Multigrid preconditioning for nonlinear (degenerate) parabolic equations with application to monument degradation

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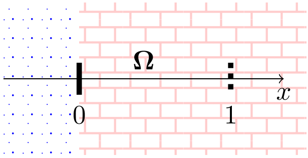
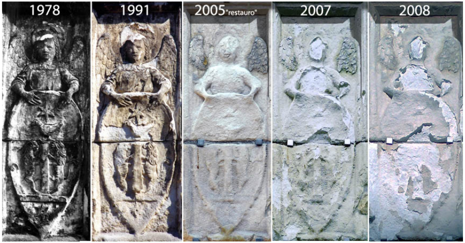
ENUMATH2013
Losanna, 26-30 August 2013

Outline

1. Marble sulfation $\Rightarrow \partial_t u = \nabla \cdot (D(u)\nabla u)$
2. Implicit discretization in time and finite differences in space
3. Uniform grids (spectral analysis of the Jacobian matrix, etc.)
4. Marble sulfation
5. Nonuniform grids
6. Future work

Marble sulfation model



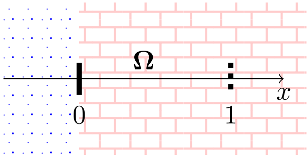


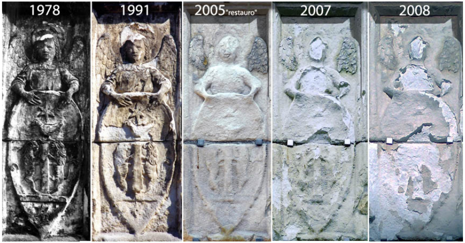
- $c(t, \mathbf{x})$ concentration of $\mathrm{CaCO_3}$, $c(0, \mathbf{x}) = c_0$
- $s(t, \mathbf{x})$ concentration of $\mathrm{SO_2}$, $s(0, \mathbf{x}) = 0$

Porosity: $\varphi(c) = \alpha c + \beta$, with $\alpha, \beta > 0$

B.C.: Dirichlet for $\mathrm{SO_2}$ at $x = 0$, free-flow at $x = 1$

Marble sulfation model





$$\begin{cases} \partial_t \varphi(c)s & = -\frac{a}{m_c}\varphi(c)sc + d\nabla \cdot (\varphi(c)\nabla s) \\ \partial_t c & = -\frac{a}{m_s}\varphi(c)sc \end{cases}$$

- $c(t, \mathbf{x})$ concentration of $\mathrm{CaCO_3}$, $c(0, \mathbf{x}) = c_0$
- $s(t, \mathbf{x})$ concentration of $\mathrm{SO_2}$, $s(0, \mathbf{x}) = 0$

Porosity: $\varphi(c) = \alpha c + \beta$, with $\alpha, \beta > 0$
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Model problem

We first consider a single equation of the form

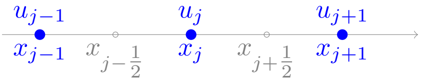
$$\partial_t u = \nabla \cdot (D(u)\nabla u)\,,$$

where $D(u)$ is a nonnegative function.
($D(u)$ differentiable and $D'(u)$ is Lipschitz continuous for convergence . . .)

Space discretization by finite differences

1. Uniform grid
2. Nonuniform grid under the assumption that the grid points can be seen as the image of a uniform grid via an invertible function.

1D finite difference discretization



$$\frac{\partial}{\partial x}\left(D(u(x))\frac{\partial u(x)}{\partial x}\right) \simeq \frac{D(u(x))\frac{\partial u}{\partial x}\Big|_{x_{j+1/2}} - D(u(x))\frac{\partial u}{\partial x}\Big|_{x_{j-1/2}}}{h}$$

$$\simeq \frac{D_{j+1/2}(u_{j+1}-u_j) - D_{j-1/2}(u_j - u_{j-1})}{h^2}$$

where $D_{j+1/2} = \dfrac{D(u_{j+1}) + D(u_j)}{2} = D(u(x_{j+1/2})) + O(h^2)$.

