CSMA 2024
16ème Colloque National en Calcul des Structures
13-17 Mai 2024, Presqu'île de Giens (Var)

A robust preconditioner for Thermo-Hydro-Mechanics problems with a second gradient of dilation regularization

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Résumé — The topic of this work is the modeling of a deep geological disposal facility built in a clay-based host rock, resulting in the solution of a nonlinear thermo-hydro-mechanical (THM) problem with a second gradient of dilation regularization. The objective is to find a robust iterative solver for the system of equations after linearization. Numerical results reflect the good performance of the proposed preconditioner that shows mesh size independence and parameter robustness.
Mots clés — Multiphysics, Preconditioning, Biot's Problem, Finite Elements, HPC.

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1 Introduction

1.1 Context

The modeling of situations involving coupled phenomena, where multiple physical variables come into play, is challenging. This is especially true for underground detailed modeling of soil mechanics.
The study of subsurface phenomena began with Terzaghi's work on one-dimensional consolidation theory [17], which was later expanded by Biot, who among other aspects integrated temperature effects [3]. Finally Coussy showed that a general theory of thermomechanics of saturated porous media could be established based on standard thermodynamics principles [5].
The main contribution of this communication is the extension of previous results of the authors [13] to another class of ground constitutive equations. Indeed, the soil behavior often requires the use of softening constitutive laws, leading to well-known numerical troubles [15]. In particular, strain localization and loss of solution uniqueness can occur, causing the solution process to fail. To avoid this, non-locally regularized equations based on a second gradient theory can be used [8]. In this approach, a new primal unknown is introduced, corresponding to the trace of the displacement gradient, together with its dual, which can be interpreted as a Lagrange multiplier. The occurrence of this saddle-point deeply affects the nature of the system of equations and special care must be taken in order to define a preconditioner. This is the key point of this work.
The communication is organized as follows. We first present the thermo-hydro-mechanical (THM) problem with a second gradient of dilation regularization. We then introduce a preconditioner in order to build a robust solver of the system. To finish, parameter sensibility of the solver is presented.

1.2 The equations

We focus on an isotropic, incompressible and saturated mono-phased porous medium. It is represented as a solid structure with fluid filled pores. For the rest of the communication, we place ourselves in a simplified case by using linear elasticity for the mechanics constitutive law.
In regard to the THM equations, the key parameters are :

- the porosity, named φ in the sequel. It is the ratio between the volume of the void and the total volume of the medium,
- the intrinsic permeability named K_{int}. It measures the material's ability to transmit fluids, with λ^H, the hydraulic permeability, being a function of it,
- the thermal conductivity named λ^T. It measures the medium's ability to conduct heat.

In regards to the second gradient of dilation equations, the key parameters are :

- the second stress tensor, named $\underline{S}$. It is the microscopic volumetric stress that follows a linear elastic law especially developed for the second gradient of dilation [8],
- the stiffness parameter, named a_1. It defines the isotropic and linear constitutive law of the second gradient of dilation such as $\underline{S}(\chi) = 3a^1\nabla\chi$,
- the penalization parameter, named r. It introduces an augmented Lagrangian to the formulation in order to eliminate any stress and strain oscillations that can appear at Gauss points.

Another significant parameter is the Biot's coefficient b, but since the medium is incompressible it will translate into $b = 1$. As well as the saturation S, that describes the moisture content of the medium who will also be $S = 1$ because the medium is saturated. These parameters, some of which appear explicitly therein, are of major importance in the balance equations. They are five in number since the medium is saturated and mono-phased : the mechanics equilibrium equation, the water mass conservation, the energy conservation, the second gradient equilibrium equation and the constraint equation that forces the equality of microscopic and macroscopic volume changes.

