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A Newton–Krylov method for reactive transport in porous media

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Outline

Work sponsored by Itasca Consultants, Groupement MoMaS (Andra – CEA – CNRS – EDF – IRSN), and ANR SHPCO2 project

Plan

Chemical equilibrium

Only take into account equilibrium, model, aqueous and sorption reactions

Chemical reactions, mass action laws

$$x_i \leftrightarrows \sum_{j=1}^{N_c} S_{ij} c_j, \qquad i = 1, \ldots, N_x,$$

$$y_i \leftrightarrows \sum_{j=1}^{N_c} A_{ij} c_j + \sum_{j=1}^{N_s} B_{ij} s_j, \qquad i = 1, \ldots, N_y,$$

c_j aqueous (mobile) components, s_j sorbed (immobile) components,
x_i aqueous secondary species, y_i fixed secondary species.

Numerical solution of nonlinear problem

System of non-linear equations

Mass action law

$$\log x = S \log c + \log K_x,$$
$$\log y = A \log c + B \log s + \log K_y.$$

Mass conservation

$$c + S^t x + A^T y = T, \qquad T \text{ known from transport}$$
$$s + B^T y = W, \qquad W \text{ imposed}$$

Take concentration logarithms as main unknowns

Use globalized Newton's method (line search, trust region).

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Role of chemical model

Given totals T (and W, known), split into

Mobile $C = c + S^T x$,

Fixed $F = A^T y$.

total concentrations

Result of chemical problem

$$F = \Psi_C(T)$$

Flow model: Darcy's law and mixed finite elements

Flow equations

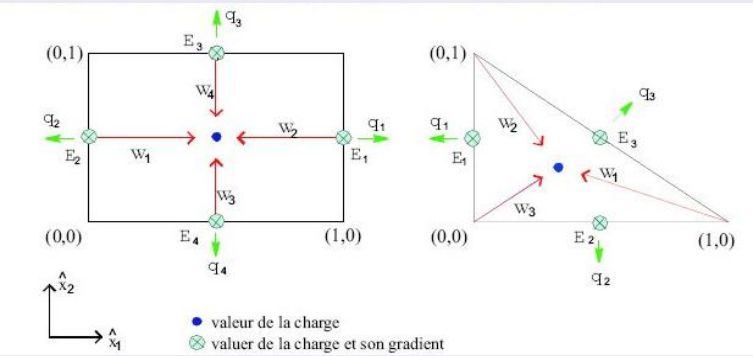
$$u = -K\nabla h, \quad \text{Darcy's law}$$

$$\nabla \cdot u = 0 \quad \text{incompressibility}$$

h piezometric head K permeability tensor u Darcy velocity

Solution by mixed finite elements

- Approximate both head and velocity
- Flux continuous across element faces
- Locally mass conservative
- Allows full diffusion tensor



Transport model

Convection–diffusion equation

$$\omega \frac{\partial c}{\partial t} - \underbrace{\operatorname{div}(\mathbf{D} \operatorname{grad} c)}_{\text{dispersion}} + \underbrace{\operatorname{div}(\mathbf{u} c)}_{\text{advection}} = f$$

- c: concentration $[\mathrm{mol/l}]$
- ω: porosity (–)
- $\mathbf{u}$ Darcy velocity $[\mathrm{m/s}]$

Dispersion tensor

$$\mathbf{D} = d_e \mathbf{I} + |\mathbf{u}|[\alpha_l \mathbf{E}(\mathbf{u}) + \alpha_t (I - \mathbf{E}(\mathbf{u}))], \quad E_{ij}(\mathbf{u}) = \frac{u_i u_j}{|\mathbf{u}|}$$

α_l, α_t dispersivity coeff. $[\mathrm{m}]$, d_e molecular diffusion $[\mathrm{m/s^2}]$

Notation: $Lc = \operatorname{div}(\mathbf{D} \operatorname{grad} c) + \operatorname{div}(\mathbf{u} c)$

