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Monolithic and splitting based solution schemes for nonlinear quasi-static thermo-poroelasticity.

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Introduction

Quasi-static thermo-poroelasticity:

- Coupling of Heat, Flow, and Mechanics within a quasi-static porous material.
- Generalization of linear quasi-static poroelasticity (Biot) to the non-isothermal case, or generalization of thermoelasticity to porous material.
- Thermal convection introduces a nonlinearity in the model which complicates the situation compared to isothermal case.

Motivation/Applications:

Efficient and robust simulation of thermo-poroelasticity highly relevant for the following applications:

- Geothermal energy storage
- Enhanced oil recovery (steam/hot water injection)
- Nuclear waste disposal
- Carbon capture and storage (CSS)
- Biomedicine
- etc.

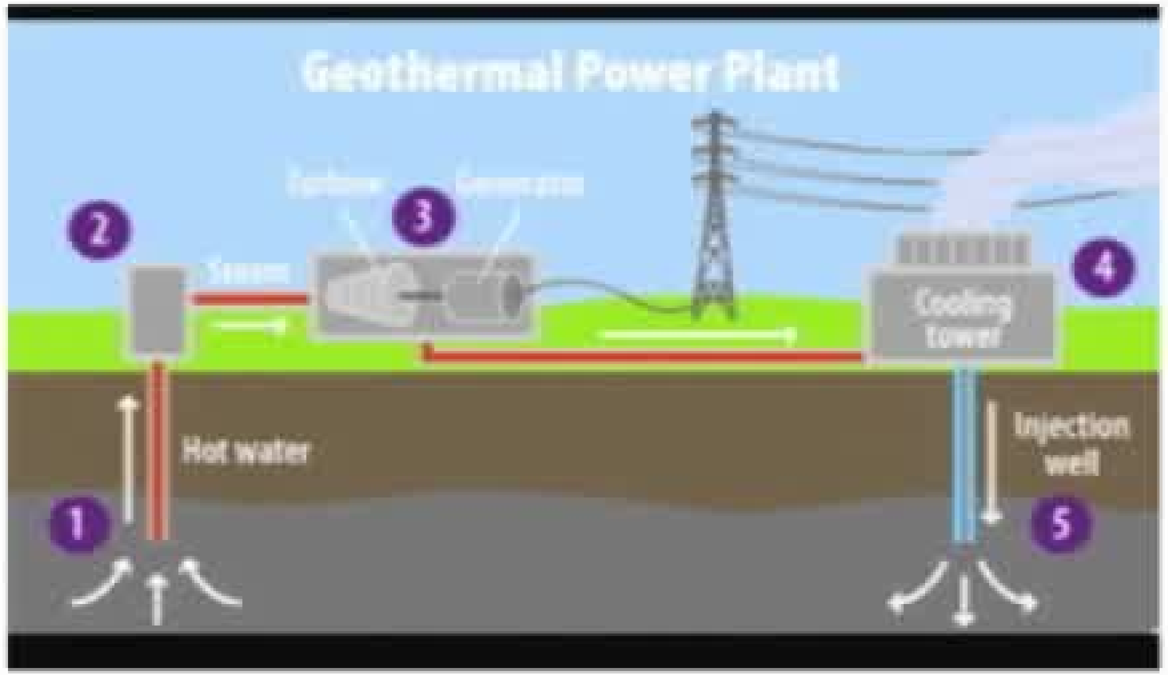

Figure: Geothermal Energy Storage.[1]

[1] Picture from archive.epa.gov

The quasi-static thermo-poroelastic equations[2]

- Energy balance (**He**at):

$$\partial_t(a_0 T - b_0 p + \beta\nabla\cdot\mathbf{u}) + \underline{c_f(\mathbf{K}\nabla p)\cdot\nabla T} - \nabla\cdot(\mathbf{\Theta}\nabla T) = z,$$

- Mass balance (**F**low):

$$\partial_t(c_0 p - b_0 T + \alpha\nabla\cdot\mathbf{u}) - \nabla\cdot(\mathbf{K}\nabla p) = g,$$

- Momentum balance (**M**echanics):

$$-\nabla\cdot(2\mu\varepsilon(\mathbf{u}) + \lambda\nabla\cdot\mathbf{u}\mathbf{I}) + \beta\nabla T + \alpha\nabla p = \mathbf{f}.$$