Thus the $N \times N$ matrix of the spatial operator is

$$L_{D(\mathbf{u})} = \mathrm{tridiag}_k^N[D_{k-1/2}(u), -D_{k-1/2}(u) - D_{k+1/2}(u), D_{k+1/2}(u)]$$

θ-method

Discretizing in time by the θ-method

$$\mathbf{u}^n - \mathbf{u}^{n-1} = \theta \frac{\Delta t}{h^2} L_{D(\mathbf{u}^n)} \mathbf{u}^n + (1-\theta) \frac{\Delta t}{h^2} L_{D(\mathbf{u}^{n-1})} \mathbf{u}^{n-1}$$

For $\theta > 0$ (e.g., Eulero, Crank-Nicolson), it holds $F(\mathbf{u}^n) = 0$ where

$$F(\mathbf{u}) = \mathbf{u} - \theta \tfrac{\Delta t}{h^2} L_{D(\mathbf{u})} \mathbf{u} - (1-\theta) \tfrac{\Delta t}{h^2} L_{D(\mathbf{u}^{n-1})} \mathbf{u}^{n-1} - \mathbf{u}^{n-1}$$

Jacobian matrix

$$F(\mathbf{u}) = \mathbf{u} - \theta\frac{\Delta t}{h^2}L_{D(\mathbf{u})}\mathbf{u} - (1-\theta)\frac{\Delta t}{h^2}L_{D(\mathbf{u}^{n-1})}\mathbf{u}^{n-1} - \mathbf{u}^{n-1}$$

where the Jacobian matrix is

$$F'(\mathbf{u}) = \underbrace{I_N - \theta\frac{\Delta t}{h^2}L_{D(\mathbf{u})}}_{X_N} + Y_N$$

$$X_N(\mathbf{u}) = \text{s.p.d.}$$

$$Y_N(\mathbf{u}) = -\theta\frac{\Delta t}{h^2}T_N(\mathbf{u})\,\text{diag}_k^N(D_k')$$

$$T_N(\mathbf{u}) = \text{tridiag}_k^N[u_{k-1}-u_k,\, u_{k-1}-2u_k+u_{k+1},\, u_{k+1}-u_k]$$

$$= \text{tridiag}_k^N[O(h), O(h^2), O(h)]$$

Newton method

Theorem (D., Semplice, Serra-Capizzano – SIMAX(2011))

If $\mathbf{u}$ *is the sampling of a solution of* $\partial_t u = \partial_x(D(u)\partial_x u)$*, with* D' *and* u' *Lipschitz. Then* $\exists\, C_1 > 0$ *independent of* h *s.t.*

$$\left\| F'(\mathbf{u})^{-1} \right\|_\infty \leq C_1 \tag{1}$$

if $\Delta t \leq C_\infty h$ *for a constant* $C_\infty > 0$*.*

Combining the previous result with Kantorovich theorem it follows

Theorem (D., Semplice, Serra-Capizzano – SIMAX(2011))

The Newton method for computing $\mathbf{u}^{(n)}$ *converges if* $\Delta t = O(h)$ *and* $\mathbf{u}^{(0)} = \mathbf{u}^{n-1}$*.*

Spectral analysis of the Jacobian matrix [SIMAX, 2011]

For the Jacobian matrix

$$F'(\mathbf{u}) = \underbrace{I_N - \theta\frac{\Delta t}{h^2}L_{D(\mathbf{u})}}_{X_N} + Y_N$$

If u is Lipschitz, $\|Y_N(\mathbf{u})\|_2 \leq C\frac{\Delta t}{h}\|D'\|_\infty$, thus if $\Delta t = O(h)$,

Y_N is negligible with respect to X_N:

$$\|Y_N(\mathbf{u})\|_2 = O(1) \text{ while } \|X_N\|_2 = O(\tfrac{1}{h}).$$

Spectrum of F'

$$\kappa_2(F') = O(N) \qquad \Sigma(F') \subset [c, CN] \times i[-d, d]$$

Spectral distribution

$$\{A_N\} \sim_\lambda (\theta, G)$$

where θ is a measurable function on $G \subset \mathbb{R}^d$, if

$$\forall F \in \mathcal{C}_0(\mathbb{C}) : \lim_{N\to\infty} \frac{1}{N} \sum_{1}^{N} F(\lambda_j(A_N)) = \frac{1}{\mu(G)} \int_G F(\theta(t))\mathrm{d}t$$

Eigenvalue cluster

If $\{A_N\} \sim_\lambda (\theta = c = \text{const}, G)$, then it is *weakly clustered* at c, i.e.

$$\#\{\lambda_j(A_N) : \lambda_j \notin D(c,\varepsilon)\} = o(N), \qquad \forall\varepsilon > 0.$$

The cluster is *strong* if $o(N) = O(1)$.

