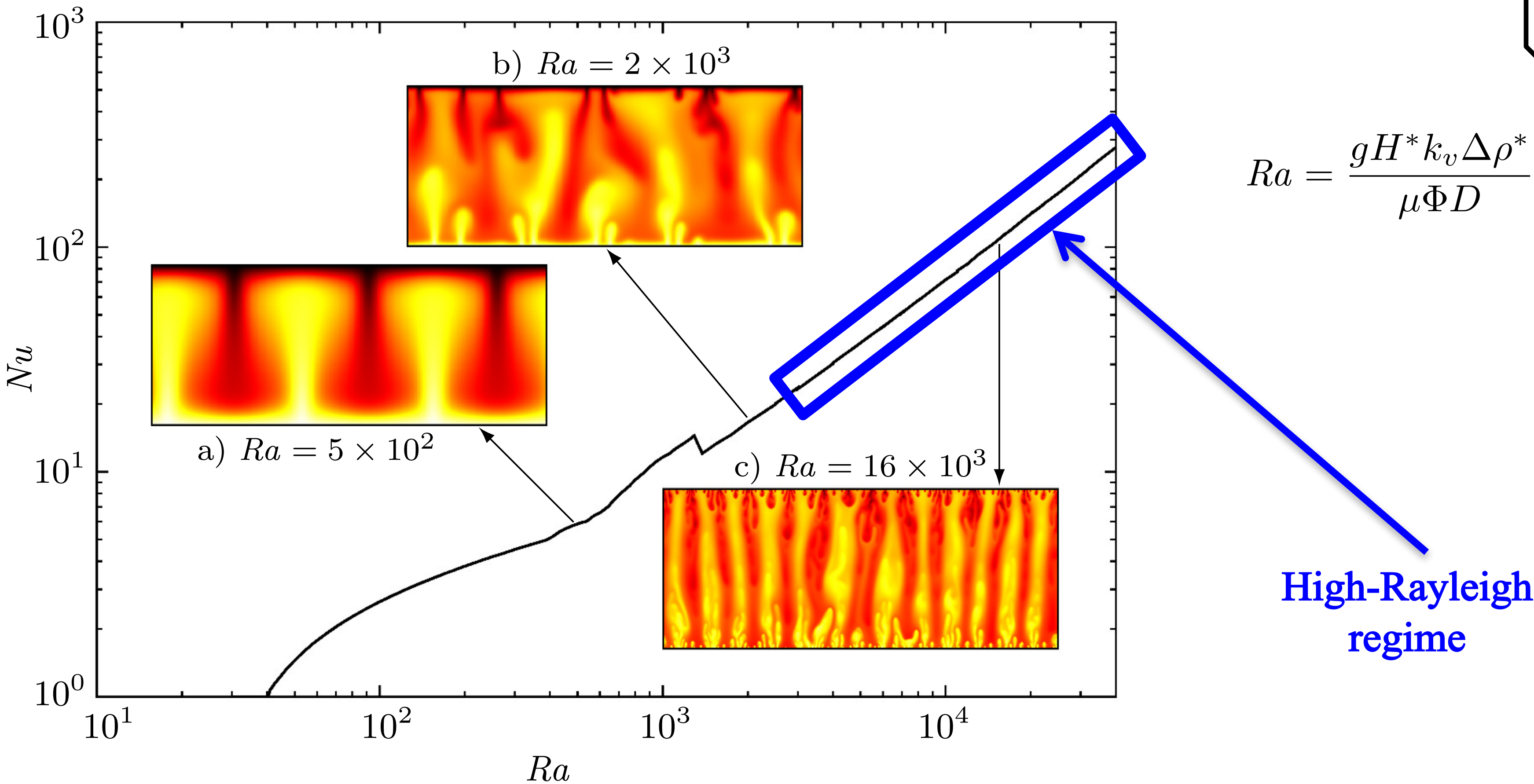
1. Modelling CO_2 storage
   - Dissolution process
   - Methodology
   - Numerical details
   - Effect of anisotropy