T	temperature	a_0	effective heat capacity
p	fluid pressure	b_0	thermal dilation coefficient
$\mathbf{u}$	displacement vector	c_0	specific storage coefficient
$\mathbf{K}$	permeability ÷ fluid viscosity	β	effective thermal stress
$\mathbf{\Theta}$	effective thermal conductivity tensor	α	Biot constant
$\varepsilon(\cdot)$	symmetric gradient	μ, λ	Lamé parameters
$\mathbf{I}$	identity tensor	c_f	volumetric heat capacity of fluid
z	heat source	g	mass source
$\mathbf{f}$	body force		

[2] Mats K. Brun et al. "Upscaling of the Coupling of Hydromechanical and Thermal Processes in a Quasi-static Poroelastic Medium". In: *Transport in Porous Media* (May 2018). ISSN: 1573-1634.

Mixed formulation

Define $\mathbf{r} := -\boldsymbol{\Theta}\nabla T$ (heat flux) and $\mathbf{w} := -\mathbf{K}\nabla p$ (Darcy flux), and let a space-time domain $\Omega \times (0, T_f)$, with final time $T_f > 0$ be given, with $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$. The thermoporoelastic problem in mixed form then reads:

Find $(T, \mathbf{r}, p, \mathbf{w}, \mathbf{u})$ such that

$$\partial_t(a_0 T - b_0 p + \beta \nabla \cdot \mathbf{u}) + c_f \mathbf{w} \cdot \boldsymbol{\Theta}^{-1}\mathbf{r} + \nabla \cdot \mathbf{r} = z, \quad \text{in } \Omega \times (0, T_f), \tag{1a}$$

$$\boldsymbol{\Theta}^{-1}\mathbf{r} + \nabla T = 0, \quad \text{in } \Omega \times (0, T_f), \tag{1b}$$

$$\partial_t(c_0 p - b_0 T + \alpha \nabla \cdot \mathbf{u}) + \nabla \cdot \mathbf{w} = g, \quad \text{in } \Omega \times (0, T_f), \tag{1c}$$

$$\mathbf{K}^{-1}\mathbf{w} + \nabla p = 0, \quad \text{in } \Omega \times (0, T_f), \tag{1d}$$

$$-\nabla \cdot (2\mu\varepsilon(\mathbf{u}) + \lambda \nabla \cdot \mathbf{u}\mathbf{I}) + \alpha \nabla p + \beta \nabla T = \mathbf{f}, \quad \text{in } \Omega \times (0, T_f), \tag{1e}$$

with suitable initial and boundary conditions.

Theorem (Existence and uniqueness)

Assuming some constraints on the coefficients and sufficient regularity of the source/initial/boundary data, the system (3a)–(3e) *admits a unique weak solution:*

$$(T, \mathbf{r}) \in H^1((0, T_f); L^2(\Omega)) \times \left(L^\infty((0, T_f); H(\text{div}; \Omega)) \cap H^1((0, T_f); L^2(\Omega))\right), \tag{2a}$$

$$(p, \mathbf{w}) \in H^1((0, T_f); L^2(\Omega)) \times \left(L^\infty((0, T_f); H(\text{div}; \Omega)) \cap H^1((0, T_f); L^2(\Omega))\right), \tag{2b}$$

$$\mathbf{u} \in H^1((0, T_f); H^1(\Omega)). \tag{2c}$$

Iterative algorithms

Various (L-type) iterative schemes

Six iterative schemes for thermo-poroelasticity, based on the L-scheme/Fixed Stress[4],[5].
Exhausting all possibilities of coupling/decoupling of the three subproblems, **H**, **F**, and **M**.

- The monolithic L-scheme:
  1) **HFM**: Linearized system solved monolithically, i.e.

     Heat/Flow/**M**echanics.
- The partially decoupled L-schemes:
  2) **HF-M**: Heat and flow subproblems solved together decoupled from mechanics, i.e.

     Heat/Flow $\to$ **M**echanics.
  3) **HM-F**: Heat and mechanics subproblems are solved together decoupled from flow, i.e.

     Heat/**M**echanics $\to$ Flow.
  4) **FM-H**: Flow and mechanics subproblems are solved together decoupled from heat, i.e.