Let Ω be a d dimensional domain, $1 \leq d \leq 3$, and t_f the final time of the simulation. The coupled system consists of , $\forall x \in \Omega$ and $\forall t > 0 \in [0, t_f]$,

$$-\operatorname{div}(\underline{\underline{\underline{\underline{A}}}} : \underline{\underline{\varepsilon}}(\underline{u})) + \nabla p + 3K_s\alpha_s\nabla T + \nabla\lambda - r\nabla(\operatorname{div}(\underline{u})) + r\nabla\chi = \underline{f}^e \qquad \text{in } \Omega \times (0, t_f) \qquad (1)$$

$$-\operatorname{div}(\rho_f\lambda_H\nabla p) + \rho_f(\operatorname{div}(\underline{\dot{u}}) + \frac{\varphi}{K_l}\dot{p} - \alpha_m 3\dot{T}) = 0 \qquad \text{in } \Omega \times (0, t_f) \qquad (2)$$

$$\begin{aligned} &-\operatorname{div}(\lambda_T\nabla T) - \operatorname{div}(\rho_f h_f \lambda_H \nabla p) \\ &+\rho_f h_f(\operatorname{div}(\underline{\dot{u}}) + \frac{\varphi}{K_l}\dot{p} - \alpha_m 3\dot{T}) \\ &+(3K_0\alpha_s\operatorname{div}(\underline{\dot{u}}) - 3\alpha_m\dot{p} - 9K_0\alpha_s^2\dot{T})T + C_\sigma^0\dot{T} = \Theta \qquad \text{in } \Omega \times (0, t_f) \qquad (3) \end{aligned}$$

$$\lambda - \operatorname{div}(\underline{S}(\chi)) - r\operatorname{div}(\underline{u}) + r\chi = 0 \qquad \text{in } \Omega \times (0, t_f) \qquad (4)$$

$$\operatorname{div}(\underline{u}) - \chi = 0 \qquad \text{in } \Omega \times (0, t_f) \qquad (5)$$

The boundary of Ω is denoted $\partial\Omega$ and six different partitions are needed to define the boundary conditions. We apply Dirichlet boundary conditions to the displacement, pressure and temperature. Neumann boundary conditions for the the displacement $\underline{u}$ follow the stress $\underline{\underline{\sigma}}$, the ones for the pressure p follow the fluid flux q, the ones for the temperature T follow the thermal flux Ψ and the ones for the microscopic volume change χ follow the stress $\underline{S}$.

We thus have, respectively, the boundary conditions on the displacement unknowns, on the pressure unknowns and on the temperature unknowns such as :

$$\begin{aligned} \partial\Omega &= \partial\Omega^{\underline{u}} \cup \partial\Omega^{\underline{t}} \text{ with } \partial\Omega^{\underline{u}} \cap \partial\Omega^{\underline{t}} = \emptyset \\ \partial\Omega &= \partial\Omega^{p} \cup \partial\Omega^{q} \text{ with } \partial\Omega^{p} \cap \partial\Omega^{q} = \emptyset \\ \partial\Omega &= \partial\Omega^{T} \cup \partial\Omega^{\Psi} \text{ with } \partial\Omega^{T} \cap \partial\Omega^{\Psi} = \emptyset \end{aligned}$$

The boundary conditions are given by :

$$
\begin{aligned}
\underline{\underline{\sigma}}(\underline{u}) \cdot \underline{n} = \underline{t}^{e} & \qquad \text{on } \partial\Omega^{\underline{t}} \times (0, t_f) \\
\underline{S}(\chi) \cdot \underline{n} = 0 & \qquad \text{on } \partial\Omega \times (0, t_f) \\
-\lambda_H \nabla p \cdot \underline{n} = q^{e} & \qquad \text{on } \partial\Omega^{q} \times (0, t_f) \\
-\lambda_T \nabla T \cdot \underline{n} = \Psi^{e} & \qquad \text{on } \partial\Omega^{\Psi} \times (0, t_f) \\
\underline{u} = \underline{u}^{e} & \qquad \text{on } \partial\Omega^{\underline{u}} \times (0, t_f) \\
p = p^{e} & \qquad \text{on } \partial\Omega^{p} \times (0, t_f) \\
T = T^{e} & \qquad \text{on } \partial\Omega^{T} \times (0, t_f) \\
\underline{u}(\,,0) = \underline{u}_0 & \qquad \text{in } \Omega \\
p(\,,0) = p_0 & \qquad \text{in } \Omega \\
T(\,,0) = T_0 & \qquad \text{in } \Omega
\end{aligned}
$$

where $\underline{n}$ is the outward normal.