2. Modelling dissolution regimes
   - Theoretical model
   - Diffuse interface model
3. Conclusions

Dissolution in porous media



$$Ra = \frac{gH^* k_v \Delta\rho^*}{\mu \Phi D}$$

$$\overline{Nu}(t) = \frac{1}{2L} \int_0^L \left(\left. \frac{\partial C(x,t)}{\partial z} \right|_{z=0} + \left. \frac{\partial C(x,t)}{\partial z} \right|_{z=1} \right) dx$$

$$Nu = \frac{1}{t_f - t_i} \int_{t_i}^{t_f} \overline{Nu}(t)\, dt$$

Methodology

Dimensional equations

$$\frac{\partial u^*}{\partial x^*} + \frac{\partial w^*}{\partial z^*} = 0$$

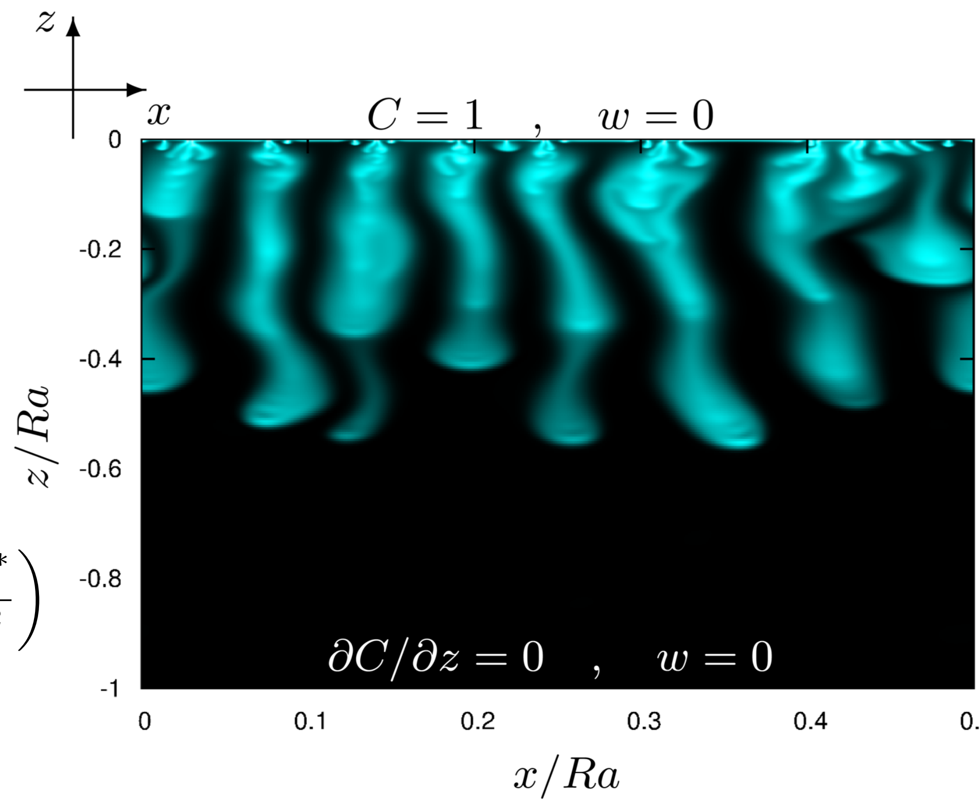
$$\frac{\mu}{k_h} u^* = -\frac{\partial p^*}{\partial x^*} \quad , \quad \frac{\mu}{k_v} w^* = -\frac{\partial p^*}{\partial z^*} - \rho^* g$$

$$\rho^* = \rho_s^* \left[1 - a(C_s^* - C^*)\right]$$

$$\Phi \frac{\partial C^*}{\partial t^*} + u^* \frac{\partial C^*}{\partial x^*} + w^* \frac{\partial C^*}{\partial z^*} = \Phi D \left(\frac{\partial^2 C^*}{\partial x^{*2}} + \frac{\partial^2 C^*}{\partial z^{*2}} \right)$$

