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### 1. Introduction

Global energy consumption has doubled in the last forty years and shows no sign of abating. A major proportion of this consumption (80%) comes from the combustion of fossil fuels, with emissions of carbon dioxide (CO<sub>2</sub>). Such emissions have led to a corresponding growth in the atmospheric concentration of CO<sub>2</sub>, likely responsible for the concomitant increase in the average global temperature of the atmosphere. With this trend showing no sign of change, remedy to this global problem is still a debated question and Carbon Capture and Storage (CCS) into natural geological reservoirs (fig. 1) was identified as a possible solution. The CO<sub>2</sub> dissolution process is a multiscale phenomenon, requiring high-resolution Direct Numerical Simulations (DNS) to be correctly investigated.

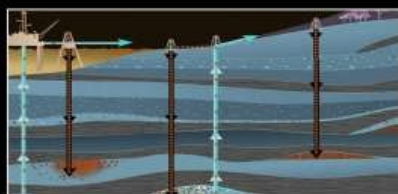
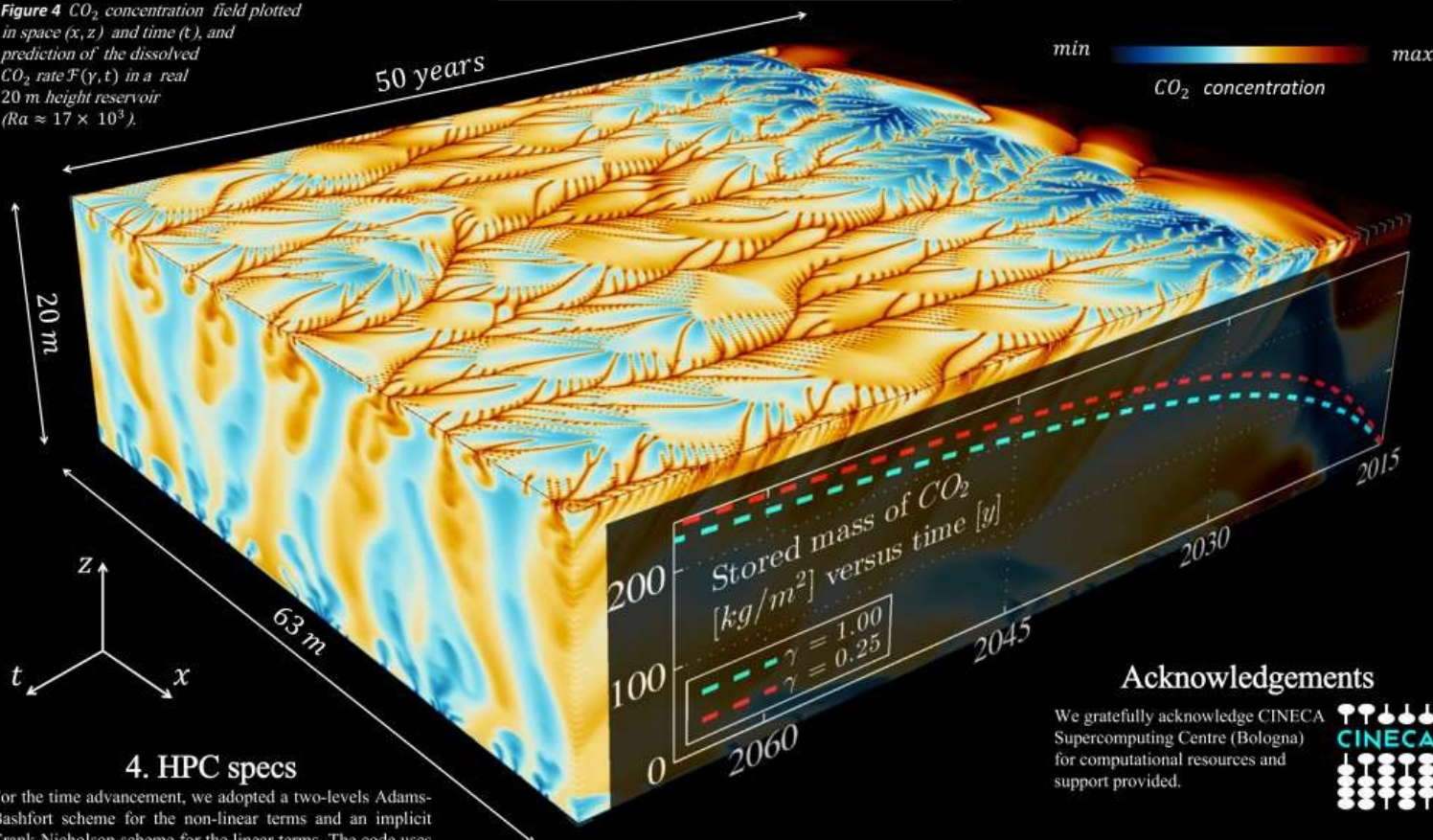


Figure 1 Geological CO<sub>2</sub> storage

Figure 4 CO<sub>2</sub> concentration field plotted in space (x, z) and time (t), and prediction of the dissolved CO<sub>2</sub> rate  $\mathcal{F}(\gamma, t)$  in a real 20 m height reservoir ( $Ra \approx 17 \times 10^3$ ).



