Iterative metohds and preconditioning for a model of transport with sorption

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Outline

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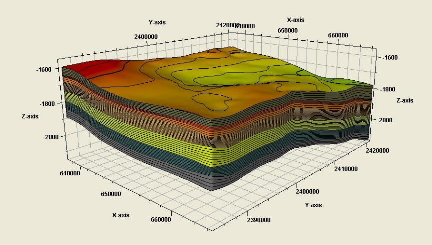
Motivation

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

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
- F source / sink (reaction) term
- **q** Darcy velocity (assumed known)

D diffusion-dispersion tensor :

$$\mathbf{D} = d_e \mathbf{I} + |q| \left[\alpha_l \mathbf{E}(q) + \alpha_t (\mathbf{I} - \mathbf{E}(q)) \right], \; E_{ij}(q) = \frac{q_i q_j}{|q|}$$

Discretization based on operator splitting

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

Dispersion step
- Mixed finite elements
- Implicit, locally conservative

A simplified 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 coupled problem for multicomponent chemistry

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 DSA

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

Eliminate c

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

Discrete system

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

Outline

Gauss–Seidel iterations (1)

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

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

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

Gauss–Seidel iterations (2)

Relax the iterations to restore convergence

Introduce total concentration, $T = c + \bar{c}$.

$$\begin{aligned}(\mathbf{M} + \Delta t\,\mathbf{L})\mathbf{c}^{\mathbf{k+1}} + \mathbf{M}\bar{\mathbf{c}}^{\mathbf{k}} - \mathbf{b}^n &= 0\\ \mathbf{T}^{\mathbf{k+1}} &= \mathbf{c}^{\mathbf{k+1}} + \bar{\mathbf{c}}^{\mathbf{k}}\\ \bar{\mathbf{c}}^{\mathbf{k+1}} &= \tilde{\Psi}(\mathbf{T}^{\mathbf{k+1}})\end{aligned}$$

Equivalent to relaxation with $\theta = \dfrac{1}{1+K}$.

Convergence

Relaxed method converges iff

$$\frac{(1-\omega)\rho_S \Delta t}{\omega + D\Delta t C_p} + \frac{1}{K} > 0$$

Always OK for any Δt,

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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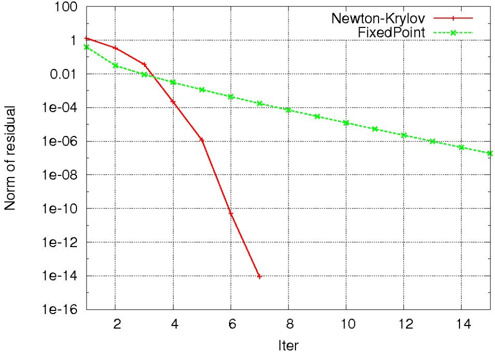
Inexact Newton

- Approximation of the Newton's direction $\|f'(x_k)d + f(x_k)\| \le \eta \|f(x_k)\|$
- 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)

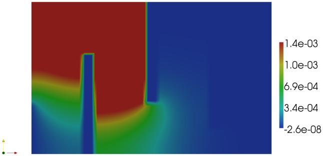
L. Amir's thesis, Amir, MK (Comp. Geosci. 09)

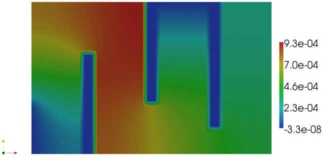
Performance of Newton's method

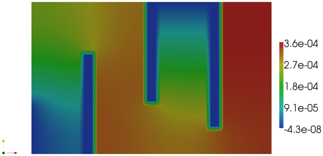


Convergence of Newton and fixed point

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







Outline

Jacobian preconditioning

Jacobian for coupled system

$$J = \begin{pmatrix} \mathbf{M} + \Delta t \mathbf{L} & \mathbf{M} \\ -\mathbf{D} & I \end{pmatrix} \qquad D = \operatorname{diag}(\Psi'(C_1), \dots, \Psi'(C_N))$$