$$\boxed{Ra = \frac{g H^* k_v \Delta \rho^*}{\mu \Phi D}}$$

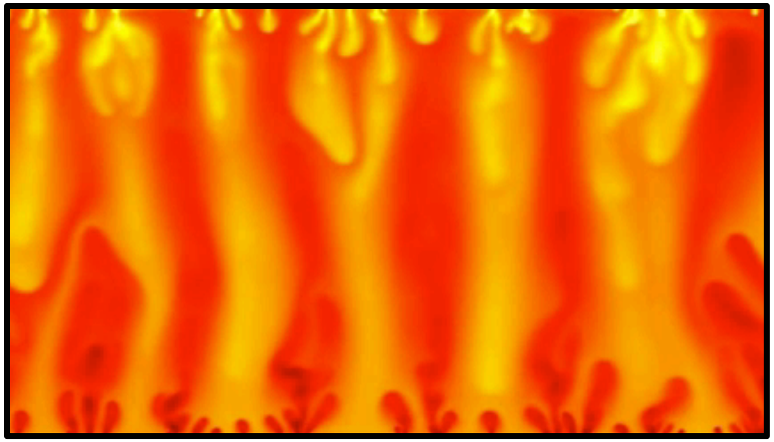
Dimensional variables



Numerical details

High-resolutions required

Large scale (~10 m) >> small scales (~ cm)



Up to 8 collocation points for a 2D simulation
Up to 200 collocation points for a 3D simulation

HPC resources

20 million CPU hours used on **Marconi**, **Fermi** (Cineca Supercomputing Centre, Bologna, Italy), **VSC3** (Vienna Scientific Cluster, Vienna Austria), **Mira** (Argonne, USA)

Numerical details

Numerical scheme

High-order methods in space
Pseudo-spectral code (Fourier + Chebyshev)
Chebyshev-Tau method

$$\nabla \cdot \mathbf{u} = 0 \qquad \mathbf{u} = -\nabla P + \mathbf{k}C$$

$$\frac{\partial C}{\partial t} + \underbrace{u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z}}_{} = \underbrace{\frac{1}{Ra}\left(\gamma\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right)}_{}$$

Adams-Bashforth (explicit) term S

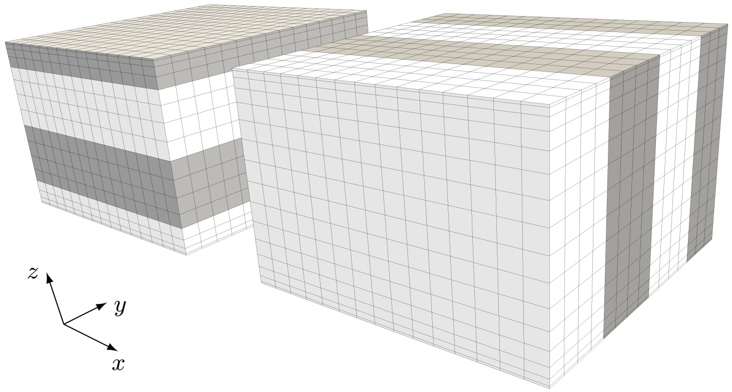
Crank-Nicolson (implicit)

Secondo order accuracy in time

$$\frac{\hat{C}^{n+1} - \hat{C}^n}{\Delta t} = \frac{3}{2}\hat{S}^n - \frac{1}{2}\hat{S}^{n-1} + \frac{1}{2\,Ra}\left(\gamma\nabla_H^2 + \frac{\partial^2}{\partial z^2}\right)(\hat{C}^{n+1} - \hat{C}^n)$$

Parallelization

MPI paradigm
FFTW3 libraries (x, y directions)
Chebyshev polynomials (z direction)



