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

Part I – Wave propagation in nonhomogeneous media

Liya Gaynutdinova, Ivana Pultarová, Martin Ladecký, Jan Zeman

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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 wave propagation in elastic heterogeneous media

In this part we study preconditioning of numerical solution of a wave propagation in a heterogeneous media.

1.1 The problem

Consider the wave equation to find u and F such that

$$
\begin{aligned}
\frac{\partial}{\partial x}\sigma(x,t)+f(x,t) &= \rho(x)\frac{\partial^2}{\partial t^2}u(x,t) && \text{for } (x,t)\in\Omega\times(0,T)\\
u(x_0,t) &= U(t) && \text{for } t\in(0,T)\\
u(x,t),\sigma(x,t) & && \Omega\text{-periodic}\\
u(x,0) &= u_0(x) && \text{for } x\in\Omega\\
\frac{\partial}{\partial t}u(x,0) &= v_0(x) && \text{for } x\in\Omega\\
\sigma(x,t) &= E(x)\frac{\partial}{\partial x}u(x,t) && \text{for } (x,t)\in\Omega\times(0,T)
\end{aligned}
$$

where $f(x,t)=F(t)\delta(x-x_0)$ where δ is a Dirac delta function. The role of $F(t)$ is to represent a load in x_0, which guarantees the condition $u(x_0,t)=U(t)$. The problem is motivated by [1]. We study the example presented in [1, Section 3.1].

The numerical algorithm is described in [1, Algorithm 1] where FFT is used to express the unknown vectors in frequency domain. Instead of it, we consider the weak form of the problem and discretize it by FEM with respect to the physical domain and by the implicit Newmark integration scheme in the time domain. We use FFT only for cheap inverting of the preconditioning matrices. Note that both approaches need twice using FFT in every iteration step.

1.2 Preconditioning and spectral bounds

The most demanding part of the solution process (see [1, Algorithm 1]) is solution of the set of linear equations of the type

$$(\beta d_t^2 \mathsf{K} + \mathsf{M})\mathsf{u} = \mathsf{M}(\mathsf{v} + d_t \mathsf{v}_d + d_t^2(0.5 - \beta)\mathsf{v}_{dd})$$

in every time step, where K and M are the stiffness and mass matrices, respectively, d_t is the time step, v, v_d, and v_{dd}, are the previous time step solution and its time derivatives, respectively, β is the Newmark integration constant. The system matrix $\beta d_t^2 \mathsf{K} + \mathsf{M}$ is symmetric and positive definite. Therefore, the most appropriate solution method is the conugate gradient method (CG). Due to M the eigenvalues of the system matrix are well separated from zero for small d_t. However, for larger time steps, the conditioning of the system matrix may worsen and thus a preconditioning can be suggested.

Since periodic boundary conditions are applied, we suggest preconditioning with a matrix which can be easily inverted using FFT, namely

$$\beta d_t^2 \mathsf{K}_p + \mathsf{M}_p$$

where K_p and M_p are the preconditioning stiffness and mass matrices, respectively, obtained for constant Young modulus E and density ρ, respectively.

The lower and upper bounds to all individual eigenvalues of the preconditioned matrix can be easily obtained by a simple algorithm based on inspecting local contributions to the matrices K and M and to their preconditioning counterparts K_p and M_p. For the detais of the estimating algorithm see e.g. [2, 3].

1.3 Numerical experiments

We consider the following setting (omitting the physical metric units): length of the physical domain $L = 2$, number of physical discretization intervals $Nx = 500$, length of the time domain $T = 1.6 \cdot 10^{-4}$, wave velocity $c_0 = 5102.6$, basic time step $\widetilde{d_t} = 4L/N_x/c_0$. For the displacement condition $U(t)$ in $x_0 = 1$ we use $\alpha = 4$, $\omega = 5\pi c_0/L$, $A = 0.001$ and

$$U(t) = \frac{A(t(\pi/\omega - t))^\alpha}{((\pi/\omega)^2/4)^\alpha}$$

for $t < \pi/\omega$ and $U(t) = 0$ otherwise. For preconditioning we use $\rho_p = 2700$ and $E = 7.3 \cdot 10^9$. Reduction of the residual norm by the factor of 10^{-9} is considered as a stopping criterium in CG.

Example 1.3.1 *We consider homogeneous density $\rho(x) = 2700$ and Young modulus $E(x) = 7.3 \cdot 10^9$ and compare the numerical solution with the exact solution [1]. In Table 1 we can see how the time step d_t influences the conditioning of the matrices and the L^2 norm of the error of the solution. Note that for small steps, the rounding errors deteriorate the accuracy.*

d_t	av. CG steps	κ	error
$\widetilde{d_t} \cdot 2$	76.8	63.9	$7.8 \cdot 10^{-6}$
$\widetilde{d_t}$	34.0	16.2	$1.7 \cdot 10^{-6}$
$\widetilde{d_t} \cdot 0.5$	14.9	4.3	$4.6 \cdot 10^{-7}$
$\widetilde{d_t} \cdot 0.1$	7.2	2.0	$3.0 \cdot 10^{-6}$

Table 1: Averaged numbers of CG steps, condition numbers of system matrices and the norm of the final error vector for different time steps $\widetilde{d_t}$.