Spectral distribution of F'

$$A_N = hF' = -L_{D(\mathbf{u})} + R_N(\mathbf{u})$$

$$\begin{aligned}\{A_N\} &\sim_\lambda (\theta, \Omega \times [0, 2\pi]) \\ \theta(x, s) &= D(u(x))(2 - 2\cos(s))\end{aligned}$$

and Ω is the domain of the PDE.

The negligible term $R_N = hI_N + hY_N$

$$\{R_N\} \sim_\lambda (0, G)$$

$$\left\{\frac{R_N}{h}\right\} \sim_\lambda \left(1 - D'(u(x))2i\sin(s)\,,\ \Omega \times [0, 2\pi]\right)$$

Multigrid Preconditioner

Preconditioner

$$P_N = -L_{D(\mathbf{u})} + hI_N,$$

$$\Sigma(P_N^{-1}A_N) \subset [1 - c_1 h,\ 1 + c_2 h] \times i[-d,\ d].$$

with c_1, c_2, and d independents of N.

Multigrid

Classical geometric multigrid (V-cycle with bilinear interpolation) with a standard smoother (Gauss-Seidel) is an optimal solver for P_N.

A robust and efficient solver for a linear system with the Jacobian matrix is GMRES with a V-cycle iteration as preconditioner.

2D case

$$\{A_N\} \sim_\lambda (\theta, \Omega \times [0,2\pi] \times [0,2\pi])$$

$$\theta = D(u(x,y))(2-2\cos(s))(2-2\cos(t))$$

- The Jacobian matrix has not a tensor product structure but they share the same sparsity pattern.
- All results about convergence of the Newton method, spectral estimation and preconditioning hold similarly to the 1D case...

Numerical example

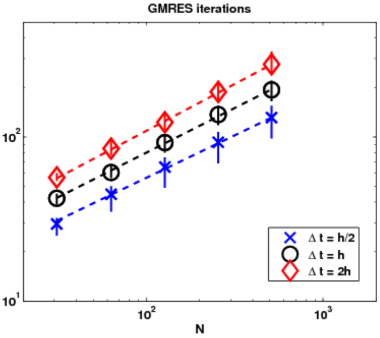
Example

- Test problem: $D(u) = 4u^3$
- $\Omega \subset \mathbb{R}^2$
- 3 choices of Δt

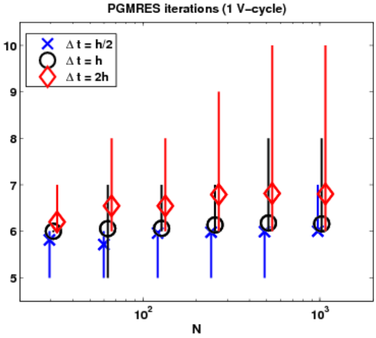
Results

- Newton converges always within 3–7 iterations (4–5 iterations for $\Delta t = h$).
- Number of GMRES iterations without preconditioning $O(\sqrt{1/h})$

Numerical example



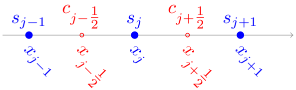
(a)



(b)

Average, min, and max number of iterations of
(a) GMRES without preconditioning
(b) GMRES preconditioned with one V-cycle iteration.