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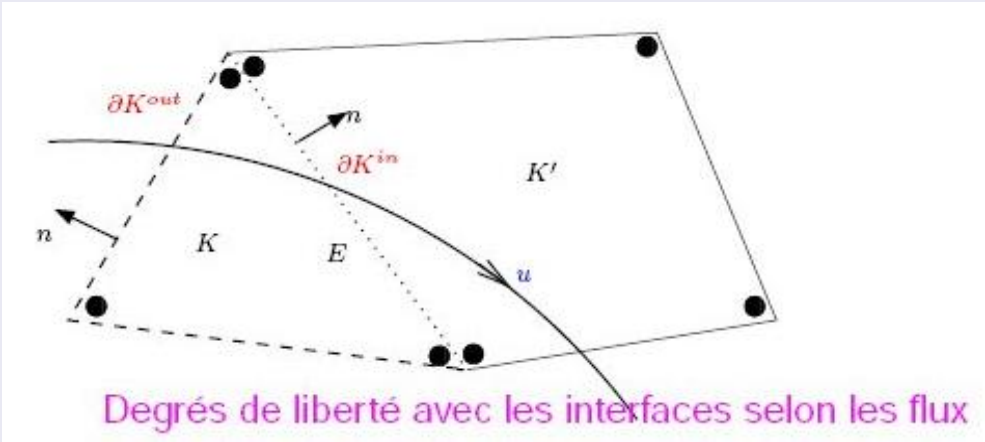
Solution by operator splitting

Advection step

Explicit, finite volumes / discontinuous Galerkine

- Locally mass conservative
- Allows unstructured meshes
- CFL condition: use sub–time–steps



Dispersion step

Like flow equation (time dependent): mixed finite elements (implicit)

See Ackerer et al., Putti et al., Arbogast et al., ...

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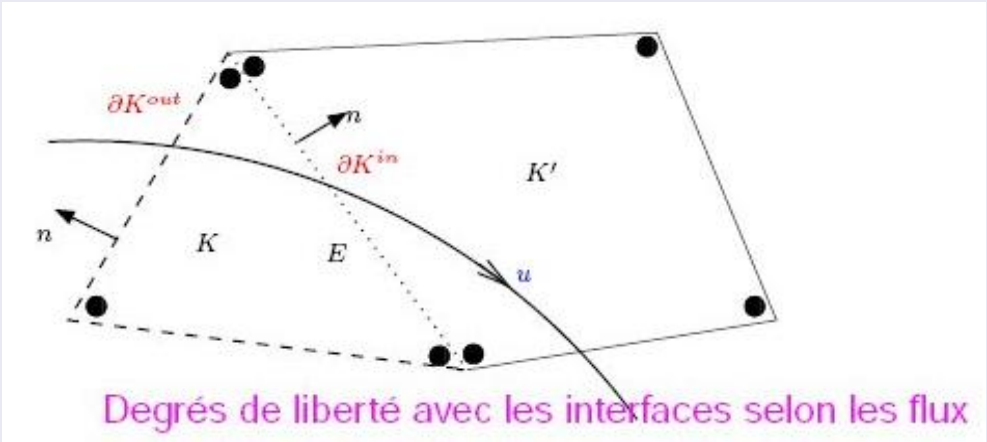


Degrés de liberté avec les interfaces selon les flux

Dispersion step

Like flow equation (time dependent): mixed finite elements (implicit)

See Ackerer et al., Putti et al., Arbogast et al., ...

Condense transport solver, one time step

$$C^{n+1} = \Psi_T(f^n, C^n)$$

Coupled problem formulationn

Benchmark formulation

$$\begin{cases} \dfrac{C^{n+1} - C^n}{\Delta t} + \dfrac{F^{n+1} - F^n}{\Delta t} + L(C^{n+1}) = 0 \\ T^{n+1} = C^{n+1} + F^{n+1} \\ F^{n+1} = \Psi_C(T^{n+1}) \end{cases}$$

Other formulations: see other MS speakers, Valocchi et al., Saaltink et al., ...

