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Iterative methods and preconditioning for a model of transport with sorption

Michel Kern, Abdelaziz Taakili

Institut National de Recherche en Informatique et Automatique

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Outline

1. Problem statement
2. Iterative methods
3. Block preconditioning

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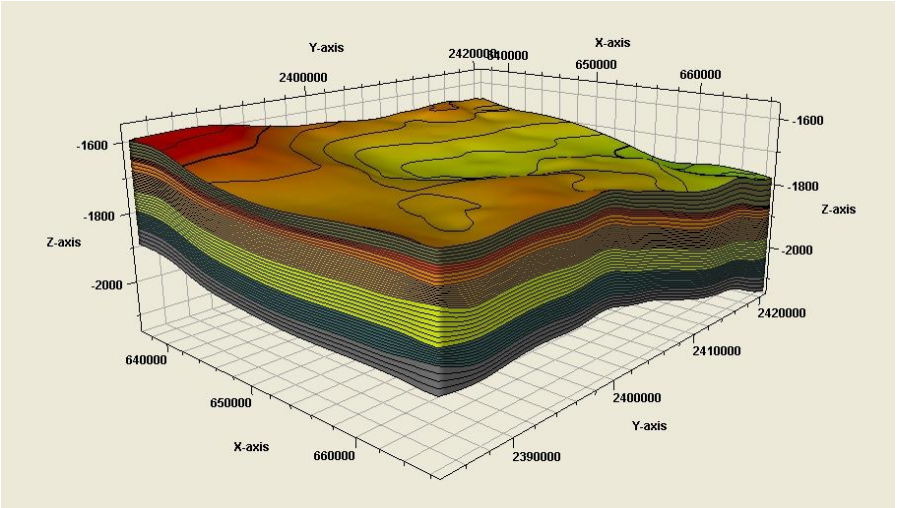
Motivation

Multi-species reactive transport

- Chemistry with equilibrium reactions
- Transport of aqueous species
- Large nonlinear system

Large scale geologic model for CO2 sequestration project (BRGM)



Difficulties

- Iterative methods: fixed point vs Newton
- Exact or inexact Newton (Newton–Krylov)?
- Preconditioning for Newton–Krylov

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Solute transport: model and solution method

Convection-difusion equation

$$\omega \partial_t c - \nabla.(\mathbf{D}\nabla c - qc) = F \text{ in } \Omega \times (0, T)$$

- c solute concentration
- ω porosity
- **D** diffusion coefficient
- **q** Darcy velocity (assumed known)

F Reaction term, from chemistry

Discretization based on operator splitting

Advection step
- Explicit finite volumes
- Locally conservative
- sub time step (respect CFL)

Diffusion step
- Mixed finite elements
- Implicit, locally conservative

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A simplified coupled model

One species model, with sorption

c mobile concentration, $\bar{c}$ fixed concentration.

$$F = -(1-\omega)\rho_S \partial_t \bar{c}$$

$\bar{c} = \Psi(c)$, Ψ sorption isotherm

$$\begin{cases} \omega \partial_t c + (1-\omega)\rho_S \partial_t \bar{c} - \nabla.(\mathbf{D}\nabla c - qc) = 0 \\ \bar{c} = \Psi(c) = \dfrac{k_f \sigma c}{k_b + k_f c} \quad \text{(Langmuir isotherm)} \end{cases}$$

Structure of nonlinear problem similar to multicomponent chemistry case

References

- J. Barrett, P. Knabner and Van Duijn
- P. Frolkovič, J. Kačur et al.

Discrete system

Coupled system

$$F\begin{pmatrix}\mathbf{c}\\ \bar{\mathbf{c}}\end{pmatrix} := \begin{pmatrix}(\mathbf{M}+\Delta t\,\mathbf{L})\mathbf{c}+\mathbf{M}\bar{\mathbf{c}}-\mathbf{b}^n\\ \bar{\mathbf{c}}-\Psi(\mathbf{c})\end{pmatrix} = 0$$

$\Psi(\mathbf{c}) = (\Psi(c_T))_T,\ T \in \mathscr{T}_h$

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Alternative formulations

Eliminate $\bar{c}$ Analogous to Direct Substitution Approach

$$(\mathbf{M}+\Delta t\,\mathbf{L})\mathbf{c}+\mathbf{M}\Psi(\mathbf{c})-\mathbf{b}^n = 0$$

Eliminate c (black-box transport and chemistry)

$$\tilde{F}(\bar{\mathbf{c}}) = \bar{\mathbf{c}}-\Psi\left((\mathbf{M}+\Delta t\,\mathbf{L})^{-1}(\mathbf{b}^n-\mathbf{M}\bar{\mathbf{c}})\right)$$