1D domain decomposition

Effect of anisotropy

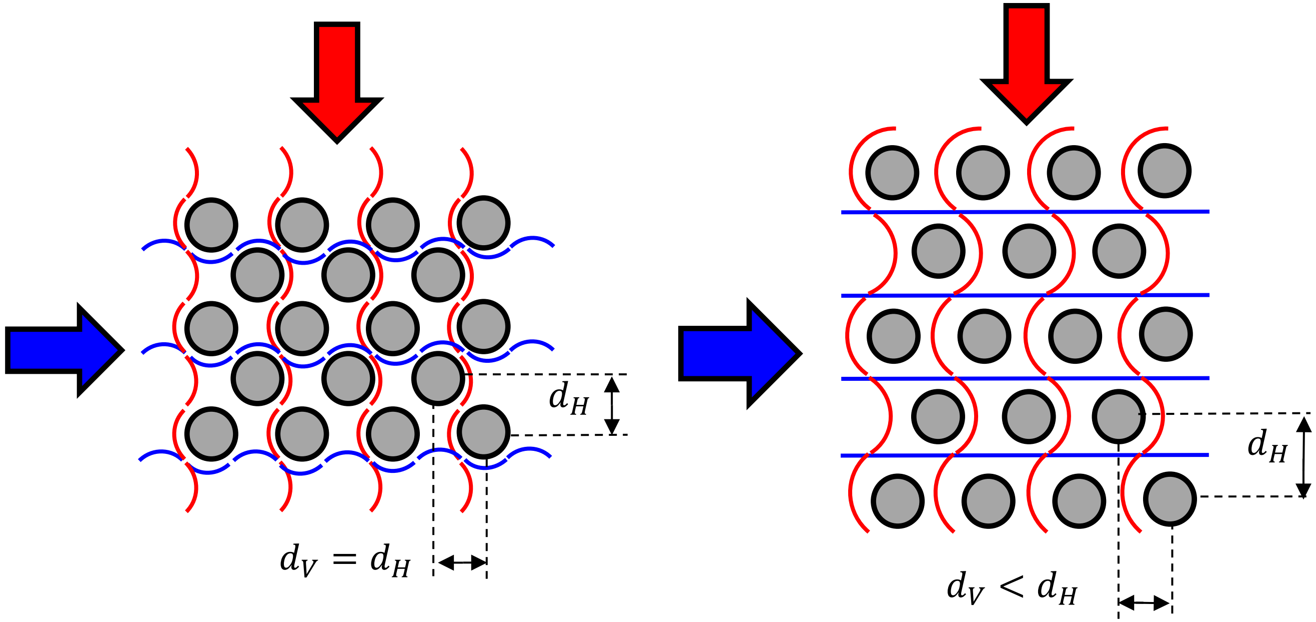
Governing Parameters

$$Ra = \frac{gH^* k_v \Delta\rho^*}{\mu \Phi D}$$

$$\gamma = k_v / k_h$$

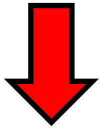
$$\mathbf{0 < \gamma \leq 1}$$

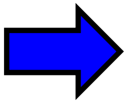
Permeability ratio interpretation



Isotropic