Equivalent form

$$\begin{cases} C^{n+1} = \Psi_T\left(\dfrac{F^{n+1} - F^n}{\Delta t}, C^n\right) \\ T^{n+1} = C^{n+1} + F^{n+1} \\ F^{n+1} = \Psi_C(T^{n+1}) \end{cases}$$

Decoupling of transport and chemistry modules

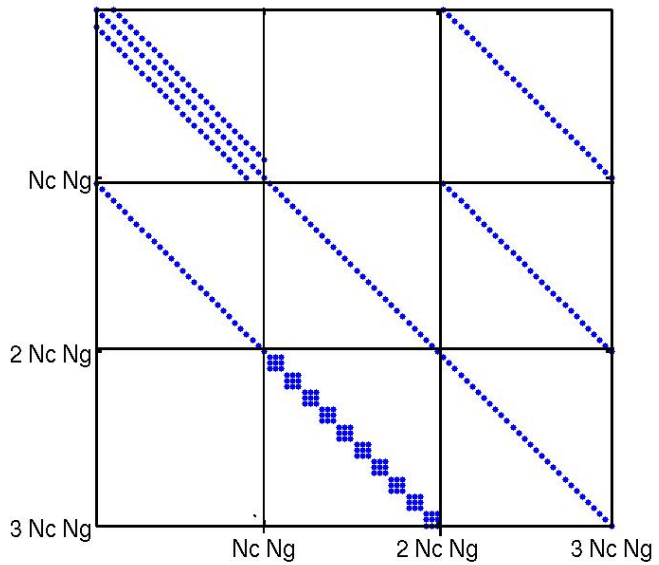
Coupled problem (2)

Solution by block Gauss–Seidel (fixed point) or by Newton–Krylov : keep transport and chemistry as black–boxes (up to Jacobian computation)

Residual computation:

1. Apply Ψ_T : solve transport for each species,
2. Apply Ψ_C: solve chemistry for each grid cell.

Jacobian structure



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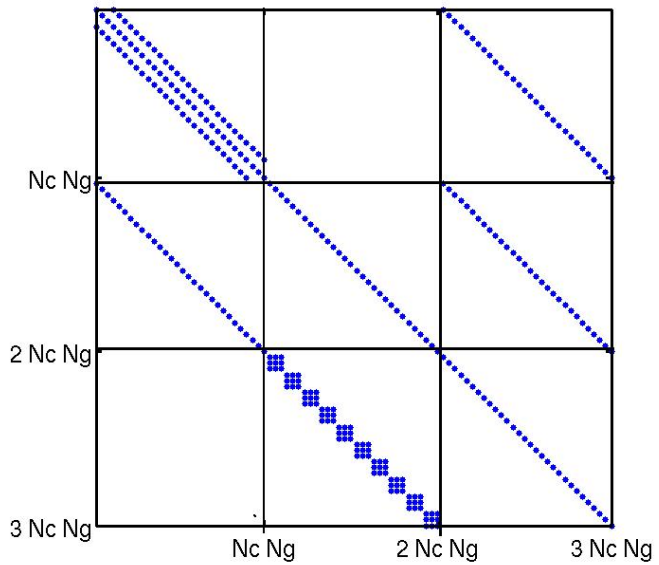

Alternative formulation

Eliminate T, C

$$F^{n+1} = \Psi_C \left(F^{n+1} + \Psi_T \left(\frac{F^{n+1} - F^n}{\Delta t}, C^n \right) \right)$$

Newton Krylov method

- Solve the linear system by an iterative method
- GMRES, TFQMR and BiCGStab require only jacobian matrix by vector products.
  Can be computed by blocks for transport and chemistry separately

Newton Krylov method

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  Can be computed by blocks for transport and chemistry separately

Inexact Newton

- Approximation of the Newton's direction:

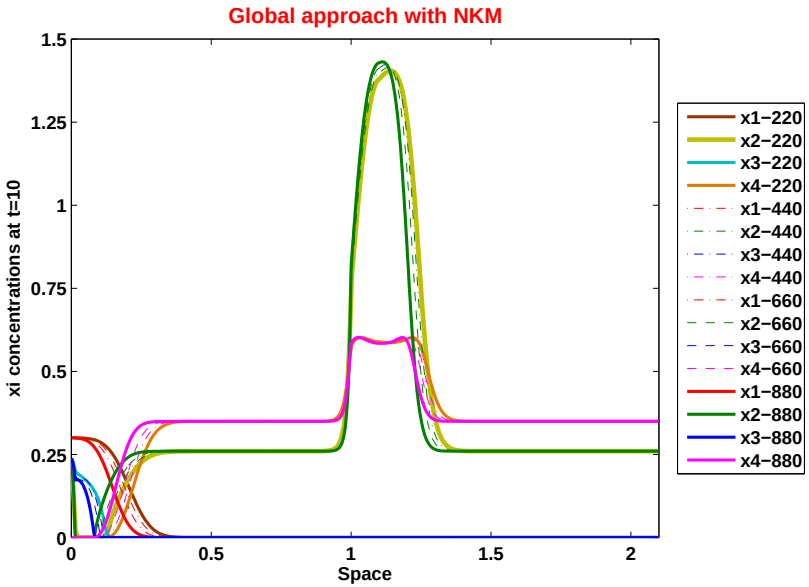
  $$\|f'(x_k)d + f(x_k)\| \leq \eta \|f(x_k)\| \quad (0<\eta<1)$$

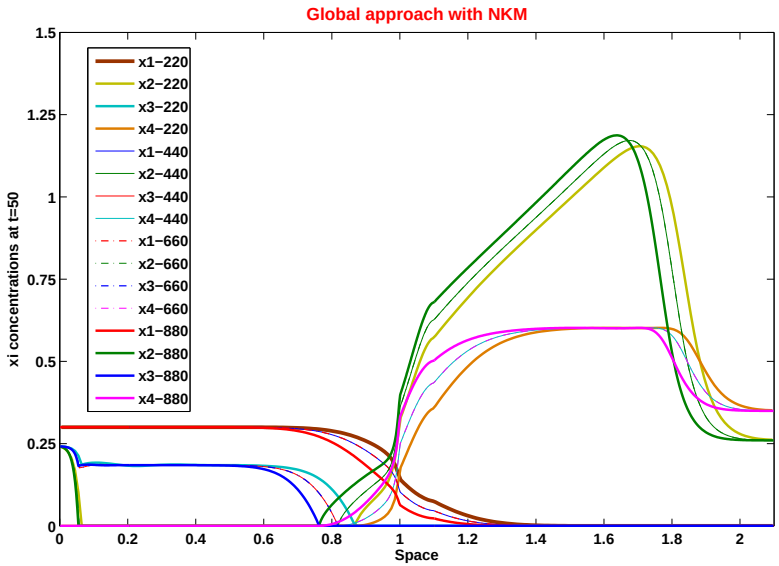
- Choice of the forcing term η?
  - Keep quadratic convergence (locally)
  - Avoid oversolving the linear system
- $\eta = \gamma \|f(x_k)\|^2 / \|f(x_{k-1})\|^2$ (Kelley, Eisenstat and Walker)

Plan

MoMaS Benchmark: easy, 1D, advective case

- 4 aqueous, 1 sorbed primary, 5 aqueous, 2 sorbed secondary species.
- Huge variation in equilibrium constants, large stoichiometric coeffs.
- Long simulation time



