Report on results of SGS project Preconditioning of time-dependent and non-symmetric problems with guaranteed spectral bounds (SGS24/001/OHK1/1T/11)

Part II – Corrosion-driven damage

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January 2, 2025

This is a report on the results of the project Preconditioning of time-dependent and non-symmetric problems with guaranteed spectral bounds solved in 2024 and supported by the SGS grant under the No. SGS24/001/OHK1/1T/11. There are two main fields of results in this report: wave propagation in elastic heterogeneous media (Part I) and a coupled problem of elasticity and erosion Part II). In both parts we apply the fast Fourier transformation (FFT) based preconditioning and study its efficiency and spectral bound of the preconditioned matrices.

1 Preconditioning of corrosion-driven fracture in porous media

We study preconditioning of a sequence of problems representing a corrosion-driven damage in a heterogeneous elastic material. The problem is motivated by [1].

1.1 Description of the problem

In this part we describe the problem of a damage of ellastic material caused by a chemical reaction (corrosion) which is motivated by [2]. In this part, we only describe the computational process. We do not consider the FFT issues yet, but pay attention only to the particular problems and to their mathematical representation and discretization.

We consider a rectangular domain $\Omega = \Omega_{\text{pore}} \cup \Omega_{\text{solid}} \subset \mathbb{R}^2$ where Ω_{pore} represents pores filled with water and Ω_{solid} represents a solid material. We set $\Omega = (0, L)^2$ where $L = 1$ (1 millimeter) is the length of the edge (not $L = 0.001$).

Diffusion of ions. The first part of the problem is to find concentration of ions $c(x)$, $x \in \Omega$, fulfilling

$$\nabla \cdot (D \cdot \nabla c(x)) = 0 \tag{1}$$

such that

$$\int_{\Omega} \nabla c(x) dx = |\Omega| \, \nabla c_{\text{mac}},$$

where ∇c_{mac} is a prescribed constant macroscopic overall concentration gradient. It is recommended to use $\nabla c_{\text{mac}} = (10^{-5}, 10^{-5})$. The diffusion tensor D is defined as

$$D(x) = \omega(x) D_{\text{solid}} I + (1 - \omega(x)) D_{\text{pore}} I,$$

where $\omega(x) = 1$ for $x \in \Omega_{\text{solid}}$ and $\omega(x) = 0$ for $x \in \Omega_{\text{pore}}$. It is recommended to use $D_{\text{solid}} = 10^{-6}$ and $D_{\text{pore}} = 1$. Since $\nabla c(x)$ satisfies the periodic boundary condition, the weak form of (1) reads

$$\int_{\Omega} \nabla v(x) \cdot D(x) \nabla c(x) \, dx = 0 \tag{2}$$

for all $v \in H^1_{\mathrm{per}}(\Omega)$. The concentration gradient is expressed as

$$\nabla c(x) = \nabla c_{\mathrm{mac}} + \nabla \phi(x), \tag{3}$$

where ϕ is a periodic fluctuation of the concentration gradient of ions and thus $\int_\Omega \phi \, dx = 0$; see [2, formula (8)]. This means that (2) becomes

$$\int_\Omega \nabla v(x) \cdot D(x) \nabla \phi(x) \, dx = -\int_\Omega \nabla v(x) \cdot D(x) \nabla c_{\mathrm{mac}} \, dx. \tag{4}$$

From (3) we get

$$c(x) = \nabla c_{\mathrm{mac}} \cdot x + \phi(x) + \beta,$$

where β is piece-wise constant as β_{pore} and β_{solid}, see [2]. Two conditions are to be fulfilled:

$$\frac{1}{|\Omega_{\mathrm{solid}}|} \int_\Omega c(x) \, dx = 0 \qquad \text{and} \qquad \frac{1}{|\Omega_{\mathrm{pore}}|} \int_\Omega c(x) \, dx = \frac{|\Omega|}{|\Omega_{\mathrm{pore}}|} c_{\mathrm{mac}}. \tag{5}$$

From (5) we get

$$\beta_{\mathrm{solid}} = \frac{-1}{|\Omega_{\mathrm{solid}}|} \int_{\Omega_{\mathrm{solid}}} \nabla c_{\mathrm{mac}} \cdot x + \phi(x) \, dx$$

$$\beta_{\mathrm{pore}} = \frac{|\Omega|}{|\Omega_{\mathrm{pore}}|} c_{\mathrm{mac}} - \frac{1}{|\Omega_{\mathrm{ore}}|} \int_{\Omega_{\mathrm{pore}}} \nabla c_{\mathrm{mac}} \cdot x + \phi(x) \, dx.$$