Anisotropic

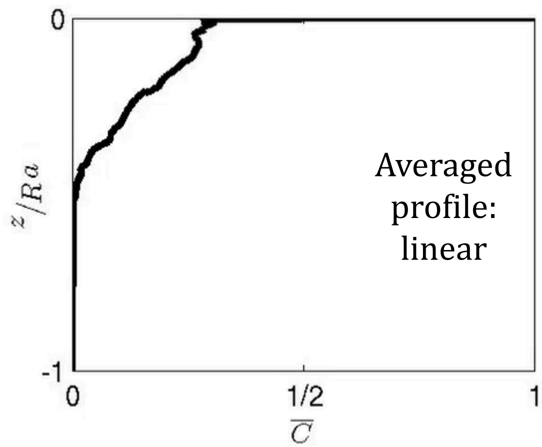

Vertical flow

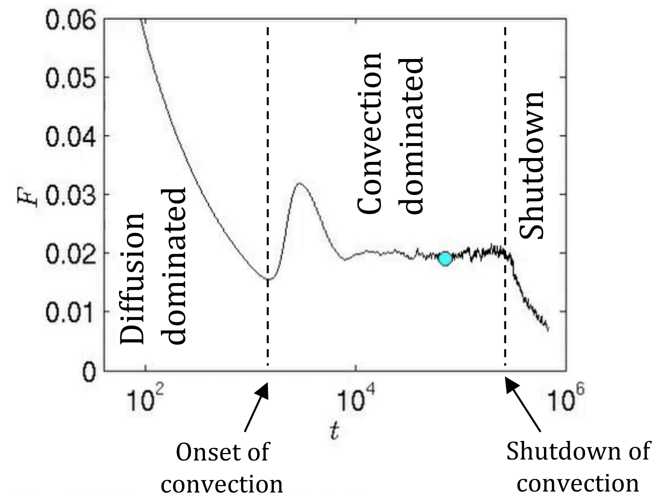

Horizontal flow

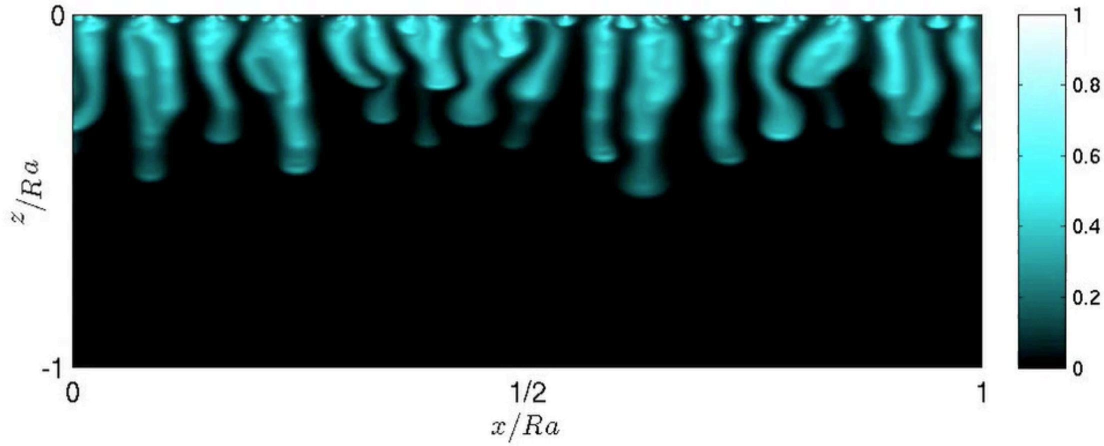
Dissolution process description

$$\overline{C}(z,t) = \frac{1}{L}\int_0^L C(x,z,t)\,dx \qquad F(t) = \frac{1}{L}\int_0^L \left.\frac{\partial C}{\partial z}\right|_{z=0} dx$$

