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COUPLING 3D AND ROTATION INVARIANT PROBABILISTIC MODELS FOR TWO-PHASE FLOWS IN RANDOM MEDIA.

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Abstract. *Modeling and simulation of two-phase flows in a porous random media is a highly challenging task due the non-linearity of the wetting process, the time and space scales at stake and the very large spatial variability and anisotropy of the intrinsic permeability. In the particular case of an injection problem being statistically invariant for any rotation around the axis of the well a coupled 3D/rotation-invariant probabilistic model is proposed following the methodology introduced in [1] and [2]. The idea of a variational coupling between a probabilistic local model and a deterministic or probabilistic model is developed here in the context of a coupling along a surface and not over a volume. 3D/2D coupling is also considered. The implementation in a general purpose Finite Element Code is then addressed and illustrated in the context of Risk assessment of geological storage of carbon dioxide.*

1 OUTLINE

Two-phase flow in porous media is classically modeled using a two-field diffusion equation:

$$d_a \frac{\partial u}{\partial t} + div(-c\nabla u + \gamma) = 0 \tag{1}$$

applying in a given domain Ω where $u(x, y, z, t)$ is vector valued, d_a, γ second-order-tensor valued and c symmetric fourth-order tensor valued. Appropriate boundary conditions on $\partial\Omega$ are also assumed, either of Dirichlet or Neumann types:

$$u = u_0, (c\nabla u) \cdot n = q_0 \tag{2}$$

where n is the outer normal vector. In the context of two-phase flow in porous media, the diffusion tensor d_a and the hydraulic conductivity tensor c are strongly non-linear functions of the pressure fields u. The classical Van Genuchten model [3] is used to represent these dependencies in the present study but more complex models could be considered. The underlying intrinsic permeability is an anisotropic tensor valued random field modeled using a non-linear filtering of independent Gaussian random fields. The non-linear mapping is defined using a the Principle of maximum entropy as already proposed for elastic tensor in [4]. Hence only a 3D probabilistic model can give access to the random field u and the related saturation front between the two phases. Moreover, in the case of geological storages, the lateral external bound of Ω ' is quite remote to be included into numerical modeling, nevertheless, no equivalent boundary conditions at finite distance have been proposed in literature in the non-linear case. The basic idea developed in this paper consists in noticing that even though the random field u is fully a 3D field, all its marginal probability density functions are invariant with respect to any rotation around a vertical axis, as long as the domain and the boundary conditions satisfy this invariance property. As a consequence, the mean field and the related mean fluxes are also rotation invariant. Assuming that the mean pressure field satisfies a diffusion equation similar to equation 1 but with rotation invariant coefficients, the general framework introduced in [1] allows the coupling of a 3D probabilistic model at moderate distances from the axis and a 2D rotation-invariant model for the mean field for large radius. Following [2], this model can easily be extended to a probabilistic 2D rotation-invariant model for large radius. This methodology has been applied to the risk assessment of geological storage of carbon dioxide (see figure 1). In particular it is shown that only a few hundreds of Monte-Carlo simulations can give access to reliable statistics on the maximum horizontal extension of the carbon dioxide cloud thanks to a tremendous variance reduction induced by the spatial variability of the permeability field.

2 COUPLING OF 2D-AXISYMMETRIC AND 3D FORMULATIONS

2.1 Axisymmetric solution at finite distance

First, let us state the equations on the 3D model so that the approximate solution satisfies the rotation-invariant conditions in the outer domain. Let us call $S \subset \Omega$ a cylindrical surface bounded by the two planes $z = z^{\pm}$ with a circular cross-section of radius R and let $\Omega_- \subset \Omega$ be the inner domain and $\tilde{\Omega}_+$ be the outer domain (Figure 1). In the outer domain $\tilde{\Omega}_+$ both physical properties and boundary conditions are assumed to have a cylindrical symmetry (therefore, tensor c has to be orthotropic with respect to the z axis). The solution u is rotation invariant only when properties and boundary conditions share the same property.