### 4. HPC specs

For the time advancement, we adopted a two-levels Adams-Bashfort scheme for the non-linear terms and an implicit Crank-Nicholson scheme for the linear terms. The code uses multiple FFTW3 libraries to perform Fast Fourier Transform. The parallel paradigm used is the MPI standard achieved by 1D domain decomposition. The domain is spaced using up to 8192 x 1025 nodes in horizontal and vertical directions respectively, and the computation is massively parallelized on the TIER-0 HPC system named «FERMI» (Bologna, Italy).

**Domain decomposition** Here is adopted a non-uniform cartesian grid due to the wall-normal discretization implemented (Chebyshev). During the computation, Fourier (x direction) and Chebyshev (z direction) transform have to be performed. In the first case, the domain is divided in horizontal slabs and the computation distributed along the MPI processes. In the case of the Chebyshev discretization, all the column nodes are required and the domain is divided in vertical sections. This procedure is performed each time step during the computation of the non-linear terms, which are calculated in the physical space.

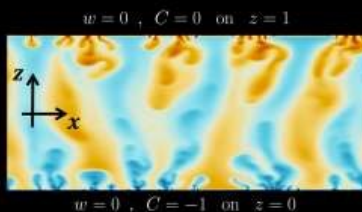


Figure 2 Boundary conditions adopted

### 2. Problem formulation

We model the reservoir as a fully saturated, anisotropic porous medium filled with a newtonian and incompressible fluid. The flow is governed by the Darcy equations (see box below), where the governing parameter is the Rayleigh number  $Ra$  (the relative intensity of advection compared to diffusion). The anisotropic parameter  $\gamma$  is the vertical-to-horizontal permeability ratio. We performed DNS using a Chebyshev-Tau pseudo-spectral method, imposing the boundary conditions shown in fig. 2 (periodicity is applied along x).

$$u = \frac{\partial P}{\partial x}, \quad w = \frac{\partial P}{\partial z} - C$$

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + w \frac{\partial C}{\partial z} = \frac{1}{Ra} \left( \gamma \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2} \right) \quad \text{Physical model implemented}$$

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

### 3. Numerical results

The efficiency of the CO<sub>2</sub> dissolution mechanism is evaluated through the Nusselt Number

$$Nu = \frac{1}{L} \left\langle \int_0^L \frac{\partial C(x, t)}{\partial z} \Big|_{z=1.0} dx \right\rangle$$

The amount of dissolved CO<sub>2</sub> is larger for smaller values of  $\gamma$  (fig. 3) and follows the correlation:

$$Nu = \alpha + \beta \gamma^{-1/4} Ra \quad \text{with } \alpha = 2.75, \quad \beta = 6.88 \times 10^{-3}$$

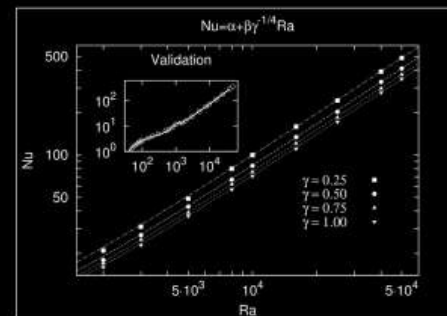


Figure 3 Nusselt number vs Rayleigh number for different values of the anisotropic parameter  $\gamma$

### 5. Conclusions

Results obtained from Direct Numerical Simulations are used to derive a model to predict the flux evolution of the CO<sub>2</sub> as a function of  $\gamma$ ,  $\mathcal{F}(\gamma, t)$ , which is estimated as:

$$\mathcal{F}(\gamma, t) = \frac{4\beta\gamma^{1/4}}{1 + 4\beta\gamma^{1/4}} Ra.$$

We found that for  $\gamma < 1$ ,  $\mathcal{F}(\gamma, t)$  increases significantly compared to the isotropic case of  $\gamma = 1$ , indicating that previous predictions of the CO<sub>2</sub> storage capability are underestimated (fig. 4).

### 6. References

De Paoli M., Zonta F. and Soldati A., "Influence of anisotropic permeability on convection in porous media: implications for geological CO<sub>2</sub> sequestration", *Physics of Fluids*, Accepted.

### Acknowledgements

We gratefully acknowledge CINECA Supercomputing Centre (Bologna) for computational resources and support provided.



Our contacts, research and activities are available in the *Multiphase Flow Laboratory* website



Further visualizations and movies are available in the *Multiphase Flow Laboratory* Youtube Channel