Marble sulfation

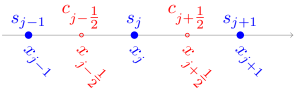


$$\partial_x(\varphi(c)\partial_x s)\big|_{x_j} = \frac{\varphi(c_{j+1/2})(s_{j+1} - s_j) - \varphi(c_{j-1/2})(s_j - s_{j-1})}{h^2}$$

$$\varphi(c)sc\big|_{x_j} = \varphi\left(\frac{c_{j-1/2}+c_{j+1/2}}{2}\right)\frac{c_{j-1/2}+c_{j+1/2}}{2}s_j$$

$$\varphi(c)sc\big|_{x_{j+1/2}} = \varphi(c_{j+1/2})c_{j+1/2}\frac{s_j+s_{j+1}}{2}$$

Marble sulfation



$$\partial_x(\varphi(c)\partial_x s)\big|_{x_j} = \frac{\varphi(c_{j+1/2})(s_{j+1}-s_j) - \varphi(c_{j-1/2})(s_j - s_{j-1})}{h^2}$$

$$\varphi(c)sc\big|_{x_j} = \varphi\left(\frac{c_{j-1/2}+c_{j+1/2}}{2}\right)\frac{c_{j-1/2}+c_{j+1/2}}{2}s_j$$

$$\varphi(c)sc\big|_{x_{j+1/2}} = \varphi(c_{j+1/2})c_{j+1/2}\frac{s_j+s_{j+1}}{2}$$

Newton method for

$$\begin{cases} 0 = \mathbf{F}^{(s)}(\mathbf{s}^n,\mathbf{c}^n) = & \Phi^n\mathbf{s}^n + \theta\Delta t\frac{a}{m_c}C^n\mathbf{s}^n + \theta\Delta t d L_{\varphi^n}\mathbf{s}^n \\ & -\Phi^{n-1}\mathbf{s}^{n-1} + (1-\theta)\Delta t\frac{a}{m_c}C^{n-1}\mathbf{s}^{n-1} + (1-\theta)\Delta t d L_{\varphi} \\ 0 = \mathbf{F}^{(c)}(\mathbf{s}^n,\mathbf{c}^n) = & \mathbf{c}^n + \theta\Delta t\frac{a}{m_s}S^n\mathbf{c}^n - \mathbf{c}^{n-1} + (1-\theta)\Delta t\frac{a}{m_s}S^{n-1}\mathbf{c}^{n-1} \end{cases}$$

where Φ^n, C^n, S^n are diagonal matrices.

Jacobian matrix

$$\mathbf{u} = \begin{pmatrix} \mathbf{s} \\ \mathbf{c} \end{pmatrix}, \; J = F' = \left[\begin{array}{c|c} J_s^s & J_c^s \\ \hline J_s^c & J_c^c \end{array}\right], \quad [J_s^s]_{j,k} = \partial_{s_k} \mathbf{F}_j^{(s)}, \; [J_c^s]_{j,k} = \partial_{c_{k+1/2}} \mathbf{F}_j^{(s)}$$

$$J_s^s = \operatorname{diag}\left\{ \frac{\varphi_{j+1/2} + \varphi_{j-1/2}}{2} \right\} + \theta \Delta t \frac{a}{m_c} \operatorname{diag}\left\{ \frac{\varphi_{j+1/2} c_{j+1/2} + \varphi_{j-1/2} c_{j-1/2}}{2} \right\}$$
$$+ \theta \frac{d \Delta t}{h^2} \operatorname{tridiag}_j \left\{ -\varphi_{j-1/2}, \varphi_{j-1/2} + \varphi_{j+1/2}, -\varphi_{j+1/2} \right\}$$

Jacobian matrix

$$\mathbf{u} = \begin{pmatrix} \mathbf{s} \\ \mathbf{c} \end{pmatrix}, \; J = F' = \left[\begin{array}{c|c} J_s^s & J_c^s \\ \hline J_s^c & J_c^c \end{array}\right], \quad [J_s^s]_{j,k} = \partial_{s_k} \mathbf{F}_j^{(s)}, \; [J_c^s]_{j,k} = \partial_{c_{k+1/2}} \mathbf{F}_j^{(s)}$$