Let us now consider an approximate 3D solution $\tilde{u}_-(x, y, z)$ satisfying the field Equation 1 in Ω_- together with the boundary conditions on $\partial\Omega \cap \partial\Omega_-$, and $\tilde{u}_+(r, z)$ an axisymmetrical

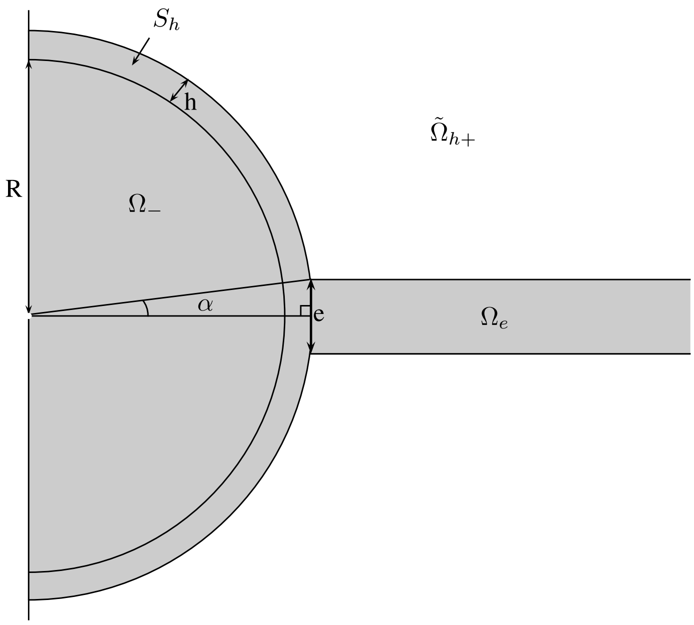

Figure 1: View from above of the considered 3D domain consisting of three parts: Ω_-, the domain where the original 3D formulation of the problem applies, S_h - zone with significant tangent conductivity, Ω_e - 3D slice of a little thickness e conceived to represent the equivalent axisymmetric solution of the problem in $\tilde{\Omega}_{h+}$

solution of Equation 1 in $\tilde{\Omega}_+$ satisfying the boundary conditions on $\partial\Omega\cap\partial\tilde{\Omega}_+$ with the following compatibility conditions on S:

$$\frac{1}{2\pi}\int_0^{2\pi} \tilde{u}_- d\theta = \tilde{u}_+(z,R) \quad , \quad \forall z \in]z^-, z^+[\tag{3}$$

$$\int_0^{2\pi} (c_-\nabla\tilde{u}_-)\cdot e_r R d\theta = q_R(z) \quad , \quad \forall z \in]z^-, z^+[\tag{4}$$

$$\frac{1}{R}\partial_\theta \tilde{u}_- = 0 \quad \text{on} \quad S \tag{5}$$

$$c_{rr}\partial_r \tilde{u}_+ = \frac{q_R(z)}{2\pi R} \quad , \quad \forall z \in]z^-, z^+[\tag{6}$$

where e_r is the outer normal vector of S. Due to orthotropy c_{rr} is the radial hydraulic conductivity and $q_R(z)$ is the vector of radial fluxes crossing S at a given depth z, the fluxes tangent to S vanish.

Penalization of rotation-invariance Equation 5 stating that the solution is rotation-invariant at R is difficult to implement in a Finite Element framework. However, noticing that its left hand side is one of the components of the gradient, a penalization technique is used. Let S_h be a tube of thickness h and internal radius R, $\tilde{\Omega}_{h+} = \tilde{\Omega}_+ \setminus S_h$ and let $c_{\epsilon h}$ be the orthotropic hydraulic conductivity tensor defined on S_h as:

$$c_{\epsilon h} = c_{zz} e_z \otimes e_z + \epsilon^{-1}(c_{\theta\theta} e_\theta \otimes e_\theta + c_{rr} e_r \otimes e_r)$$

for any small ϵ. Equation 5 is replaced by the following field equations and boundary conditions on S_h

$$\operatorname{div}(-c_{\epsilon h}\nabla u_h) = 0 \qquad \text{in } S_h \tag{7}$$
$$u_h = \tilde{u}_- \qquad \text{for } r = R \tag{8}$$
$$u_h = \tilde{u}_+ \qquad \text{for } r = R + h \tag{9}$$
$$(c_-\nabla\tilde{u}_- - c_{\epsilon h}\nabla u_h)\cdot e_r = 0 \qquad \text{for } r = R \tag{10}$$
$$(c_+\nabla\tilde{u}_+ - c_{\epsilon h}\nabla u_h)\cdot e_r = 0 \qquad \text{for } r = R + h \tag{11}$$