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Can be solved by block Gauss Seidel or by Newton's method

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Gauss–Seidel iterations

Gauss–Seidel on coupled system $\Longleftrightarrow$ fixed–point on $\bar{c}$ equation

$$\bar{\mathbf{c}}^{\mathbf{k+1}} = \bar{\mathbf{c}}^{\mathbf{k}} - \Psi\left((\mathbf{M} + \Delta t\,\mathbf{L})^{-1}(\mathbf{b}^n - \mathbf{M}\bar{\mathbf{c}}^{\mathbf{k}})\right)$$

Convergence analysis (for continuous problem)

Fixed–point converges iff

$$\Delta t > \frac{(1-\omega)\rho_s K - \omega}{DC_p}$$

- $K = \max_{c \in \mathbf{R}} |\Psi'(c)|$,
- C_p Poincaré's constant

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Relax the iterations to restore convergence: introduce total concentration, $T = c + \bar{c}$, equivalent to relaxation with $\theta = \dfrac{1}{1+K}$.

Relaxed method always converges

Solution by Newton–Krylov

- Solve the linear system by an iterative method (GMRES)
- Requires only jacobian matrix by vector products.

Used for CFD, shallow water, radiative transfer (Keyes, Knoll, JCP 04), and for reactive transport (Hammond, Valocchi, Lichtner, Adv. Wat. Res. 05)

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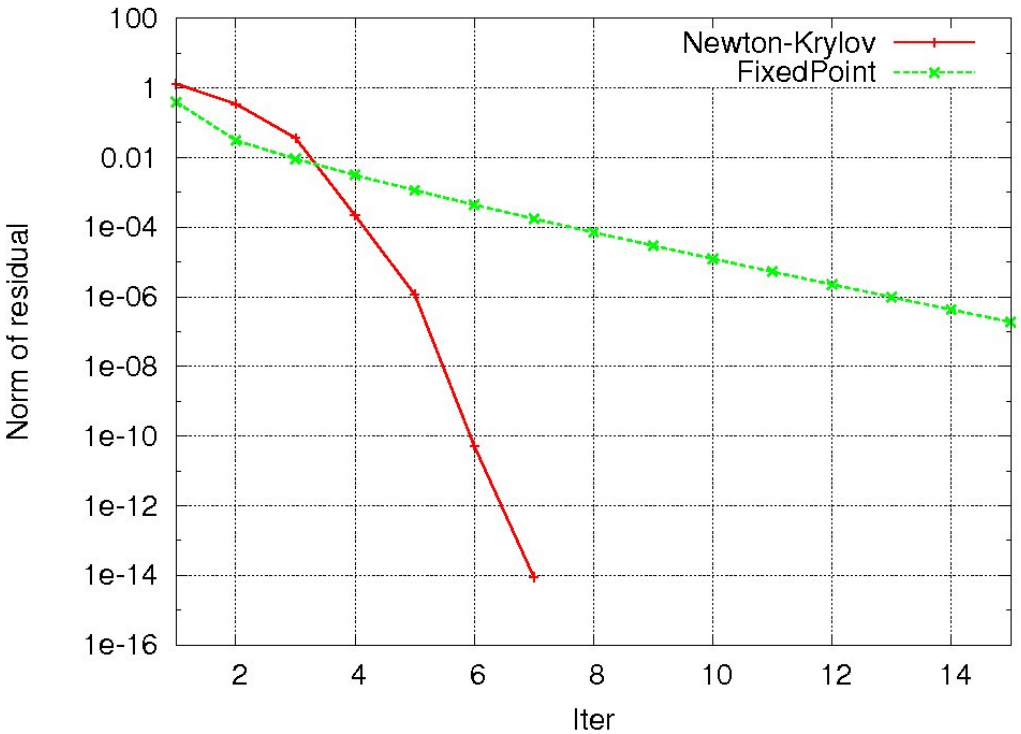
Inexact Newton

- Approximation of the Newton's direction $\|f'(x_k)d + f(x_k)\| \leq \eta \|f(x_k)\|$
- Choice of the forcing term η?
  - Keep quadratic convergence (locally)
  - Avoid oversolving the linear system
- $\eta = \gamma \|f(x_k)\|^2 / \|f(x_{k-1})\|^2$ (Kelley, Eisenstat and Walker)