As a result, concentration of ions within the pores is

$$c(x) = \nabla c_{\mathrm{mac}} \cdot x + \phi(x) + \frac{|\Omega|}{|\Omega_{\mathrm{pore}}|} c_{\mathrm{mac}} - \frac{1}{|\Omega_{\mathrm{ore}}|} \int_{\Omega_{\mathrm{pore}}} \nabla c_{\mathrm{mac}} \cdot x + \phi(x) \, dx, \quad x \in \Omega_{\mathrm{pore}}.$$

(It is an open question for now, how we can obtain c_{mac}. The only information we have is ∇c_{mac}. Then it can be $c_{\mathrm{mac}} = \nabla c_{\mathrm{mac}} \cdot x + \widetilde{c}$, where $\widetilde{c} \in \mathbb{R}$. Then it is not clear enough why in [2, formula (12)] the authors use both terms "$\nabla c_{\mathrm{mac}} \cdot x$" and "$c_{\mathrm{mac}}$".) In our computation, we set $c_{\mathrm{mac}} = 2 \cdot 10^{-5}$.

We obtain

$$\int_\Omega \beta \, dx = |\Omega| \, c_{\mathrm{mac}} - \int_\Omega \nabla c_{\mathrm{mac}} \cdot x \, dx - \int_\Omega \phi(x) \, dx. \tag{6}$$

From [2, text after formula (12)] we have

$$\int_\Omega \beta \, dx = 0 \tag{7}$$

$$\int_\Omega \phi(x) \, dx = 0 \tag{8}$$

$$\frac{1}{|\Omega|} \int_\Omega c(x) \, dx = c_{\mathrm{mac}}. \tag{9}$$

Formula (9) is obtained from (5). (From (9) we get that c_{mac} is constant. But it is in a contradiction with the assumption that ∇c_{mac} is a given constant macroscopic gradient.) Formula (8) can be obtained because of the pseudo-inversion of the system matrix. In other words, the system is solvable but not uniquely. The uniqueness is achieved, for example, by requiring (8). (Finally, it is not clear where (7) comes from in [2].) Despite of some insufficient clarity in [2], we can introduce the following example where the main computational issues are used.

Example 1.1.1 *In this example, we consider $\Omega = (0,1)^2$, $\nabla c_{\mathrm{mac}} = (0,1)$, $D_{\mathrm{solid}} = 10^{-3}$, $D_{\mathrm{pore}} = 1$, $N_1 = N_2 = 36$. In Figure 1, the local concentration of ions is graphically displayed.*
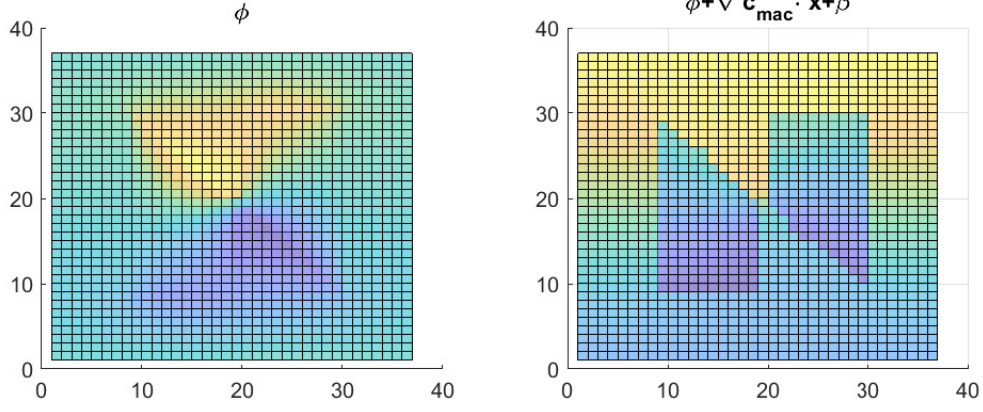
Figure 1: Numerical results of Example 1.1.1.

