A posteriori error estimators and adaptivity for CO_2 sequestration

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Mathematical and numerical methods for multi-scale multi-physics, nonlinear coupled processes (MS07)

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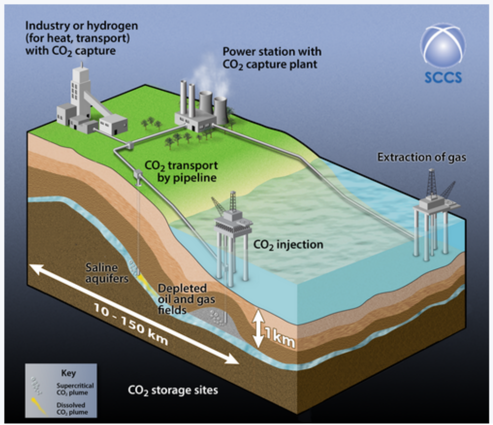
Contribution of this work

Extend the application of a posteriori error estimates for more complex problems

Motivation: Ensuring long-term storage of the injected CO_2 $\hookrightarrow$ expensive numerical simulations



Goals

- Quantify the relative error using fully computable a posteriori error estimates [Vohralík and Yousef2025; Di Pietro et al.2014]
- Quantify the contribution of each relative error component (space, time, and linearization)
- Improve the computational efficiency of the Geoxim code by introducing adaptive stopping criteria based on a posteriori error estimates for both Newton and time loops

Outline of the talk

1. Context
   - The multiphase flow model and its approximation
   - A posteriori error estimates based on equilibrated fluxes
2. Numerical results for SPE11
   - Description of the SPE11 benchmark: *11th SPE Comparative Solution project (CSP)*
   - Quantification of the error simulations
   - Adaptive iterative approximation
3. Current work

- Unsteady nonlinear coupled degenerate advection-diffusion- reaction problem
- Unkonwns of the system $\boldsymbol{\mathcal{X}} := \left(P, \, (S_p)_{p\in\mathcal{P}} \, , \, (C_{p,c})_{p\in\mathcal{P},\, c\in\mathcal{C}} \right)$

Coats model [Coats1989]

Set of PDEs for each component $c \in \mathcal{C}$

$$\partial_t \underbrace{\left(\sum_{p\in\mathcal{P}_c} \phi \zeta_p S_p C_{p,c} \right)}_{l_c} + \nabla \cdot \underbrace{\left(\sum_{p\in\mathcal{P}_c} \nu_p C_{p,c} \boldsymbol{v}_p \right)}_{\boldsymbol{\theta}_c} = q_c$$

$$\boxed{\boldsymbol{v}_p = -\underline{\mathbf{K}} \left(\nabla P_p + \rho_p g \nabla z \right)} \quad \boxed{Pc_p = P - P_p}$$

$$\boxed{\nu_p = \zeta_p kr_p / \mu_p}$$

System of algebraic eqs.

$$\begin{cases} \sum_{p\in\mathcal{P}} S_p = 1 \\ \sum_{c\in\mathcal{C}_p} C_{p,c} = 1, \ \forall p \in \mathcal{P} \\ + \text{equilibrium eq.} \end{cases}$$

- Thermal effects, dispersive fluxes & chemical reactions are not included

Approximations

- Spatial $\hookrightarrow$ Finite Volume scheme
- Temporal $\hookrightarrow$ Backward Euler scheme
- System of nonlinear algebraic equations $\hookrightarrow$ Newton' algorithm
- System of linear algebraic equations $\hookrightarrow$ Iterative solvers

Difficulties (among others)

- **Newton slow convergence or divergence or unstability**
  - Nonlinear Pc_p & kr_p $\hookrightarrow$ nonlinear flux
  - Discontinuous $\underline{\mathbf{K}}$ $\hookrightarrow$ discontinuious flux function
  - For immobile phases ($kr_p \longrightarrow 0$) $\hookrightarrow$ $\nabla \cdot (\underline{\mathbf{K}} \nabla P_p)$ becomes degenerate elliptic
  - Gravitational forces lead to the presence of **kinks** (discontinuities in the flux first-order derivative) $\hookrightarrow$ non-differentiable numerical flux

- **Small time steps (heuristic timestep control techniques!)**
  - nonconvergence of Newton solver if the timestep is large $\hookrightarrow$ Newton scheme is restarted with a smaller time step

A posteriori error estimates

Error control and adaptivity

- Unknown exact solution $\hookrightarrow$ a posteriori error estimates based on equilibrated fluxes
  - Error control

$$\boxed{\frac{|||\boldsymbol{u} - \boldsymbol{u}_{h\tau}^{n,k}|||}{|||\boldsymbol{u}_{h\tau}^{n,k}|||} \leq \eta^{n,k}}$$