$$\begin{aligned} J_s^s =& \operatorname{diag}\left\{ \frac{\varphi_{j+1/2}+\varphi_{j-1/2}}{2} \right\} + \theta \Delta t \frac{a}{m_c} \operatorname{diag}\left\{ \frac{\varphi_{j+1/2} c_{j+1/2} + \varphi_{j-1/2} c_{j-1/2}}{2} \right\} \\ & + \theta \frac{d \Delta t}{h^2} \operatorname{tridiag}_j \left\{ -\varphi_{j-1/2}, \varphi_{j-1/2} + \varphi_{j+1/2}, -\varphi_{j+1/2} \right\} \\ J_c^s =& \operatorname{tridiag}\left\{ 0, \varphi'_{j+1/2} s_j, +\varphi'_{j-1/2} s_j \right\} \\ & + \theta \Delta t \frac{a}{m_c} \operatorname{tridiag}\left\{ 0, \frac{(\varphi'_{j+1/2} c_{j+1/2} + \varphi_{j+1/2})}{2}, \frac{(\varphi'_{j-1/2} c_{j-1/2} + \varphi_{j-1/2}) \delta_{j,k+1}}{2} \right\} \\ & + \theta \frac{d \Delta t}{h^2} \operatorname{tridiag}\left\{ 0, -\varphi'_{j+1/2}(s_{j+1} - s_j), \varphi'_{j-1/2}(s_j - s_{j-1}) \right\} \\ J_s^c =& \theta \Delta t \frac{a}{m_s} \operatorname{tridiag}\left\{ \varphi_{j+1/2} c_{j+1/2}, \varphi_{j+1/2} c_{j+1/2}, 0 \right\} \\ J_c^c =& \operatorname{diag}\left\{ 1 + \theta \Delta t \frac{a}{m_s} (\varphi'_{j+1/2} c_{j+1/2} + \varphi_{j+1/2}) \frac{s_{j+1} + s_j}{2} \right\} \end{aligned}$$

Block preconditioner

- J_s^c has entries that decay as $O(\Delta t)$,
- J_c^c is the identity matrix plus a diagonal matrix with $O(\Delta t)$ entries.

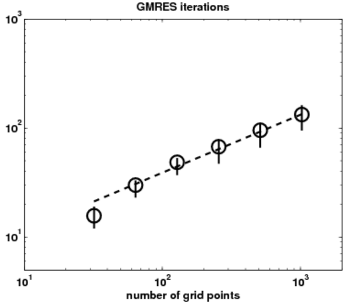
Theorem

If $\Delta t = O(h)$, the block upper triangular part of J, namely

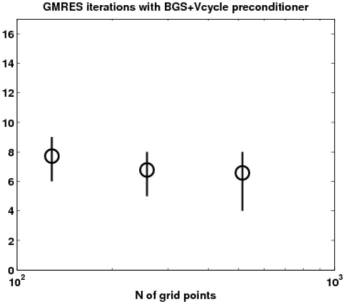
$$P = \left[\begin{array}{c|c} J_s^s & J_c^s \\ \hline \mathbf{0} & J_c^c \end{array}\right], \tag{2}$$

is an optimal preconditioner for J if $\varphi(c)$ is strictly positive (i.e., the porosity of the marble-gypsum mixture does not vanish).

Numerical results for a 2D corner



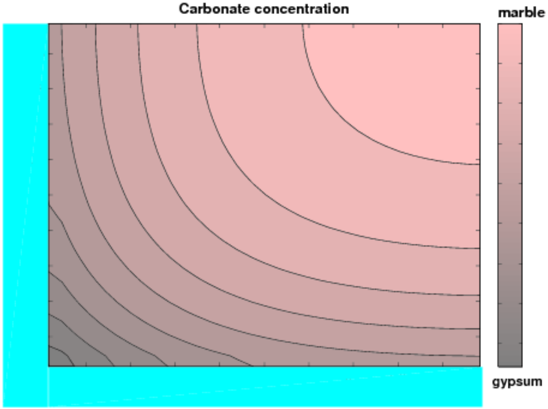
(a)



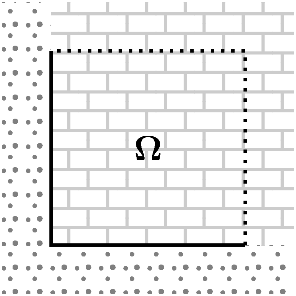
(b)

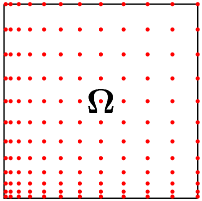
Number of iterations (average, min, and max) for
(a) GMRES without preconditioning
(b) Preconditioner P and one step of AMG for J_s^s

Numerical results for a 2D corner



A nonuniform grid can help . . .