Strain computation. After obtaining the concentration $c(x)$, $x \in \Omega$, we determine the pressurization of pores due to the expansion of the corrosion products. We calculate an isotropic eigenstrain

$$\varepsilon_{\mathrm{eig}} = (c(x)M_{\mathrm{ppt}} - 1)_+ I$$

where M_{ppt} is the molar volume of the precipitate (probably not defined in [2]) and the sign $+$ means that we take only the positive part of it.

We can summarize the choice of some constant from [2]:

```
threshold_concentration = 1e-9
molar_masss = 89
density = 3.4e-3
cell_volume = h1*h2
precipitation = concentration - threshold_concentration
moles_precitipation = precipitation*cell_volume
volume_precipitation = moles_precitipation*molar_mass/density
eigen_strain = (volume_precipitation-)/cell_volume ... zero if negative, or solid
precipitate_fraction = abs(volume_precipitation)/cell_volume ... max 0.9, 0 for pores
porosity_reduction =  1-precipitate_fraction .. 1 for pores
```

We note that the numerical results are very sensitive with respect to the choice of these constants.

Then the stress development is computed. We assume an overall constant macroscopic strain $\varepsilon_{\mathrm{mac}}$. It is recommended to use $E = 10$ and $\nu = 0.2$ for solid and $E = 1$ and $\nu = 0.45$ for pores. The stiffness tensor is

$$C(x) = \omega(x)C_{\mathrm{solid}} + (1 - \omega(x))C_{\mathrm{pore}}.$$

We solve the equation

$$\nabla_s C : (\varepsilon(x) - \varepsilon_{\mathrm{eig}}(x)) = 0, \qquad \frac{1}{|\Omega|}\int_\Omega \varepsilon(x)\, dx = \varepsilon_{\mathrm{mac}}$$

which can be expressed in the weak form with $\varepsilon(x) = \psi(x) + \varepsilon_{\mathrm{mac}}(x)$

$$\int_\Omega \nabla_s v(x) : C(x) : \psi(x)\, dx = \int_\Omega \nabla_s v(x) : C(x) : (\varepsilon_{\mathrm{eig}}(x) - \varepsilon_{\mathrm{mac}}(x))\, dx. \tag{10}$$

Damage computation. Finally, crack initiation and propagation is computed. First we compute the positive part of the strain energy density

$$\psi^+ = \frac{1}{2}(\lambda + \mu)[\mathrm{tr}(\varepsilon)]_+^2 + \mu(\varepsilon^{\mathrm{dev}} : \varepsilon^{\mathrm{dev}}),$$

3

where $[*]_+ = (* + \| * \|)/2$ and $\varepsilon^{\text{dev}} = \varepsilon - \text{tr}(\varepsilon)I/2$. The history field $H^+(x,T) = \max_{t \in (0,T)} \psi^+(x,t)$. Then we compute damage $\widetilde{d}$ from the weak formulation

$$\frac{G_c l_0}{2} \int_\Omega \nabla \widetilde{d} \nabla v \, dx dx + (\frac{G_c}{2l_0} + H^+) \int_\Omega \widetilde{d} v \, dx = \int_\Omega H^+ v \, dx. \tag{11}$$