     Flow/**M**echanics $\to$ Heat.
- The fully decoupled L-schemes:
  5) **H-F-M**: At each iteration all three subproblems are decoupled and solved in the order

     Heat $\to$ Flow $\to$ **M**echanics.
  6) **F-H-M**: At each iteration all three subproblems are decoupled and solved in the order

     Flow $\to$ Heat $\to$ **M**echanics.

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[4] Jakub Wiktor Both et al. "Robust fixed stress splitting for Biot's equations in heterogeneous media". In: *Appl. Math. Lett.* 68 (2017), pp. 101–108. ISSN: 0893-9659.
[5] Florian List and Florin A. Radu. "A study on iterative methods for solving Richards' equation". In: *Comput. Geosci.* 20.2 (2016), pp. 341–353. ISSN: 1420-0597.

H-F-M: Heat $\to$ Flow $\to$ Mechanics

Initialize: $(T^{n,0}, \mathbf{r}^{n,0}) := (T^{n-1}, \mathbf{r}^{n-1})$, $(p^{n,0}, \mathbf{w}^{n,0}) := (p^{n-1}, \mathbf{w}^{n-1})$, and $\mathbf{u}^{n,0} := \mathbf{u}^{n-1}$.

- **Step 1**: Given $(T^{n,i-1}, p^{n,i-1}, \mathbf{w}^{n,i-1}, \mathbf{u}^{n,i-1})$ find $(T^{n,i}, \mathbf{r}^{n,i})$ such that

$$
\begin{aligned}
&(a_0 + \underline{L_T})(T^{n,i}, S) + \tau c_f(\mathcal{M}(\mathbf{w}^{n,i-1}) \cdot \mathbf{\Theta}^{-1}\mathcal{M}(\mathbf{r}^{n,i}), S) + \tau(\nabla \cdot \mathbf{r}^{n,i}, S) \\
&\quad = \underline{L_T}(T^{n,i-1}, S) + b_0(p^{n,i-1}, S) - \beta(\nabla \mathbf{u}^{n,i-1}, S) \\
&\quad + \tau(z, S) + a_0(T^{n-1}, S) - b_0(p^{n-1}, S) + \beta(\nabla \cdot \mathbf{u}^{n-1}, S), && \forall S \in \mathcal{T}_h, \\
&(\mathbf{\Theta}^{-1}\mathbf{r}^{n,i}, \mathbf{y}) - (T^{n,i}, \nabla \cdot \mathbf{y}) = 0, && \forall \mathbf{y} \in \mathcal{R}_h,
\end{aligned}
$$

- **Step 2**: Given $(T^{n,i}, p^{n,i-1}, \mathbf{u}^{n,i-1})$ find $(p^{n,i}, \mathbf{w}^{n,i})$ such that

$$
\begin{aligned}
&(c_0 + \underline{L_p})(p^{n,i}, q) + \tau(\nabla \cdot \mathbf{w}^{n,i}, q) = \underline{L_p}(p^{n,i-1}, q) + b_0(T^{n,i}, q) - \alpha(\nabla \cdot \mathbf{u}^{n,i-1}, q) \\
&\quad + \tau(g, q) + c_0(p^{n-1}, q) - b_0(T^{n-1}, q) + \alpha(\nabla \cdot \mathbf{u}^{n-1}, q) && \forall q \in \mathcal{P}_h, \\
&(\mathbf{K}^{-1}\mathbf{w}^{n,i}, \mathbf{z}) - (p^{n,i}, \nabla \cdot \mathbf{z}) = 0, && \forall \mathbf{z} \in \mathcal{W}_h.
\end{aligned}
$$

- **Step 3**: Given $(T^{n,i}, p^{n,i})$ find $\mathbf{u}^{n,i}$ such that

$$
2\mu(\varepsilon(\mathbf{u}^{n,i}), \varepsilon(\mathbf{v})) + \lambda(\nabla \cdot \mathbf{u}^{n,i}, \nabla \cdot \mathbf{v}) = (\mathbf{f}, \mathbf{v}) + \beta(T^{n,i}, \nabla \cdot \mathbf{v}) + \alpha(p^{n,i}, \nabla \cdot \mathbf{v}), \quad \forall \mathbf{v} \in \mathcal{U}_h,
$$

where $\underline{L_T}, \underline{L_p} > 0$ are stabilization/linearization parameters. Cut-off operator $\mathcal{M}$ def. by[6]:

$$
\mathcal{M}(\mathbf{z})(x) := \begin{cases} \mathbf{z}(x), & |\mathbf{z}(x)| \leq M \\ M\mathbf{z}(x)/|\mathbf{z}(x)|, & |\mathbf{z}(x)| > M. \end{cases}
$$

[6] Shuyu Sun, Béatrice Rivière, and Mary F. Wheeler. "A combined mixed finite element and discontinuous Galerkin method for miscible displacement problem in porous media". In: *Recent progress in computational and applied PDEs (Zhangjiajie, 2001)*. Kluwer/Plenum, New York, 2002, pp. 323–351.