The system is linearized using Newton's method. Time discretization is done trough an implicit Euler method and space discretization trough a finite element method with Lagrange $P2$-$P1$-$P1$-$P1$-$P1$ elements. This translates into using continuous piecewise quadratics to approximate the displacement and continuous piecewise linears to approximate the pressure, the temperature, the microscopic volume changes and the Lagrange multipliers. The linearized system finally expresses as :

$$
A = \begin{bmatrix}
\boldsymbol{A}_{\underline{uu}} & \boldsymbol{A}_{\underline{u}p} & \boldsymbol{A}_{\underline{u}T} & \boldsymbol{A}_{\underline{u}\chi} & \boldsymbol{A}_{\underline{u}\lambda} \\
\boldsymbol{A}_{p\underline{u}} & \boldsymbol{A}_{pp} & \boldsymbol{A}_{pT} & 0 & 0 \\
\boldsymbol{A}_{T\underline{u}} & \boldsymbol{A}_{Tp} & \boldsymbol{A}_{TT} & 0 & 0 \\
\boldsymbol{A}_{\chi\underline{u}} & 0 & 0 & \boldsymbol{A}_{\chi\chi} & \boldsymbol{A}_{\chi\lambda} \\
\boldsymbol{A}_{\lambda\underline{u}} & 0 & 0 & \boldsymbol{A}_{\lambda\chi} & \boldsymbol{A}_{\lambda\lambda}
\end{bmatrix},
$$

2 The Preconditioner

In the realm of preconditioning for coupled multi-physics problems, the literature highlights two main approaches. First, using block preconditioners with multigrid preconditioning within each block [13]. Secondly, employing a multigrid algorithm with block preconditioners as smoothers [10]. For ease of integration into code_aster, the first option is the one we follow.
One of the main challenges we face is the saddle point aspect of the system introduced by the second gradient of dilation regularization. It is present due to the use of Lagrange multipliers and becomes explicit in equation (5) of the system. A preconditioner for this particular saddle-point, relying on the use of a discrete mass matrix, is proven to be parameter-robust in the sense of Mardal [12] under the condition that the Young's modulus E is greater as the penalisation parameter r when applied to mechanics problems [14].
For the other equations, we rely on the approach we have previously proposed [13] and emphasize the interest of the strategy, which allows each block to be treated in a specific manner.

In the end, the Block Gauss-Seidel preconditioner expresses as :

$$
P = \begin{bmatrix}
\boldsymbol{A}_{\underline{uu}} & 0 & 0 & 0 & 0 \\
\boldsymbol{A}_{p\underline{u}} & \boldsymbol{A}_{pp} & 0 & 0 & 0 \\
\boldsymbol{A}_{Tu} & \boldsymbol{A}_{Tp} & \boldsymbol{A}_{TT} & 0 & 0 \\
\boldsymbol{A}_{\chi\underline{u}} & 0 & 0 & \boldsymbol{A}_{\chi\chi} & 0 \\
\boldsymbol{A}_{\lambda\underline{u}} & 0 & 0 & \boldsymbol{A}_{\lambda\chi} & \boldsymbol{M}_{\lambda}
\end{bmatrix},
$$

where $\boldsymbol{M}_{\lambda}$ represents the discrete mass matrix.

TABLE 1 – Parameters

Symbol	Definition	Value	Unit
$\underline{\underline{\underline{A}}}$	Forth order Hooke's tensor	-	Pa
$\underline{\underline{\varepsilon}}$	Strain tensor	-	-
$\underline{S}$	Second stress tensor	-	-
a^1	Stiffness parameter	500	-
r	Penalization parameter	$[1.e^8, 1.e^{10}, 1.e^{11}]$	-
E	Young's modulus	$[1.e^9, 25.e^9, 50.e^9]$	Pa
ν	Poisson's ratio	0.3	-
K_0	Drained bulk modulus of the continuum	K_s	Pa
K_l	Bulk modulus of the fluid	2.10^9	Pa
K_s	Bulk modulus of the solid matrix	$\frac{E}{3(1-2\nu)}$	Pa
K_{int}	Intrinsic permeability	$[4.e^{-21}, 4.e^{-18}, 4.e^{-15}]$	-
φ	Porosity	0.18	-
μ_l	Fluid dynamic viscosity	10^{-3}	Pa.s
h_f	Specific enthalpy of the fluid	$\frac{p_{atm}}{\rho_f}$	J.kg^{-1}
p_{atm}	Atmospheric pressure	10^5	Pa
C_σ^0	Specific heat of the medium to constant constraint	2981980	J.K^{-1}.m^{-3}
ρ_f	Fluid density	1000	kg.m^{-3}
λ_H	Hydraulic conductivity	K_{int}/μ_l	Pa^{-1}.m².s^{-1}
λ_T	Thermal conductivity	1.6	W.m^{-1}.K
α_s	Dilation coefficient of the solid	10^{-5}	K^{-1}
α_l	Dilation coefficient of the fluid	10^{-4}	K^{-1}
α_m	Homogenized dilation coefficient of the medium	$\varphi\alpha_l + (1-\varphi)\alpha_s$	K^{-1}