Error control and adaptivity

- Unknown exact solution $\hookrightarrow$ a posteriori error estimates based on equilibrated fluxes
  - Error control

$$\boxed{\frac{|||\boldsymbol{u}-\boldsymbol{u}_{h\tau}^{n,k}|||}{|||\boldsymbol{u}_{h\tau}^{n,k}|||} \le \eta^{n,k}}$$

  - Distinguishing error components

$$\boxed{\frac{|||\boldsymbol{u}-\boldsymbol{u}_{h\tau}^{n,k}|||}{|||\boldsymbol{u}_{h\tau}^{n,k}|||} \le \eta^{n,k} = \eta_{\mathrm{sp}}^{n,k} + \eta_{\mathrm{tm}}^{n,k} + \eta_{\mathrm{lin}}^{n,k}}$$

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- Component temporal error estimate on cell K, for component $c \in \mathcal{C}$

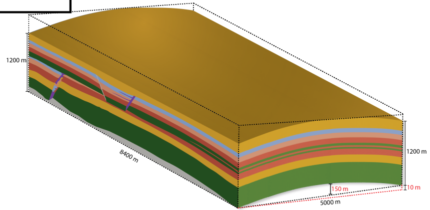
$$\left(\eta_{\mathrm{tm},c,K}^{n,k}\right)^2 = \left\|\boldsymbol{\theta}_{c,K,\sigma,\uparrow}\left(\boldsymbol{\mathcal{X}}_H^{n,k}\right) - \boldsymbol{\theta}_{c,K,\sigma,\uparrow}\left(\boldsymbol{\mathcal{X}}_H^{n-1}\right)\right\|_{\underline{\mathbf{K}}^{-\frac{1}{2}},K}^2 = \left(\mathrm{U}_{p,K,\mathrm{tm}}^{n,k}\right)^T \widehat{\mathbb{A}}_{\mathrm{MFE},K}\left(\mathrm{U}_{p,K,\mathrm{tm}}^{n,k}\right)$$

Advantage $\hookrightarrow$ easy coding, fast evaluation, use in practical simulations

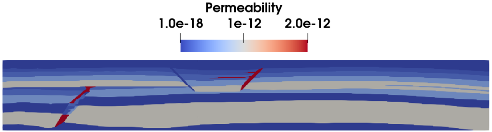
Description of the SPE11 benchemark

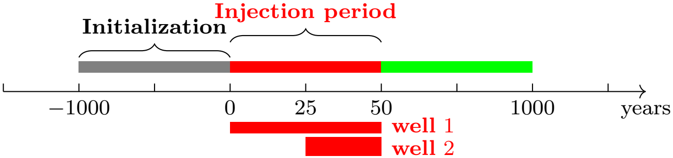
International exercise [2023-2025] proposed by [Nordbotten et al.2024]

Two-phase two-component miscible flow

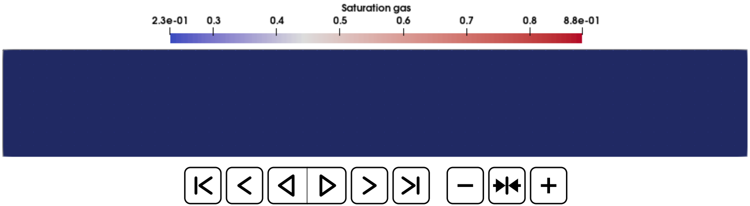


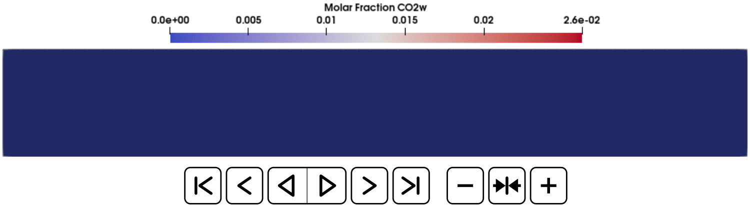
- Pure water in the reservoir (aquifer) and pure CO_2 injection
- Synthetic cases representative of a geological structure in Norway
- **The 11B version of the benchmark:**
  2D field scale model <u>without</u> thermal effects
- Heterogeneous medium, two injection wells
- Simulation timeline