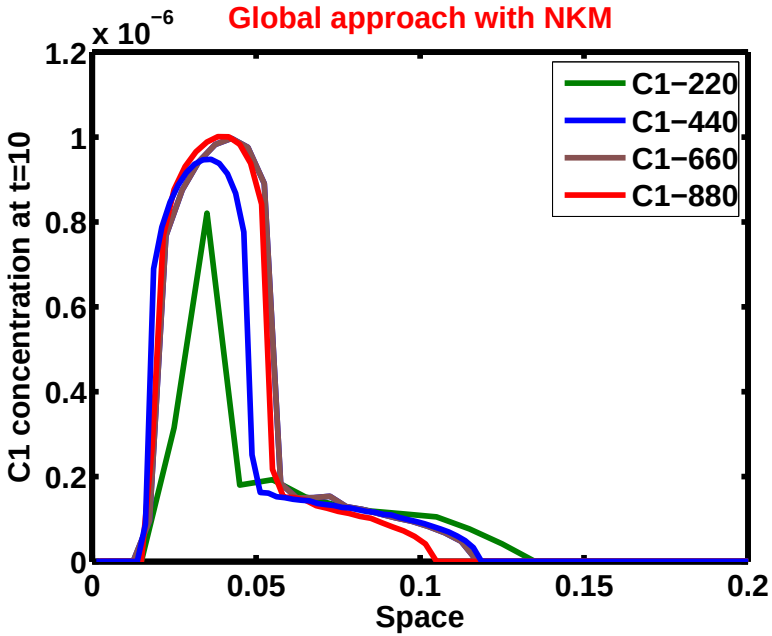


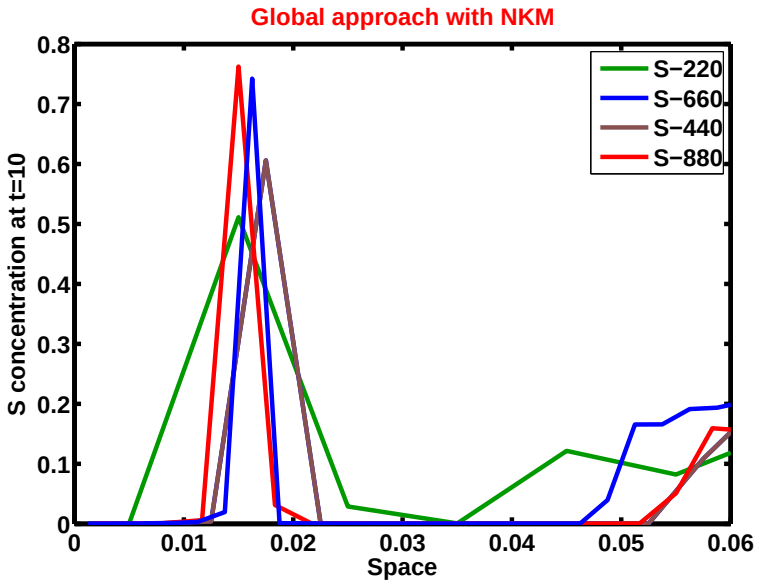
Snapshots of components concentrations. Left $t = 10$, right $t = 50$

Laila Amir's thesis (December '08).

MoMaS benchmark (2)