Convergence of iterative algorithms

(A1) $c_0 - b_0 > 0$ and $a_0 - b_0 > 0$.
(A2) $\mathbf{K}, \mathbf{\Theta} \in (L^\infty(\Omega))^{d\times d}$ such that $\theta_M/\theta_m := \max/\min \Lambda(\mathbf{\Theta})$, $k_M/k_m := \max/\min \Lambda(\mathbf{K})$.
(A3) Time step satisfies: $0 < \tau < \dfrac{2(a_0 - b_0)}{c_f^2 M^2 (k_M/\theta_m + 1) - \theta_m/4c_{\Omega,d}}$
(A4) Stabilization parameters satisfy: $L_T \geq \dfrac{4\beta^2}{3(2\mu/d + \lambda)}$ and $L_p \geq \dfrac{4\alpha^2}{3(2\mu/d + \lambda)}$

Theorem (Convergence of the scheme H-F-M[7])

Assuming that ***(A1)–(A4)*** *holds true, then the scheme* ***H-F-M*** *is a contraction given by*

$$\left(a_0 - b_0 + \frac{L_T}{2} + \frac{\tau\theta_m}{4c_{\Omega,d}} - \frac{\tau c_f^2 M^2}{2}\left(\frac{k_M}{\theta_m} + 1\right)\right)\left\|e_T^i\right\|^2 + \left(c_0 - \frac{b_0}{2} + \frac{L_p}{2}\right)\left\|e_p^i\right\|^2 + \tau\left\|\mathbf{e}_\mathbf{w}^i\right\|_{\mathbf{K}^{-1}}^2$$
$$\leq \frac{L_T}{2}\left\|e_T^{i-1}\right\|^2 + \left(\frac{L_p}{2} + \frac{b_0}{2}\right)\left\|e_p^{i-1}\right\|^2 + \frac{\tau}{2}\left\|\mathbf{e}_\mathbf{w}^{i-1}\right\|_{\mathbf{K}^{-1}}^2.$$

Furthermore, $$\frac{\mu}{2}\left\|\varepsilon(\mathbf{e}_\mathbf{u}^i)\right\|^2 + \frac{\lambda}{4}\left\|\nabla\cdot\mathbf{e}_\mathbf{u}^i\right\|^2 \leq \frac{2\alpha^2}{3(\frac{2\mu}{d}+\lambda)}\left\|e_p^i\right\|^2 + \frac{2\beta^2}{3(\frac{2\mu}{d}+\lambda)}\left\|e_T^i\right\|^2,$$

where $(e_T^i, \mathbf{e}_\mathbf{r}^i, e_p^i, \mathbf{e}_\mathbf{w}^i, \mathbf{e}_\mathbf{u}^i) := (T^{n,i} - T^n, \mathbf{r}^{n,i} - \mathbf{r}^n, p^{n,i} - p^n, \mathbf{w}^{n,i} - \mathbf{w}^n, \mathbf{u}^{n,i} - \mathbf{u}^n)$.

[7] Mats K. Brun et al. "Monolithic and splitting based solution schemes for fully coupled quasi-static thermo-poroelasticity with nonlinear convective transport". In: *arXiv e-prints*, arXiv:1902.05783 (Feb. 2019), arXiv:1902.05783. arXiv: 1902.05783 [math.NA].