Example 1.3.2 *We consider nonhomogeneous density $\rho(x) = 2700$ for $x \in (0.6, 1.4)$ and $\rho(x) = 0$ otherwise, and Young modulus $E(x) = 7.3 \cdot 10^9$ for $x \in (0.6, 1.4)$ and $E(x) = 211.4 \cdot 10^9$ otherwise. In Table 2 we can see how the time steps d_t influence the conditioning of the matrices and how the preconditioning reduces it.*

d_t	no preconditioning av. CG steps	κ	$\beta d_t^2 \mathsf{K}_p + \mathsf{M}_p$ av. CG steps	κ	κ_{estim}
$\widetilde{d_t} \cdot 2$	128.9	191.8	4.2	3.0	3.0
$\widetilde{d_t}$	59.2	48.7	3.8	3.0	3.0
$\widetilde{d_t} \cdot 0.5$	25.6	13.0	3.7	3.0	3.0
$\widetilde{d_t} \cdot 0.1$	13.5	5.9	3.6	2.9	2.9

Table 2: Averaged numbers of CG steps, condition numbers of (preconditioned) system matrices and their estimates for different time steps $\widetilde{d_t}$.

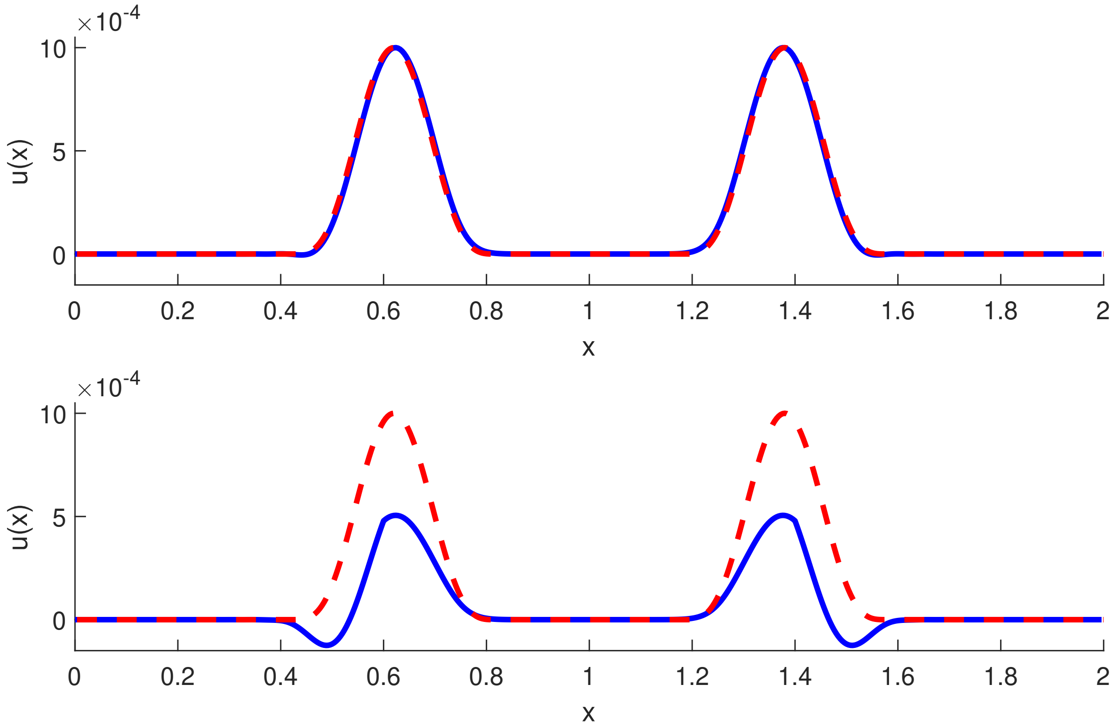

Figure 1: Graphical plots of final solutions u (blue lines) in Examples 1.3.2 (first plot) and **??** (second plot) and the exact solution of Example 1.3.2 (red dashed line).

1.4 Conclusion

We study preconditioning of numerical solution of wave propagation in heterogeneous elastic media. We have shown that FFT-based preconditioning with matrices $\mathsf{K}p$ and M_p obtained for a suitable reference material improves the convergence of the CG method. Moreover, the condition numbers and even every eigenvalue can be estimated in advance using a cheap algorithm. This can help to predict the efficiency of a preconditioner. We note that for the growing time step d_t the condition number and the accuracy of the system deteriorate. Thus, it is nor expected that systems with high condition numbers are to be solved. On the other hand, very small time step can lead to a large rounding error; see Example 1.3.2. In addition, even if the time step is small enough to yield a sufficient approximation, the preconditioning can significantly reduce the number of CG iterations.

We have also studied the two-dimensional setting and conclude that the same strategy can be used to obtain an effective preconditioning which is even more desired in the 2D case.

The results of this study can be further developed and/or applied in particular practical problems. For example, we can theoretically study the balance between accuracy, time steps, and CG steps.

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References

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