Example 1.1.2 Let us consider $\Omega = (0,1)^2$, $\nabla c_{\text{mac}} = (0,1)10^{-5}$ or $(1,1)10^{-5}$, $D_{\text{solid}} = 10^{-6}$, $D_{\text{pore}} = 1$, $N_1 = N_2 = 36$, $\varepsilon_{\text{mac}} = 10^{-5}[1,0;0,1]$, $\nu_{\text{solid}} = 0.2$, $\nu_{\text{pore}} = 0.2$, $C_{\text{solid}}(x) = 1$, $C_{\text{pore}}(x) = 10^{-5}$, $G_c = 0.01$, $l_0 = 0.01$, $\mu = E/2/(1+\nu)$, $\lambda = E\nu/(1+\nu)/(1-2\nu)$. The numerical results are presented on Figures 2 and 3 for two different shapes of the porous subdomain.
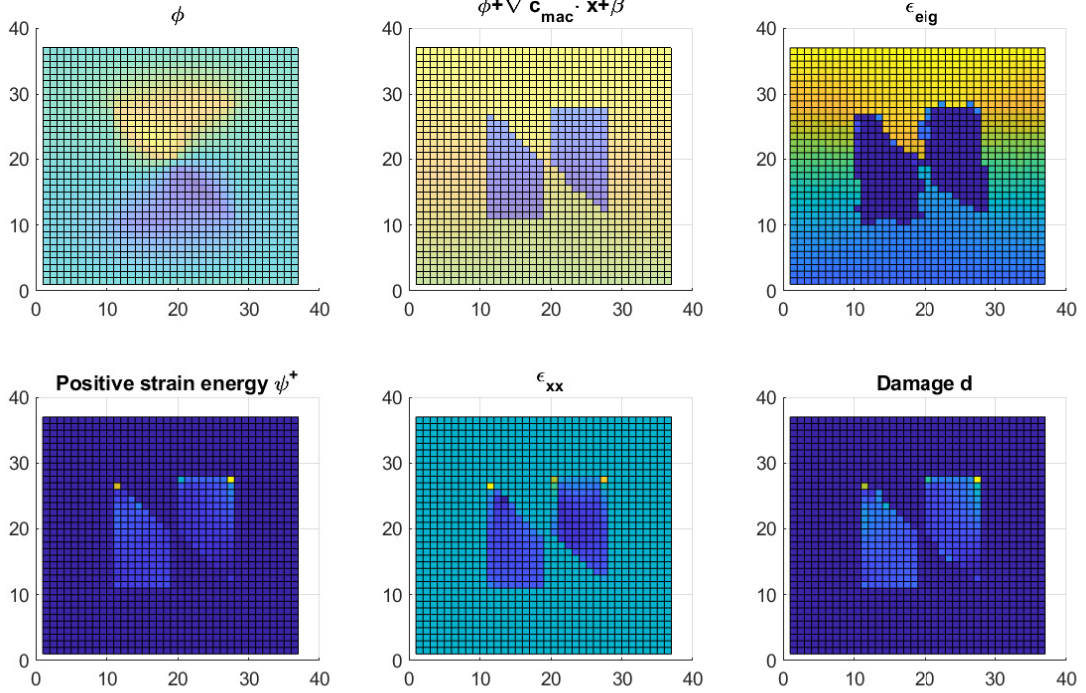

Figure 2: Numerical results of Example 1.1.2.

1.2 Numerical experiments with preconditioning of the three steps

In this part we study influence of preconditioning of the three main part of the problem:
(a) Diffusion of ions (diffusion equation), see (4)
(b) Strain (linear elasticity equation), see (10)
(c) Damage (diffusion and reaction term), see (11).
All three problems are preconditioned with matrices that belong to the respective homogeneous problems. Due to periodic boundary conditions, the inversion of such matices can be cheaply obtained using the fast Fourier transformation (FFT).

We consider the domain with two interconnected discs, see Figure 3, $D_{\text{solid}} = 10^{-6}$ and $D_{\text{pore}} = 1$. The numbers of steps of the conjugate gradient (CG) method without or with the preconditioning to reach the relative residual error 10^{-8} are show in the table below. We can see that preconditioning is helpful in problems (a) and (b), but it has almost no effect on the equation (c) which is due to the reaction term well conditioned itself.

Tables 1 and 2 show numbers of steps and solution times of (p)CG, respectively. Sparse format of matrices is used. Solution time is not shown for the damage problem, because preconditioning does not make any sense here.
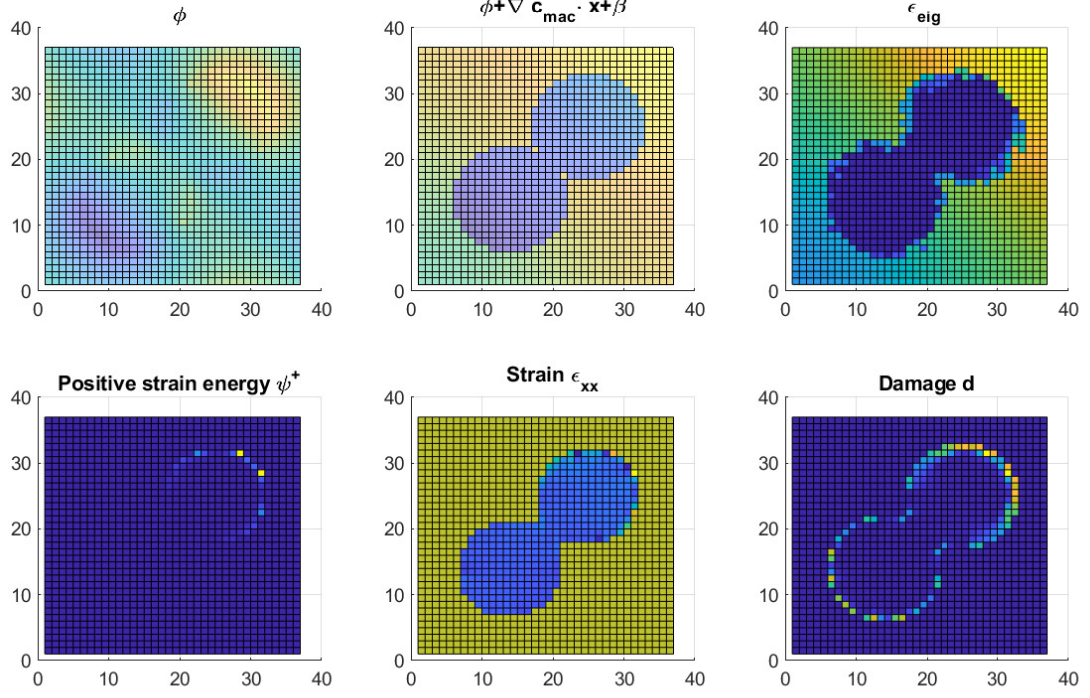
Figure 3: Numerical results of Example 1.1.2.