The outer Krylov method is a Flexible GMRES (FGMRES) [16], with the notation : FGMRES($\boldsymbol{A}$,$\boldsymbol{P}$), where $\boldsymbol{A}$ is the system to solve, and $\boldsymbol{P}$ the preconditioner. A relative convergence tolerance of 10^{-6} is the stopping criteria.

In order to apply the preconditioner, the approximation of the inverse of each diagonal block is needed. $\boldsymbol{A}_{\underline{uu}}^{-1}$, $\boldsymbol{A}_{pp}^{-1}$, $\boldsymbol{A}_{TT}^{-1}$ and $\boldsymbol{A}_{\chi\chi}^{-1}$ are approximated with FGMRES($\boldsymbol{A}_{**}$,Boomer). Boomer refers to the algebraic multigrid preconditioner BoomerAMG of the Hypre library [7]. Denoting $\tilde{*}^{-1}$ the approximation of the inverse of each block, $\tilde{\boldsymbol{A}}_{\underline{uu}}^{-1}$ and $\tilde{\boldsymbol{A}}_{\chi\chi}^{-1}$ are approximated with 10 iterations of FGMRES whereas only 3 iterations are used for $\tilde{\boldsymbol{A}}_{pp}^{-1}$ and $\tilde{\boldsymbol{A}}_{TT}^{-1}$. $\tilde{\boldsymbol{M}}_{\lambda}^{-1}$ is approximated with one V-cycle of Boomer.

3 Numerical results

We now present the parameter sensibility of the proposed preconditioner on a simple but representative test case. The method is implemented in code_aster, the massively parallel open source general purpose finite element solver developed at EDF R&D [4].

3.1 Test case

The test case should reflect the industrial problem in question. Therefore it needs to be complex enough but simple enough to allow the mesh to be easily refined.

To do so, a 3D rectangular box as seen in figure 1, with a 0.1 m length following x, a 0.1 m height following y and 0.05 m large following z is chosen. The tetrahedral mesh was generated using Gmsh 4.4.1. The displacement was set to 0 on the bottom surface ($y = 0$), a mechanical pressure of 5 MPa was applied on the top surface ($y = 0.1$) and a temperature of 80°C is imposed on the whole surface of the sample.

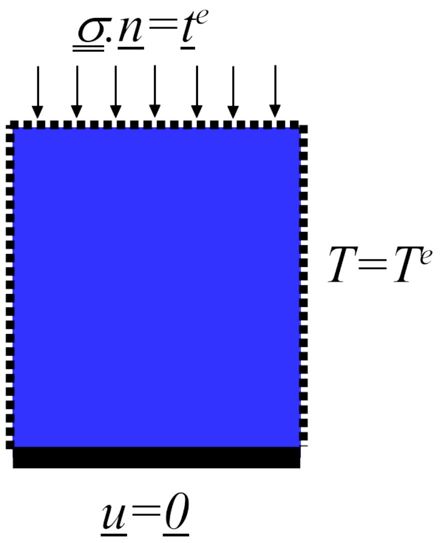

FIGURE 1 – Test case

The sample consists of clay only. We emphasize that the value of the material parameters are of great importance in the industrial applications. They are displayed in Table 1, and are representative of a typical industrial problem of geological waste disposal [9]. The tests were solved with code_aster using the Thermo-Hydro-Mechanics with a second gradient of dilation regularization framework presented above, where $P2$-$P1$-$P1$-$P1$-$P1$ finite elements are used.