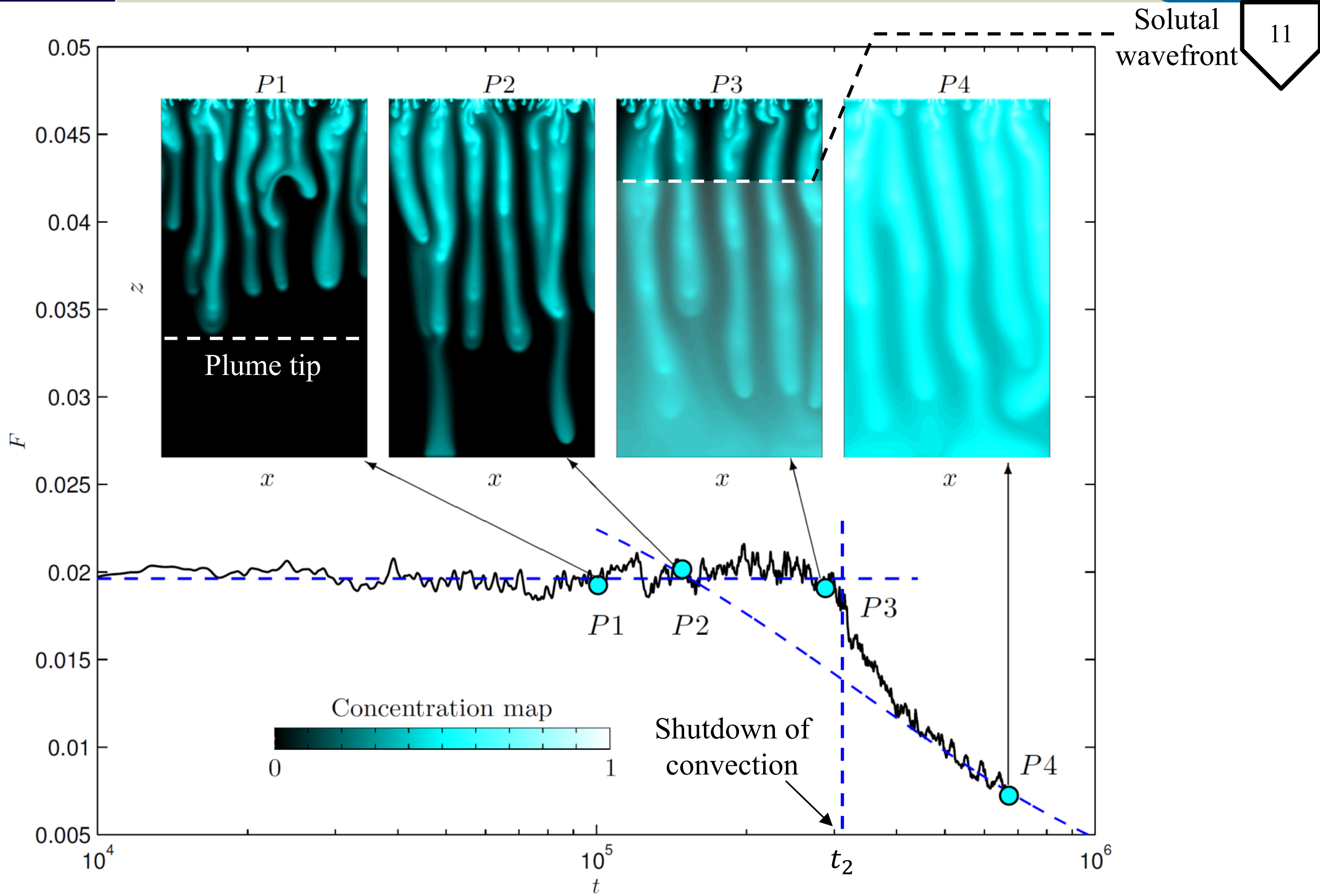
$Ra = 2\times10^4$



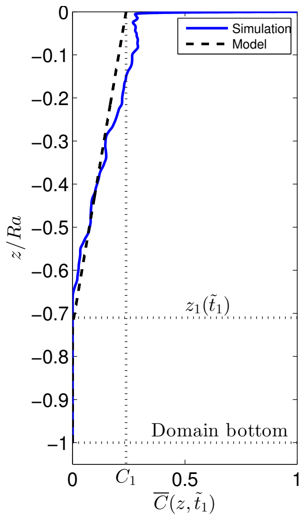




Shutdown of convection



Model for falling plumes



Linear concentration profile

$$\overline{C}(z,t) = -\frac{C_1(t)}{z_1(t)}[z - z_1(t)]$$

Average dissolution flux

$$F(t) = \frac{1}{L}\int_0^L \left.\frac{\partial C}{\partial z}\right|_{z=0} dx$$

Solute conservation equation

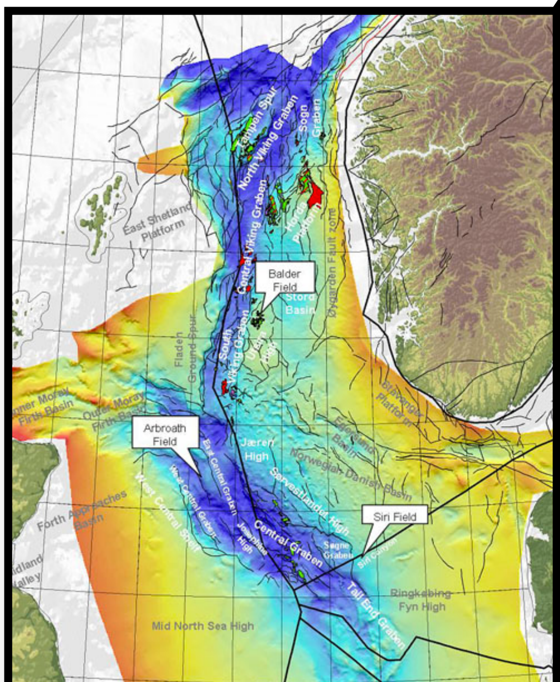
$$\underbrace{\int_0^t \left(\int_L \left.\frac{\partial C(x,z,\tau)}{\partial z}\right|_{z=0} dx \right) d\tau}_{\text{Amount of CO2 dissolved from } \tau = 0 \text{ to } \tau = t} = \underbrace{\int_V C(x,z,t)dV}_{\text{Mass of CO2 contained within the domain at } \tau = t}$$

$$\boxed{t_2 = \frac{(2+\eta)C_1}{0.017} Ra}$$

De Paoli et al. (2017),
Phys. Fluids **29** (026601)