1.3 Conclusion

We study numerical solution of the problem of corrosion-driven damage of elastic material. We proved that the preconditioning with matrices corresponding to the respective homogeneous problems fasten the convergence of CG for the two first parts of the computation (diffusion of ions and linear elasticity). Moreover, spectra of the preconditioned system can be estimated in advance, see [3] and in the reference therein. Since the solution is very sensitive with respect to the constants used, a future work will focus on suggesting appropriate reconditioning data in connection to the data of real-life problems.

References

[1] P. Farrell, C. Maurini, Linear and nonlinear solvers for variational phase-field models of brittle fracture, International Journal for Numerical Methods in Engineering 109 (5) (2017) 648–667. `doi:10.1002/nme.5300`.

[2] M. Pundir, D. S. Kammer, U. Angst, An fft-based framework for predicting corrosion-driven damage in fractal porous media, Journal of the Mechanics and Physics of Solids 179 (2023) 105388. `doi:https://doi.org/10.1016/j.jmps.2023.105388`.
URL `https://www.sciencedirect.com/science/article/pii/S0022509623001928`

[3] L. Gaynutdinova, M. Ladecký, I. Pultarová, M. Vlasák, J. Zeman, Preconditioned discontinuous galerkin method and convection-diffusion-reaction problems with guaranteed bounds to resulting spectra, Numerical Linear Algebra with Applications 31 (4) (2024) e2549.

$N_1 = N_2$	Diffusion of ions		Strain		Damage	
	# CG	# PCG	# CG	# PCG	# CG	# PCG
20	437	17	366	60	34	30
30	930	18	624	60	34	31
40	1601	19	858	59	33	32
50	2374	24	1114	62	32	31
60	3373	22	1352	62	33	31
70	4363	20	1568	62	33	31
80	5658	21	1830	62	36	31
90	7067	28	2124	65	34	31
100	8603	23	2364	64	34	31
110	10221	21	2564	63	37	31
120	12037	23	2795	63	37	31

Table 1: Numbers of steps (P)CG for diffusion of ions, strain and damage computation.

$N_1 = N_2$	Diffusion of ions		Strain	
	time CG	time PCG	time CG	time PCG
20	1.8E-2	2.8E-3	3.7E-2	2.2E-2
30	5.6E-2	4.8E-3	9.0E-2	2.6E-2
40	1.5E-1	7.8E-3	2.2E-1	3.9E-2
50	3.5E-1	9.9E-3	4.7E-1	5.8E-2
60	7.2E-1	1.1E-2	7.9E-1	8.1E-2
70	1.4E0	1.5E-2	1.3E0	1.0E-1
80	2.3E0	2.2E-2	1.9E0	1.2E-1
90	3.4E0	3.2E-2	2.4E0	1.7E-1
100	4.3E0	3.0E-2	3.9E0	2.5E-1
110	6.1E0	3.3E-2	5.3E0	4.0E-1
120	8.4E0	3.7E-2	9.6E0	2.3E0

Table 2: Numbers of steps and solution times of (P)CG for diffusion of ions and strain computation.