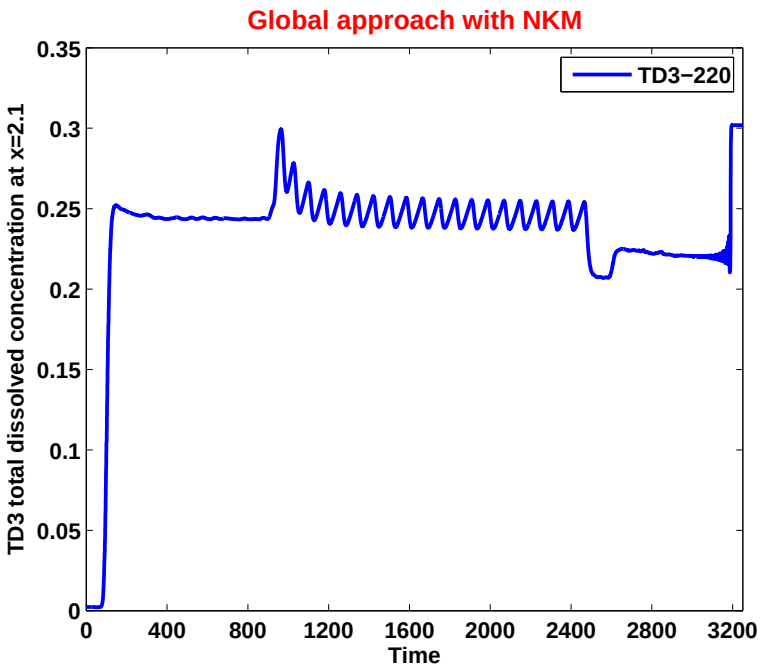
Mesh dependence

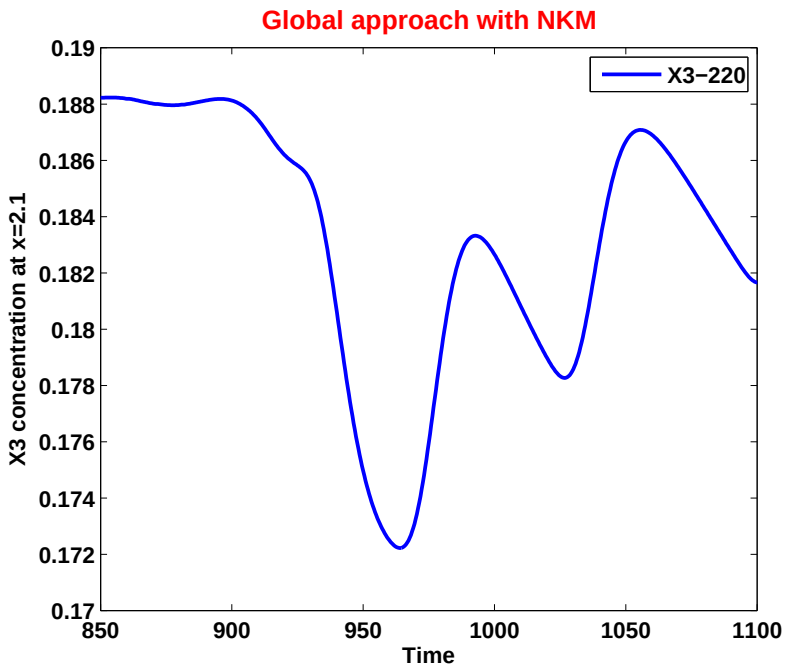




	220 points		440 points		660 points	
Step	Non lin	lin	Non lin	lin	Non lin	lin
101	18	377	22	682	25	814
103	25	494	18	551	25	636
105	15	426	22	583	21	741

MoMaS benchmark (3)





Oscillations due to discretization (cf V. Lagneau)

Plan

A simpler system

Key issue for Newton–Krylov is preconditioning

Single species with sorption

Conservation law $\omega \partial_t u + \omega \partial_t v + Lu = 0 \quad \text{in } \Omega \times (0, T)$

Sorption models $v = \psi(u)$, ψ known explicitely

Linear isotherm $\psi(u) = k_f u$

Langmuir isotherm $v = \psi(u) = \dfrac{k_f \sigma_0 u}{k_f u + k_b},$

Freundlich isotherm $\psi(u) = k_f u^p, \quad p < 1.$

Alternative formulations

Coupled system

$$F\begin{pmatrix}\mathbf{u}\\ \mathbf{v}\end{pmatrix} = \begin{pmatrix}(\mathbf{M}+\Delta t\,\mathbf{L})\mathbf{u}+\mathbf{M}\mathbf{v}-\mathbf{b}^n\\ \mathbf{v}-\Psi(\mathbf{u})\end{pmatrix}$$

Jacobian $J = \begin{pmatrix}\mathbf{M}+\Delta t\,\mathbf{L} & \mathbf{M}\\ -\mathbf{D} & 0\end{pmatrix} = I - \Delta t\, J_T + J_T,$

$\mathbf{D} = \mathrm{diag}(\psi'(u_1),\ldots,\psi'(u_N))$.

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$\mathbf{D} = \mathrm{diag}(\psi'(u_1),\ldots,\psi'(u_N))$.