Application

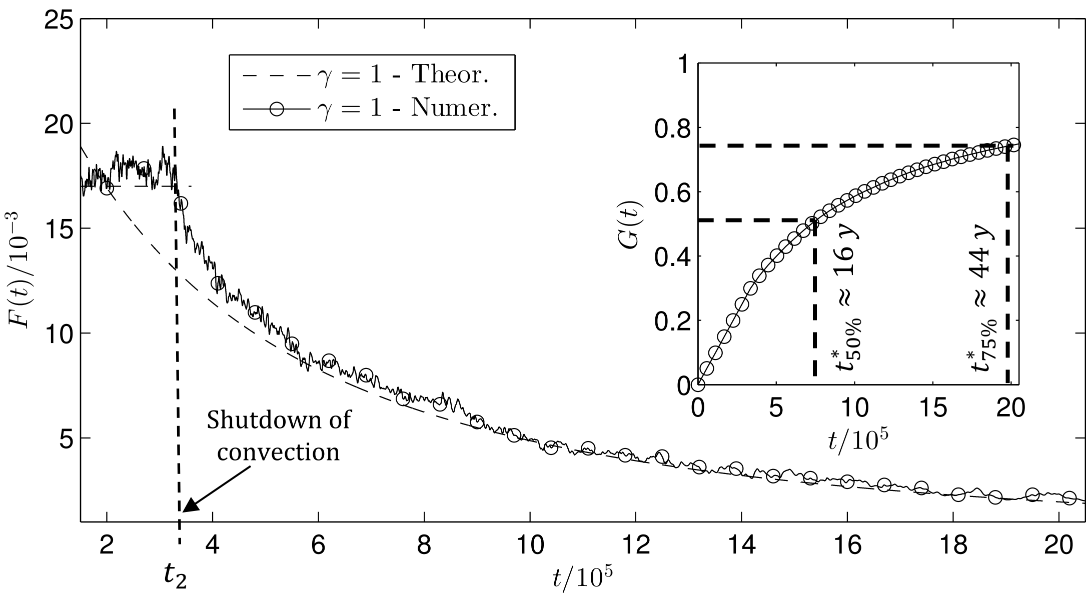
$\Delta\rho = 10.45\ kg/m^3$
$\mu = 5.95\times10^{-4}\ Pa\times s$
$D = 2\times10^{-9}\ m^2/s$
$H = 20\ m$
$\phi = 0.3$
$k_v = 3\times10^{-12}\ m^2$
$Ra \approx 17\times10^3$



[Data refer to a depth of 1 km at the Sleipner Site (North Sea)]

Conclusions

We generalized an existing model [Hewitt et al. , JFM, 2013] for the prediction of the CO_2 dissolution rate using the new scaling law



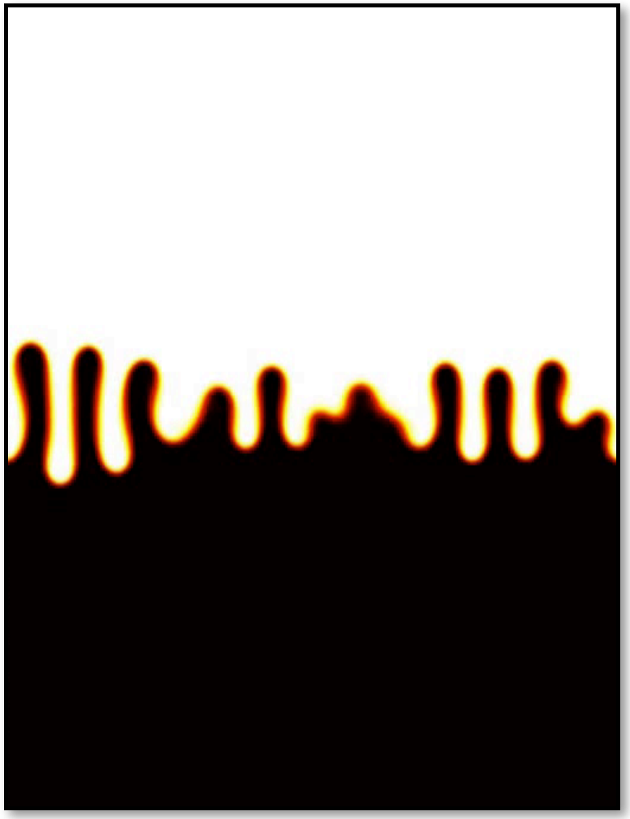
$$C(t) \approx \frac{1}{1 + 4\alpha\gamma^n Ra\, t}$$