Discretizzation on a nonuniform grid

$$\partial_x \left(D(u) \frac{\partial u}{\partial x} \right) \Big|_{x_j} \simeq \frac{D_{j+1/2} \frac{u_{j+1} - u_j}{h_{j+1}} - D_{j-1/2} \frac{u_j - u_{j-1}}{h_j}}{(h_j + h_{j+1})/2}$$

$$-L^{(1)}_{D(\mathbf{u})} = \mathrm{diag}_k^N \left[\frac{2}{h_k + h_{k+1}} \right] \mathrm{tridiag}_k^N \left[-\frac{D_{k-1/2}}{h_k}, \frac{D_{k-1/2}}{h_k} + \frac{D_{k+1/2}}{h_{k+1}}, -\frac{D_{k+1/2}}{h_{k+1}} \right]$$

Properties of $L_{D(\mathbf{u})}$

- it is not symmetric
- it can be symmetrized, by a similarity transformation, only in the 1D case.

Nonuniform grid

Consider the grid points as a map of a uniform grid

$$x_j = g(j/N), \qquad g : [0,1] \to \Omega$$

If g is piecewise C^1, the discretizzation of $\partial_x(D(x)\partial_x u)$ on the nonuniform grid is spectrally equivalent to the discretization of

$$\partial_x \left(w^D(x) \frac{\partial u}{\partial x} \right)$$

on a uniform grid, with

$$w^D(x) = \frac{D(g(x))}{[g'(x)]^2}$$

[Serra Capizzano, Tablino Possio – Lin. Alg. Appl. (2003)]

Jacobian matrix

$$F' = \underbrace{I_N - \theta \Delta t L_{w_D(\mathbf{u},g)}}_{X_N} + Y_N$$

- X_N is an M-matrix,
- Y_N is negligible with respect to X_N.

Choosing $\Delta t = \frac{1}{N}$

$\Omega \in \mathbb{R}$ $\{X_N^{-1} F'_N\} \sim_\lambda (1, G)$

$\Omega \in \mathbb{R}^2$ $\{X_N^{-1} F'_N\} \sim_\sigma (1, G)$ (singular value distribution)

It follows that the Algebraic Multigrid (AMG) is an affective preconditioner for the GMRES.

Conditioning of F'

$$\frac{1}{N}F' = \frac{1}{N}I_N - L_{w_D} + \text{negligible nonsymmetric perturbation}$$

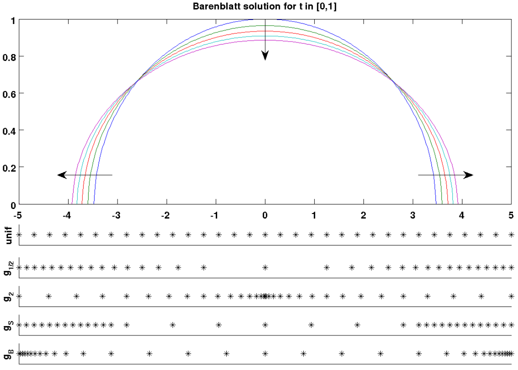
$$\{\tfrac{1}{N}F'\} \sim_\lambda \left(\theta\frac{D(g(x))}{[g'(x)]^2}(2-2\cos(s))\,,\ \Omega\times[0,2\pi]\right)$$

$\lambda_{\min} \sim \frac{1}{N}$
$\lambda_{\max}$ grows like the maximum of $\frac{D(g(x))}{[g'(x)]^2}$ and hence like N^{2q} if g' has a zero of order q where the numerator does not vanish.

$$\Rightarrow \kappa_2(F') \sim N^{2q+1}$$

Note: $g'(x)$ vanishes where the grid points accumulate.