Only block preconditioning, respect structure of coupled system

Block preconditioning

Jacobi $\mathbf{P}_J = \begin{pmatrix} \mathbf{M} + \Delta t \mathbf{L} & 0 \\ 0 & \mathbf{I} \end{pmatrix}$

Gauss–Seidel $\mathbf{P}_{GS} = \begin{pmatrix} \mathbf{M} + \Delta t \mathbf{L} & 0 \\ -\mathbf{D} & \mathbf{I} \end{pmatrix}$

Block Gauss–Seidel needs “jacobian of chemistry”

OK for Newton–Krylov

Preconditioned operators

Block Jacobi

$$JP_{\mathbf{J}}^{-1} = \begin{pmatrix} I & \mathbf{M} \\ -\mathbf{D}(\mathbf{M}+\Delta t\,\mathbf{L})^{-1} & I \end{pmatrix}$$

Block Gauss-Seidel

$$JP_{\mathbf{GS}}^{-1} = \begin{pmatrix} I+\mathbf{MD}(\mathbf{M}+\Delta t\,\mathbf{L})^{-1} & \mathbf{M} \\ 0 & I \end{pmatrix}$$

Solve transport at each iteration, reuse transport solver.

Preconditioned operators

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Solve transport at each iteration, reuse transport solver.

Alternative formulation

$\tilde{J} = I + \mathbf{D}(\mathbf{M}+\Delta t\mathbf{L})^{-1}\mathbf{M}$ is Schur complement of JP^{-1}
Equivalent to Schur complement of Gauss–Seidel, at the non-linear level.

Gmres convergence and eigenvalues

GMRES convergence

Let $A = JP^{-1}$, $A = V\Lambda V^{-1}$, $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_N)$.

$$\frac{\|r_k\|_2}{\|r_0\|_2} \leq \kappa(V) \min_{p \in \mathscr{P}_k, p(0)=1} \max_{\lambda \in \Lambda(A)} |p(\lambda)|$$

$\kappa(V)$: eigenvector condition number.

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A normal $\Rightarrow \kappa(V) = 1$.

In general, convergence of GMRES not determined by eigenvalues: any nonincreasing convergence curve is possible (Greenbaum, Strakos)

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Nevertheless ...

Eingevalue analysis

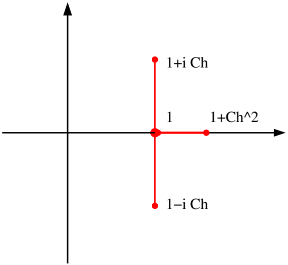
Assumption $\lambda(\mathbf{M} + \Delta t\mathbf{L}) \simeq O(h^{-2})$ (True for FD discretization)

Eigenvalues of preconditioned operators

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 $\mu_{GS} = 1)$, 1 is multiple ev.

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



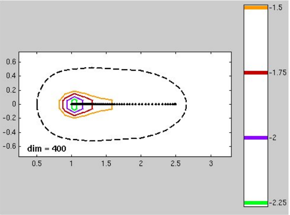
Bounded away from 0 independent of h.

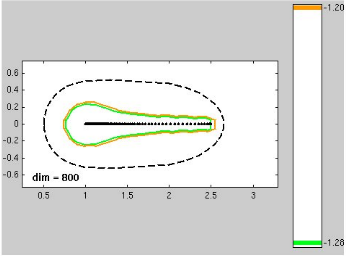
Field of value analysis

GMRES convergence

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

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





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 $\Delta t = 0.0135$.

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

Mesh dependance : constant forcing term

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

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BGS	3	48	3	48	3	48	3	45

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Elimination	3	41	3	41	3	41	3	40

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	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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	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

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	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 : constant 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

Mesh dependance : adaptive forcing term

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