Elimination of u

$$F_2(\mathbf{v}) = \mathbf{v} - \Psi((\mathbf{M}+\Delta t\,\mathbf{L})^{-1}(\mathbf{b}^n - \mathbf{M}\mathbf{v}))$$

Schur complement of coupled system

Jacobian $J_2 = I + \mathbf{D}\left(\mathbf{M}+\Delta t\,\mathbf{L}\right)^{-1})\,\mathbf{M}$

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Preconditioners for coupled system

Block Jacobi

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

Solve transport at each step

Preconditioners for coupled system

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Block Gauss–Seidel preconditioner

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Solve transport at each step, some coupling

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Block Gauss–Seidel preconditioner

$$\mathbf{P} = \begin{pmatrix} \mathbf{M} + \Delta t\, \mathbf{L} & 0 \\ -\mathbf{D} & \mathbf{I} \end{pmatrix}$$

Solve transport at each step, some coupling

Physics based preconditioner

$$\mathbf{P} = (I - \Delta t\, J_T)(I + J_C),$$

Operator splitting, $O(\Delta t)$ error

Numerical results

Geometry of MoMaS benchmark, $T = 200$, $\Delta t = 1.$, $K_L = 0.25$, $\sigma = 1.$

LifeV C++ library (EPFL, INRIA), and Kinsol (LLNL) nonlinear solver.

Cemracs 2008, J. B. Apoung-Kamga, P. Havé, J. Houot, M. K., A. Semin.
Kinsol interface by A. Taakili

Solver behavior as function of K_L

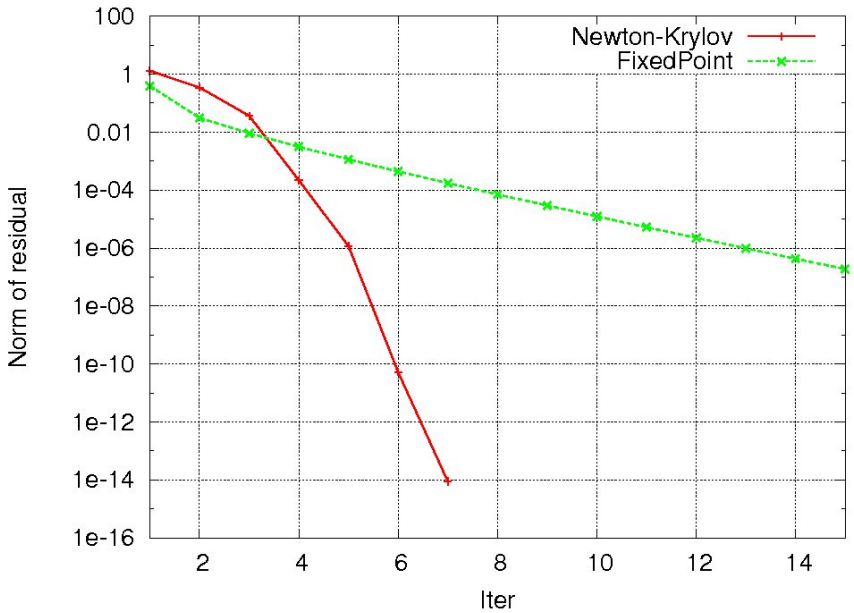
	$K_L = 0.25$			$K_L = 1.0$			$K_L = 2.5$		
PC	NNI	NLI	RT	NNI	NLI	RT	NNI	NLI	RT
None	13	218	85	27	315	130	50	770	317
BJ	9	21	16	23	84	53	46	259	150
BGS	9	12	12	24	49	41	46	139	106
OS	9	12	15	24	49	54	46	138	140