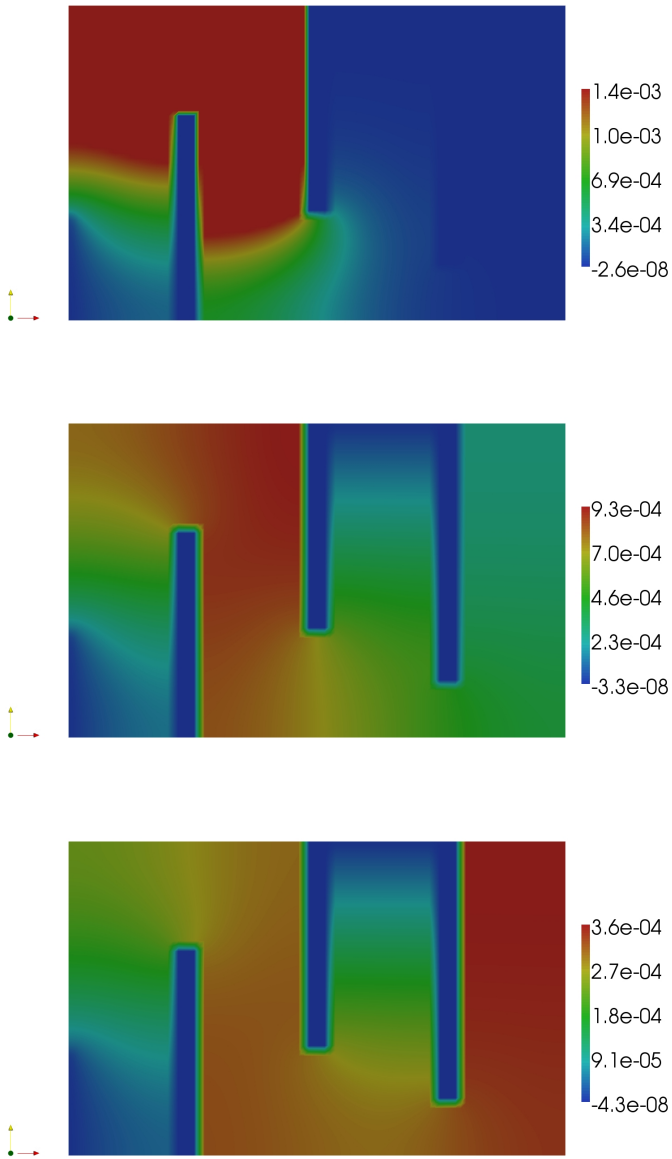
L. Amir's thesis, Amir, MK (Comp. Geosci. 09)

Performance of Newton's method



Convergence of Newton and fixed point

LifeV (EPFL, MOX, INRIA),
KINSOL (Sundials, LLNL)



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Jacobian preconditioning

Jacobian for coupled system ($A = M + \Delta t\, L$)

$$J = \begin{pmatrix} A & M \\ -D & I \end{pmatrix} \qquad D = \mathrm{diag}(\Psi'(c_1), \ldots, \Psi'(c_N))$$

Only block preconditioning, respect structure of coupled system

Block preconditioning

Jacobi $P_J = \begin{pmatrix} A & 0 \\ 0 & I \end{pmatrix} \qquad P_J^{-1} J = \begin{pmatrix} I & A^{-1}M \\ -D & I \end{pmatrix}$

Gauss–Seidel $P_{GS} = \begin{pmatrix} A & 0 \\ -D & I \end{pmatrix} \qquad P_{GS}^{-1} J = \begin{pmatrix} I & A^{-1}M \\ 0 & I + DA^{-1}M \end{pmatrix}$

Solve transport at each iteration, reuse transport solver.

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Solve transport at each iteration, reuse transport solver.

Alternative formulation, $\tilde{J} = I + DA^{-1}M$ is Schur complement of JP^{-1}

Equivalent to Schur complement of GS, at the non-linear level.

Gmres convergence and eigenvalues

In general, convergence of GMRES not determined by eigenvalues (Greenbaum, Strakos).

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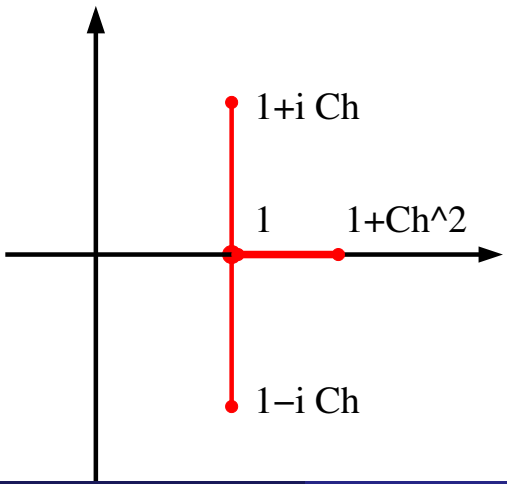
Eigenvalues of preconditioned operators

Assumption $\lambda(A) \simeq O(h^{-2})$ (True for FD discretization)

Jacobi $\Lambda(P_J^{-1}J) \subset [1 - iCh, 1 + iCh]$ $(\mu_J = 1 \pm \frac{i}{\sqrt{\lambda_A}})$.