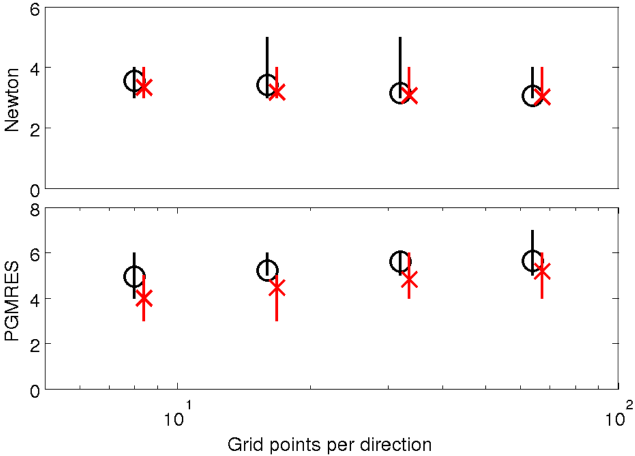
1D mesh	cond(J)	GMRES iterations no P	GMRES iterations Jac	GMRES iterations AMG	Newton iterations	GMRES CPU time no P	GMRES CPU time Jac	GMRES CPU time AMG
unif	$N^{0.97}$	$N^{0.42}$	$N^{0.47}$	2.54	2.24	1058	1892	45
Shish	$N^{1.14}$	$N^{0.46}$	$N^{0.48}$	2.73	3.00	1466	2590	93
Bakh	$N^{0.85}$	$N^{0.29}$	$N^{0.41}$	2.37	2.00	925	1821	55
$g_{1/2}$	$N^{0.94}$	$N^{0.38}$	$N^{0.44}$	2.50	2.99	1343	2194	85
g_2	$N^{3.00}$	$N^{0.76}$	$N^{0.70}$	3.47	2.01	17558	41721	86
g_3	$N^{5.00}$	$N^{0.83}$	$N^{0.78}$	3.83	2.02	n/a	159993	88



$$g_\alpha(t) = \mathtt{sign}(t)|t|^\alpha$$

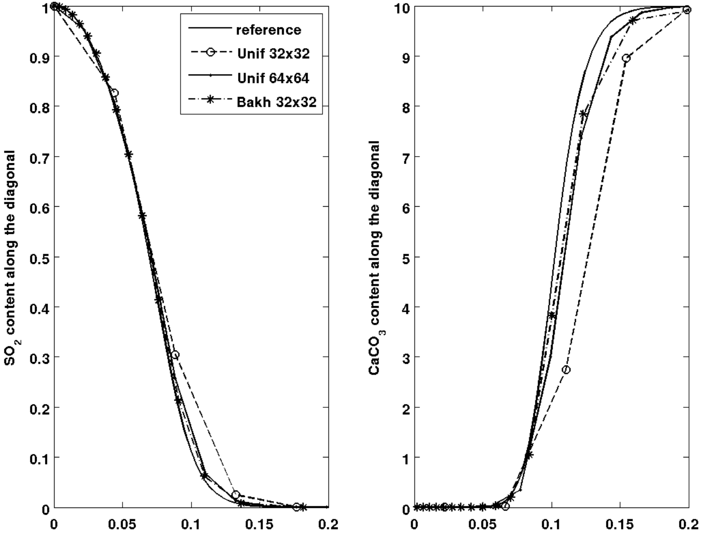
$$\partial_t = \partial_x(u^2 \partial_x u)$$

Marble sulfation



Number of iterations of Newton and PGMRES on uniform grids (red) and nonuniform grids (black).

Profile of the solution along the diagonal $x = y$



Future work

- 3D case
- Finite element discretization
- Application to 3D laser scanning of monuments (e.g., Donatello's David)
- Free boundary models of marble sulfation (the computational domain enlarges with the time)

References

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- M. Semplice Preconditioned implicit solvers for nonlinear PDEs in monument conservation SIAM J. Sci. Comp. 32 (2010) 3071–3091
- M. Donatelli, M. Semplice, S. Serra-Capizzano AMG preconditioning for nonlinear degenerate parabolic equations on nonuniform grids with application to monument degradation Appl. Numer. Math. 68 (2013) 1–18