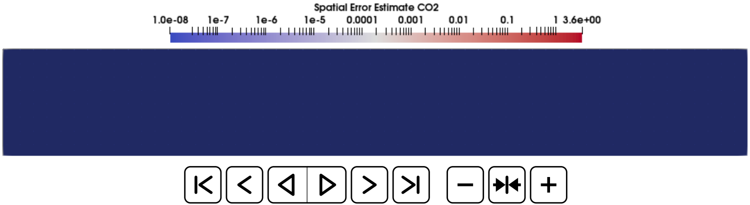




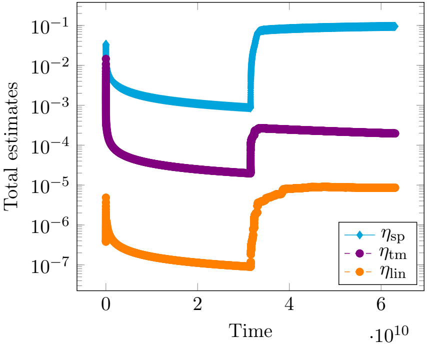
Gas saturation, CO_2 Molar fraction in water, CO_2 Spatial estimate







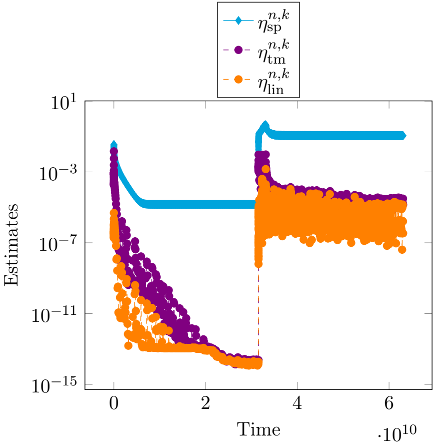
How large the simulation error is?

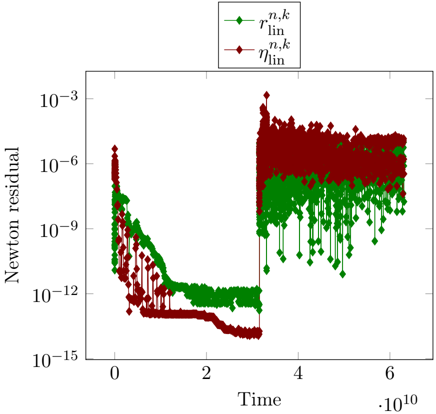


Mesh size	840×120
Spatial	9%
Temporal	0.02%
Linearization	0.001%

	Resolution time	**Estimators evaluation**
Standard resolution	4664, 48s	525.9s (11%)

Behavior of the a posteriori error estimates





- Mesh size $= 840 \times 120$
- Newton tolerance $= 1e-5$
- Linear solver tolerance $=$ $= 1e-6$

Algorithm 1 Adaptive stopping criteria for the time and Newton loops

```
while k < k_max do
    if [ η_lin^{n,k} < γ_lin η_sp^{n,k} ] then
        Break Newton loop
    end if
end while
```

- $\gamma_{\text{lin}}, \gamma_{\text{tm}} \in (0, 1)$
- In what follows: $\gamma_{\text{lin}} = 0.001$ & $\gamma_{\text{tm}} = 0.05$

Algorithm 2 Adaptive stopping criteria for the time and Newton loops

```
while t^n < t_F do
    while k < k_max do
        if [ η_lin^{n,k} < γ_lin η_sp^{n,k} ] then
            Break Newton loop
        end if
    end while
    if [ η_tm^{n,k̄} < γ_tm η_sp^{n,k̄} ] then
        τ^{n+1} ← τ^n × τ̄
    else if [ η_sp^{n,k̄} ≥ η_tm^{n,k̄} ≥ γ_tm η_sp^{n,k̄} ] then
        τ^{n+1} ← τ^n / τ̃
    else
        τ^n ← τ^n / τ̃
    end if
    n ← n + 1
end while
```

while $t^n < t_F$ **do**

  while $k < k_{\max}$ **do**

    if $\eta_{\text{lin}}^{n,k} < \gamma_{\text{lin}}\, \eta_{\text{sp}}^{n,k}$ **then**

      Break Newton loop

    end if

  end while

  if $\eta_{\text{tm}}^{n,\bar{k}} < \gamma_{\text{tm}}\, \eta_{\text{sp}}^{n,\bar{k}}$ **then**

    $\tau^{n+1} \leftarrow \tau^n \times \bar{\tau}$

  else if $\eta_{\text{sp}}^{n,\bar{k}} \geq \eta_{\text{tm}}^{n,\bar{k}} \geq \gamma_{\text{tm}}\, \eta_{\text{sp}}^{n,\bar{k}}$ **then**