Numerical experiments

Test case 1: example with a manufactured solution

As a first test case, we let the domain be a regular triangularization of the unit square, i.e., $\Omega = [0,1] \times [0,1] \subset \mathbb{R}^2$, and prescribe the following smooth solutions for the temperature, pressure and displacements:

$$T(x,t) = tx_1(1-x_1)x_2(1-x_2),$$
$$p(x,t) = tx_1(1-x_1)x_2(1-x_2),$$
$$\mathbf{u}(x,t) = tx_1(1-x_1)x_2(1-x_2)[1,1]^\top,$$

where $x := (x_1, x_2) \in \mathbb{R}^2$, $t \geq 0$.
For the analysis and comparison of our algorithms, we consider dimensionless equations, i.e. all parameters are set to $1.0e-1$, except for the three coupling coefficients $\{\alpha, \beta, b_0\}$, which we vary in order to *weaken/strengthen* the coupling between the three subproblems. In particular, we consider five different parameter regimes, **PR1 – PR5**, specified below:

	PR1	PR2	PR3	PR4	PR5
α	1.0	0.1	0.1	1.0	0.1
β	1.0	0.1	1.0	0.1	0.1
b_0	1.0	1.0	0.1	0.1	0.1

Table: Parameter regimes for varying strong/weak coupling between subproblems.

Discretization: Heat/flow: $\mathbb{RT}_0 \times \mathbb{P}_0$, Mechanics: $\mathbb{P}_1$.

Iteration counts for stabilized algorithms

	PR1	PR2	PR3	PR4	PR5	PR1	PR2	PR3	PR4	PR5
h	HFM					HF-M				
1/4	7	3	8	8	3	31	4	11	11	4
1/8	7	3	7	7	3	35	4	13	13	4
1/16	6	3	7	7	3	40	4	13	13	4
1/32	6	3	7	7	3	41	4	13	13	4
1/64	6	3	7	7	3	41	4	13	13	4
h	HM-F					FM-H				
1/4	9	6	8	11	4	9	6	11	8	4
1/8	9	6	7	11	4	9	6	11	7	4
1/16	9	6	7	11	4	9	6	11	7	4
1/32	9	6	7	11	4	9	6	11	7	4
1/64	9	6	7	11	4	9	6	11	7	4
h	H-F-M					F-H-M				
1/4	20	6	11	11	4	20	6	11	11	4
1/8	22	6	12	12	4	22	6	12	12	4
1/16	24	6	13	13	4	24	6	13	13	4
1/32	24	6	13	13	4	24	6	13	13	4
1/64	24	6	13	13	4	24	6	13	13	4

Table: Number of iterations with decreasing mesh sizes for parameter regimes **PR1 – PR5**. Stabilization from theory.

Iteration counts for strong/weak nonlinear effects

Parameters	PR1	PR5	PR1	PR5
#	**HFM**		**HF-M**	
Non-stabilized	4	4	-	5
Stabilized	7	4	41	5
#	**HM-F**		**FM-H**	
Non-stabilized	11	4	10	4
Stabilized	9	4	8	4
#	**H-F-M**		**F-H-M**	
Non-stabilized	48	5	36	4
Stabilized	25	5	22	4

Table: Number of iterations with strong nonlinear effects, i.e. $c_f = 10$, and mesh size $h = 1/16$.

h	$e_{h,T}$	r_T	$e_{h,\mathbf{r}}$	$r_{\mathbf{r}}$	$e_{h,p}$	r_p	$e_{h,\mathbf{w}}$	$r_{\mathbf{w}}$	$e_{h,\mathbf{u}}$	$r_{\mathbf{u}}$
1/4	8.5e-3	-	3.5e-3	-	8.5e-3	-	3.5e-3	-	5.6e-3	-
1/8	4.4e-3	1.93	1.8e-3	1.94	4.4e-3	1.93	1.8e-3	1.94	1.4e-3	4.0
1/16	2.2e-3	2.0	9.3e-4	1.94	2.2e-3	2.0	9.3e-4	1.94	3.6e-4	3.89
1/32	1.1e-3	2.0	4.7e-4	1.98	1.1e-3	2.0	4.7e-4	1.98	9.1e-5	3.96
1/64	5.5e-4	2.0	2.3e-4	2.04	5.5e-4	2.0	2.3e-4	2.04	2.3e-5	3.96

Table: Discretization errors using algorithm **H-F-M**. Convergence rates are optimal.

Conclusion

- Thermo-poroelasticity is a complex problem, which involves the (nonlinear) coupling of heat, flow, and mechanics.
- In total, five combinations of iterative splitting procedures, plus monolithic linearization yields six iterative algorithms, which we have analyzed and implemented.
- Without stabilizing terms the iterative schemes are very sensitive to coupling strength between the subproblems
- Using stabilizing terms from our theory improves robustness and efficiency, and reduces sensitivity to coupling strength.

Thank you!