

A posteriori error estimators and adaptivity for CO₂ sequestration

Eric FLAURAUD, IFP Energies nouvelles - Rueil-Malmaison
Ibtissem LANNABI, Inria/IFP Energies nouvelles - Paris/Rueil-Malmaison

Martin VOHRALÍK, Inria - Paris
Soleiman YOUSEF, IFP Energies nouvelles - Rueil-Malmaison

Geological carbon storage (GCS) technology has become increasingly relevant due to global warming. Numerical simulations play a crucial role in understanding and implementing this technology, as well as in assessing long-term storage risks. To provide a common baseline for GCS numerical simulations, the Society of Petroleum Engineers launched the 11th Comparative Solution Project (SPE11) [6].

The problem considered is modeled by a highly nonlinear system of degenerate partial differential equations governing a multicomponent, multiphase porous media flow. The numerical simulation of such models is computationally expensive, particularly for long-time simulations. The central question in the numerical approximation is how large the simulation error is.

In this work, we focus on the Coats model [2] for the SPE11 benchmark, approximated using a finite volume scheme in space and a backward Euler scheme in time. The resulting nonlinear equations are solved using Newton's iterative algorithm, and the linear systems obtained after linearization are solved with an iterative algebraic solver. Another important question that arises at this stage is whether it is possible to improve the computational efficiency without compromising the accuracy of the results. To answer the two above questions, we first propose to bound the total relative error by extending the fully computable a posteriori error estimate developed in [3]. We then quantify the contribution of each individual error component, namely those arising from spatial, temporal, and linearization approximations. Next, based on these a posteriori error estimate components, we propose to improve the computational efficiency through adaptive stopping criterion for the Newton algorithm and adaptive control of the time-step size.

Finally, since the complex model involves nonsmooth, highly nonlinear, and possibly degenerate constitutive laws, Newton's algorithm may face convergence difficulties. To address this issue, we propose an adaptive regularization of these stiff nonlinearities, as proposed in [4] for Richards equation.

Numerical results are performed using the Geoxim platform, which is based on Arcane [5, 1].

- [1] CEA/IFPEN. *Arcane Framework organization*, Accessed 2025-12-19. GitHub repository.
- [2] K. H. Coats. *Implicit compositional simulation of single-porosity and dual-porosity reservoirs*. In *SPE Symposium on Reservoir Simulation*, 1989. doi :10.2118/18427-MS. Paper SPE-18427-MS.
- [3] D. A. Di Pietro, E. Flauraud, M. Vohralík, S. Yousef. *A posteriori error estimates, stopping criteria, and adaptivity for multiphase compositional Darcy flows in porous media*. *J. Comput. Phys.*, **276**, 163–187, 2014. doi :10.1016/j.jcp.2014.06.061.
- [4] F. Févotte, A. Rappaport, M. Vohralík. *Adaptive regularization for the richards equation*. *Computational Geosciences*, **28(6)**, 1371–1388, 2024.
- [5] G. Gropellier, B. Lelandais. *The Arcane development framework*. In *Proceedings of the 8th Workshop on Parallel/High-Performance Object-Oriented Scientific Computing*, POOSC '09. Association for Computing Machinery, New York, NY, USA, 2009. doi :10.1145/1595655.1595659.
- [6] J. M. Nordbotten, M. A. Ferno, B. Flemisch, A. R. Kovscek, K.-A. Lie. *The 11th Society of Petroleum Engineers Comparative Solution Project : Problem Definition*. *SPE Journal*, **29(05)**, 2507–2524, 2024. doi :10.2118/218015-PA.