3.2 Parameter sensibility

The robustness of the solver is mainly measured by its parameter sensibility and mesh size independence. It is tested trough three parameters that can have different sets of values, the Young modulus E, the intrinsic permeability K_{int} and the penalization parameter r. We have chosen to vary these parameters since they have a major influence therein. The tests are done using the test case of Figure 1 and the remaining parameters from Table 1. For each set of parameters and mesh fineness, we give the average number of outer FGMRES iterations per Newton iteration followed by the total number of Newton iterations of the preconditioned system in parentheses. The results are compiled in Table 2.

In order to analyze the results in Table 2, we propose first a row-wise reading then a column-wise reading. The row-wise reading provides information on the influence of the mesh size, the material parameters being fixed. There is overall good independence with respect to the mesh size. The mesh size independence is excellent when r=1.e+10 and r=1.e+11. For r=1.e+8, the average number of outer FGMRES iterations increases but we consider it to remain constant enough given the multiplication of the size of the system by 100.
The column-wise reading provides information on the influence of the material parameters, the mesh size being fixed. Two cases are observed. First, the total number of Newton iterations shows a good independence with respect to the parameters variations. Even though an extra iteration is needed when E=1.e+9. Second, the average number of outer FGMRES iterations is observed, remaining overall between 10 and 50. The exceptions being when (E=1.e+9, r=1.e+11) where they go up to 146 and when (r=1.e+8, K_{int}=4.e-21) where a slight increase is also present. The preconditioner shows overall a good robustness in regards to the parameters variations.

TABLE 2 – Lower Block Gauss-Seidel parameter sensibility

Parameters			DoF		
E	r	Int. Perm.	9 207	64 407	971 577
1.0e+09	1.0e+08	4.0e-15	20 (3)	31 (3)	39 (3)
		4.0e-18	19 (3)	29 (3)	36 (3)
		4.0e-21	64 (3)	137 (3)	128 (3)
	1.0e+10	4.0e-15	32 (3)	33 (3)	38 (3)
		4.0e-18	31 (3)	33 (3)	37 (3)
		4.0e-21	22 (3)	24 (3)	25 (3)
	1.0e+11	4.0e-15	107 (3)	146 (3)	136 (3)
		4.0e-18	106 (3)	146 (3)	143 (3)
		4.0e-21	83 (3)	96 (3)	76 (3)
2.5e+10	1.0e+08	4.0e-15	18 (2)	30 (2)	50 (2)
		4.0e-18	18 (2)	29 (2)	50 (2)
		4.0e-21	29 (2)	56 (2)	83 (2)
	1.0e+10	4.0e-15	12 (2)	14 (2)	17 (2)
		4.0e-18	12 (2)	14 (2)	18 (2)
		4.0e-21	11 (2)	13 (2)	21 (2)
	1.0e+11	4.0e-15	25 (2)	25 (2)	30 (2)
		4.0e-18	25 (2)	25 (2)	30 (2)
		4.0e-21	21 (2)	24 (2)	29 (2)
5.0e+10	1.0e+08	4.0e-15	18 (2)	31 (2)	52 (2)
		4.0e-18	18 (2)	31 (2)	51 (2)
		4.0e-21	26 (2)	47 (2)	73 (2)
	1.0e+10	4.0e-15	11 (2)	13 (2)	15 (2)
		4.0e-18	11 (2)	13 (2)	15 (2)
		4.0e-21	10 (2)	13 (2)	14 (2)
	1.0e+11	4.0e-15	16 (2)	16 (2)	19 (2)
		4.0e-18	16 (2)	16 (2)	19 (2)
		4.0e-21	15 (2)	15 (2)	18 (2)

4 Conclusion

This communication shows the effectiveness of a lower Block Gauss-Seidel preconditioner designed for THM problems with a second gradient of dilation regularization. A simple yet representative test case has been set up, on which the preconditioner shows good mesh size independence and good enough parameter robustness. While these results have been established in the linear regime, they are very valuable when considering to move to nonlinear constitutive laws. Research is currently underway in this direction and promising results have been found.

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