Gauss-Seidel $\Lambda(P_{GS}^{-1}J) \subset [1, 1 + Ch^2]$, $(\mu_{GS} = 1 + \frac{1}{\lambda_A}$, or $\mu_{GS} = 1$,n-fold),

Schur $\Lambda(\tilde{J}) \subset [1, 1 + Ch^2]$ $(\mu_{Sch} = \mu_{GS}, \mu_{Sch} \neq 1)$.



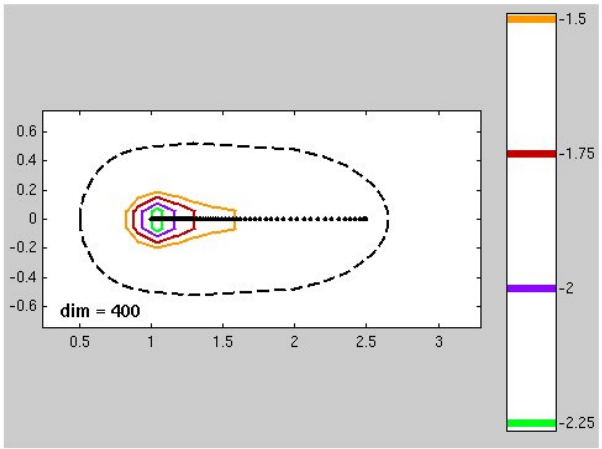
Bounded away from 0 independently of h.

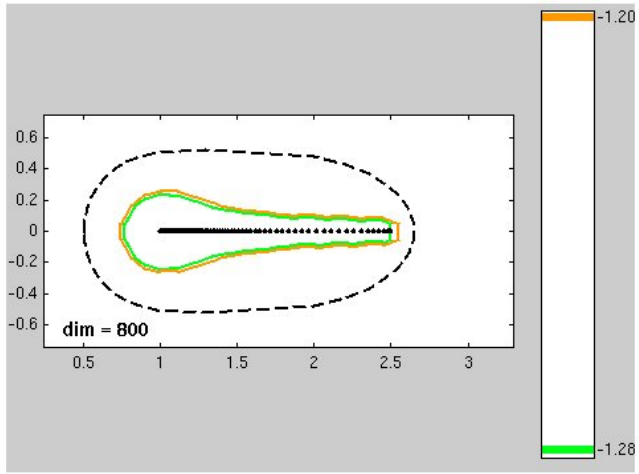
Field of value analysis

GMRES convergence

$W(A) \equiv \left\{ \frac{x^* A x}{x^* x} | x \in \mathbb{C}^n, x \neq 0 \right\}$, convex set, contains eigenvalues of A

$$\frac{\|r_k\|_2}{\|r_0\|_2} \leq 2 \min_{p \in \mathscr{P}_k^*} \max_{z \in W(A)} |p(z)| .$$





Eingenvalues, field of values and pseudospectrum for GS preconditioning

Preconditioner performance

1D model (Matlab + Sundials), $h = 0.05$, $K_L = 1.$, $\sigma = 1.5$, and $\Delta t = 0.0135$.

Mesh dependance : constant forcing term

	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	3	104	3	167	3	267	3	453

NI: # nonlinear iters, NLI: total # linear iters.

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BGS	3	48	3	48	3	48	3	45

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BGS	3	48	3	48	3	48	3	45
Elimination	3	41	3	41	3	41	3	40

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Mesh dependance : adaptive forcing term

	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	8	42	8	76	10	105	10	177

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	NI	LI	NI	LI	NI	LI	NI	LI
None	8	42	8	76	10	105	10	177
BGS	8	23	7	24	7	22	8	25

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	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	3	104	3	167	3	267	3	453
BGS	3	48	3	48	3	48	3	45
Elimination	3	41	3	41	3	41	3	40

Mesh dependance : adaptive forcing term

	h		$h/2$		$h/4$		$h/8$	
	NI	LI	NI	LI	NI	LI	NI	LI
None	8	42	8	76	10	105	10	177
BGS	8	23	7	24	7	22	8	25
Elimination	5	15	5	15	5	15	5	15

NI: # nonlinear iters, NLI: total # linear iters.

Conclusions

- Newton–Krylov method can be applied on “fixed–point” formulation
- Connection between block–preconditioning and elimination at non-linear level
- Inverting transport gives mesh independent convergence for both linear (LI) and nonlinear (NI) iterations.
- In practice: approximate inverse should give spectral equivalence
- Future work: Prove FOV results, extension to mulitcomponent chemistry

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