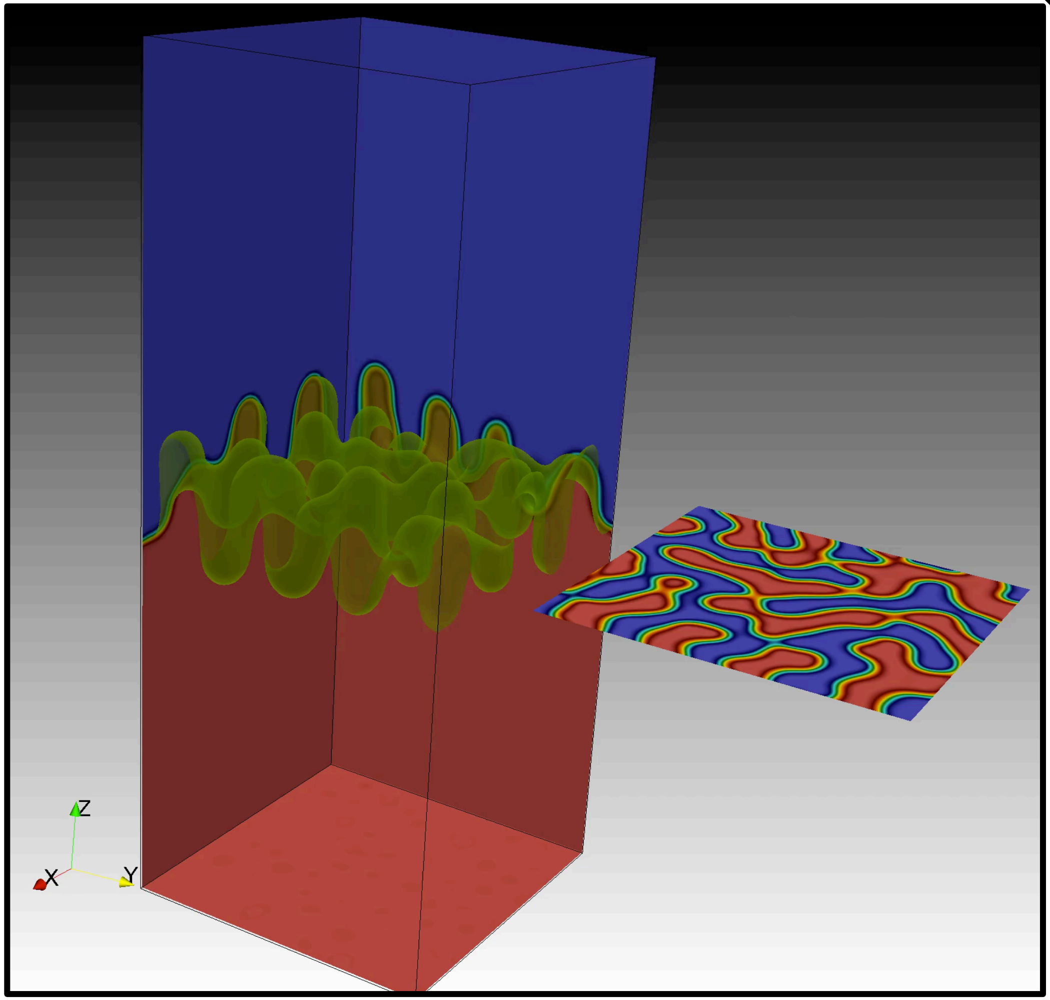
$$F(t) \approx \frac{4\,\alpha\,\gamma^{-1/4} Ra}{[1 + 4\alpha\gamma^{-1/4} t]^2}$$

$$G(t) = \int_{t_0}^{t} F(\tau)\,d\tau$$

De Paoli et al. (2016), *Phys. Fluids* **28** (056601).

$$t_2 = \frac{(2+\eta)C_1}{0.017}\, Ra$$





How does the interface evolve? What is the plume impingement time?

Conclusions

- Phenomenological model for the shutdown time in porous media

$$t_2 = \frac{(2+\eta)C_1}{0.017} Ra$$

- Analytical model for the dissolution flux during the shutdown regime in anisotropic porous media

$$F(\gamma, t) \approx \frac{4\alpha\gamma^n Ra}{\left[1 + 4\alpha\gamma^n t\right]^2}$$

Role of HPC

- Investigate possible dissolution scenarios in geological reservoirs
- Explore the evolution of injected CO2 for long times ($t \sim 10^3$ y)

References

De Paoli, M., Zonta, F., and Soldati, A. (2016). Influence of anisotropic permeability on convection in porous media: Implications for geological CO2 sequestration. *Physics of Fluids (1994-present)*, 28(5):056601.

De Paoli, M., Zonta, F., and Soldati, A. (2017). Dissolution in anisotropic porous media: Modelling convection regimes from onset to shutdown. *Physics of Fluids (1994-present)*, 29(2):026601.

Acknowledgments

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Thank you for your attention