    $\tau^{n+1} \leftarrow \tau^n / \tilde{\tau}$

  else

    $\tau^n \leftarrow \tau^n / \tilde{\tau}$

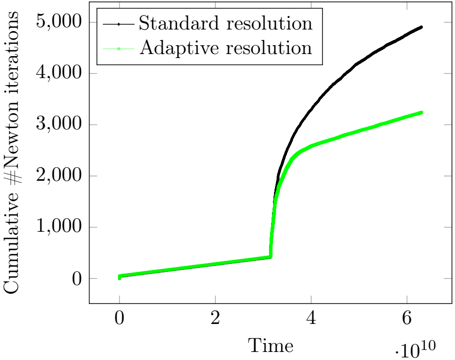
  end if

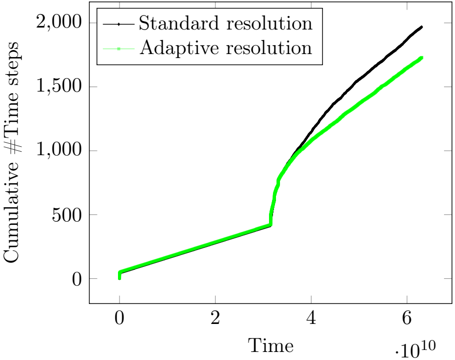
  $n \leftarrow n + 1$

end while

- $\gamma_{\text{lin}}, \gamma_{\text{tm}} \in (0, 1)$
- In what follows: $\gamma_{\text{lin}} = 0.001$ & $\gamma_{\text{tm}} = 0.05$

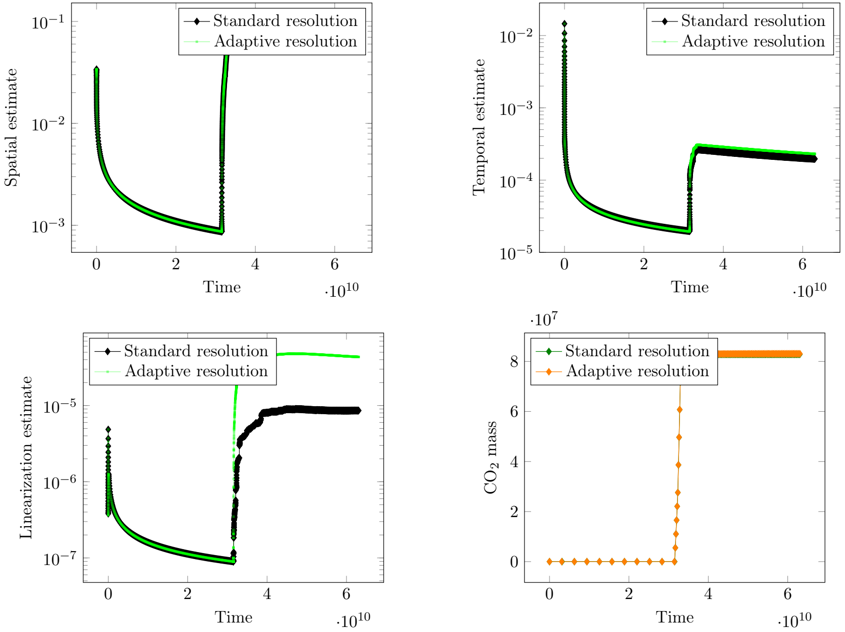
Do we reduce the computational cost?



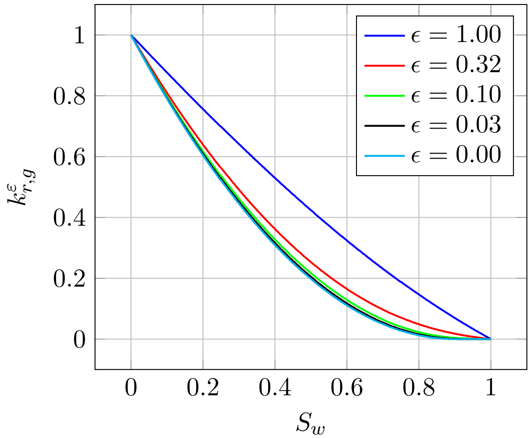


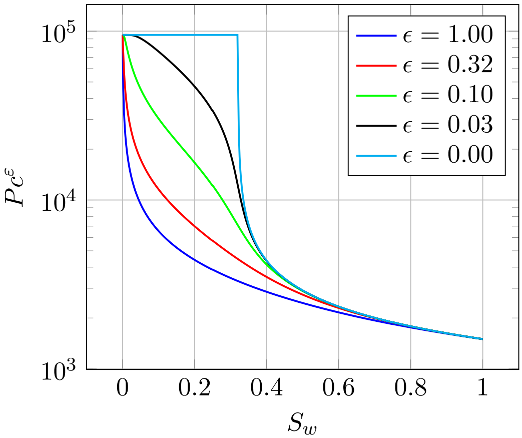
	Resolution time	**Estimators evaluation**	**Gain**
Standard resolution	$4664, 48$s	525.9s	
Adaptive resolution	$3413, 3$s (gain $26, 8\%$)	345.6s	16%

Do we impact the overall simulation accuracy?



Outlook: Address Newton nonconvergence issues by introducing regularization strategies for stiff nonlinear laws





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