NNI Nonlinear iterations

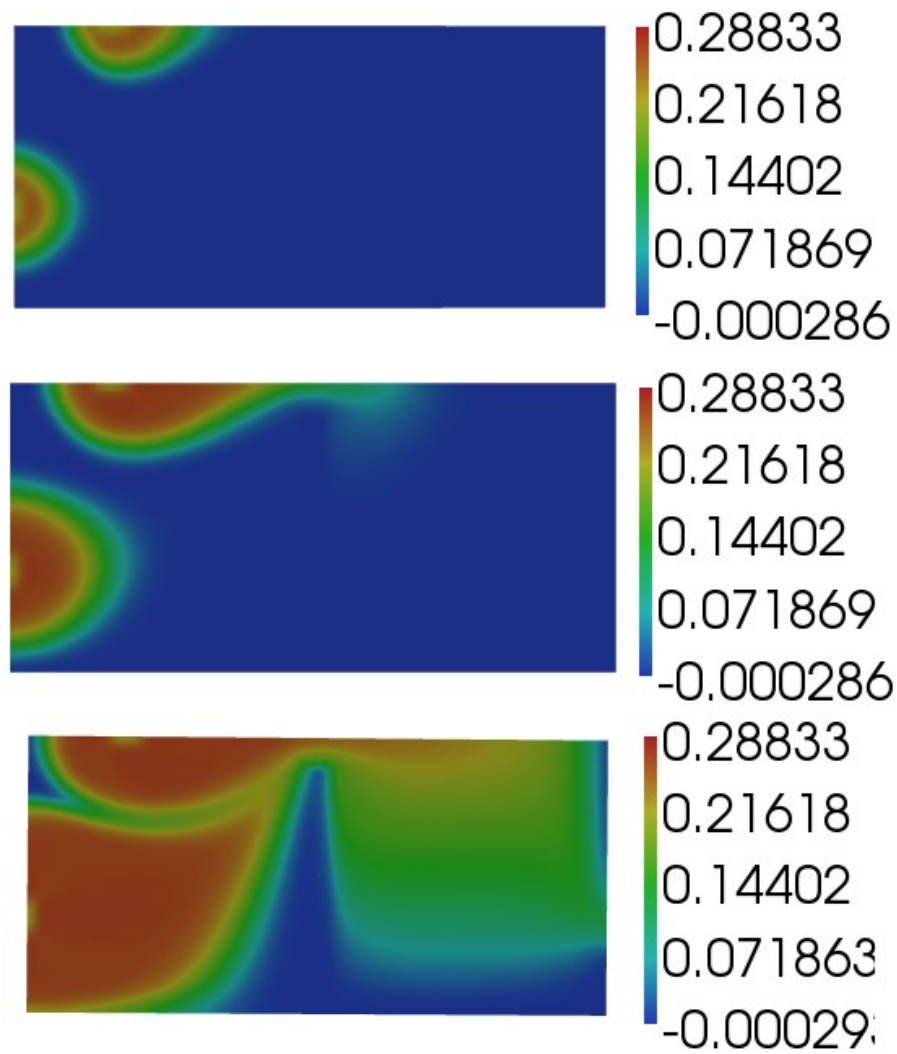
NLI Linear (inner) iterations

RT Run time (Matlab, 1D)

Numerical results



Convergence of Newton and fixed point



Preconditioner performance: mesh dependence

Mesh dependence for coupled formulation

Mesh/PC	h		$h/2$		$h/4$		$h/8$	
	NNI	NLI	NNI	NLI	NNI	NLI	NNI	NLI
None	8	54	10	100	17	238	33	658
BJ	8	22	9	26	13	38	20	62
BGS	8	11	10	15	14	22	21	36
OS	8	11	10	15	14	22	21	26

Good performance of BGS, dependence on mesh ?

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Mesh dependence for **v** formulation

Mesh	h	$h/2$	$h/4$	$h/8$	$h/16$	$h/32$
NNI	6	6	6	6	6	6
NLI	25	25	25	25	26	26

The behavior of the solver is independant of mesh

Plan

Conclusions – perspectives

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- Global formulation for equilibrium reactive transport, enabling software decoupling
- Preliminary results on MoMaS benchmark
- Comparison of precondiioners for one species sorption model

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Perspectives

- Implement Newton–Krylov for 2D/3D platform
- Fully solve MoMaS benchmark
- Extension to mixed equilibrium – kinetics models
- Further analysis of preconditioners (eigenvalues of Jacobian)