Taking the variational form for any virtual field $v = v_o(z) + v_1(\theta, z)\frac{x-R}{h}$ leads to:

$$\begin{aligned}\int_S (\frac{R+h}{R}c_+\nabla\tilde{u}_+ - c_-\nabla\tilde{u}_-)\cdot e_r v_o dS &+\\ \int_S (\frac{R+h}{R}c_+\nabla\tilde{u}_+)\cdot e_r v_1 dS &=\\ \int_{S_h}(c_{zz}\partial_z u_h\cdot\partial_z v + \epsilon^{-1}c_{rr}(\frac{1}{h}\partial_r u_h v_1 + \frac{r-R}{hr^2}\partial_\theta u_h\partial_\theta v_1))dV&\end{aligned} \tag{12}$$

Taking $v_1 = 0$ and $h \to 0$ leads to the balance of fluxes assuming that $\partial_z u_h \cdot \partial_z v$ is bounded:

$$(c_+\nabla\tilde{u}_+ - c_-\nabla\tilde{u}_-)\cdot e_r = 0 \qquad \text{on } S \tag{13}$$

leading to Equation 4.

Hence taking now $v_o = 0$ yields:

$$\begin{aligned}(1+\frac{h}{R})\int_S (c_-\nabla\tilde{u}_-)\cdot e_r v_1 dS &=\\ \int_S (c_{zz}\partial_z\left(\int_R^{R+h} u_h(r-R)\frac{r}{R}dr\right)\partial_z v_1 dS &+\\ \int_{S_h}(\epsilon h)^{-1}c_{rr}(\partial_r u_h v_1 + \frac{r-R}{r^2}\partial_\theta u_h\partial_\theta v_1))dV&\end{aligned} \tag{14}$$

After some calculations the leading terms are:

$$\begin{aligned}\int_S (c_-\nabla\tilde{u}_-)\cdot e_r v_1 dS &=\\ \int_S (c_{zz}\partial_z u_h\partial_z v_1 dS &+\\ (\epsilon)^{-1}\int_S c_{rr}(\partial_r u_h v_1 + \frac{1}{R}\partial_\theta u_h\partial_\theta v_1)dS&\end{aligned} \tag{15}$$

Taking the limit for $\epsilon \to 0$ leads to:

$$\partial_r u_h = 0 \tag{16}$$
$$\frac{1}{R}\partial_\theta u_h = 0 \tag{17}$$

Hence $\tilde{u}_+ = u_h = \tilde{u}_-$ and $\frac{1}{R}\partial_\theta\tilde{u}_- = 0$ yielding Equations 3 and 5.

2.2 Equivalent equations on an outer slice

To implement the coupling in a general purpose 3D Finite Element software, the equations for the rotation invariant part also need to be expressed in 3D. In this section we find new coefficients for equivalent 3D equations in the outer domain $\tilde{\Omega}_+$.

The divergence of any function of cylindrical coordinates $g(r,z)$ can be expressed through the 2D divergence by definition:

$$\mathrm{div} g = \frac{1}{r}\left(\partial_r + \partial_z\right)(rg) = \frac{1}{r}\mathrm{div}_{2\mathrm{D}}(rg) \tag{18}$$

Hence Equation 1 for $\tilde{u}_+$ on Ω_+ can be written as:

$$rd_a\frac{\partial \tilde{u}_+}{\partial t} + \mathrm{div}_{2\mathrm{D}}(-cr\nabla\tilde{u}_+ + r\gamma) = 0 \tag{19}$$

Therefore, the field u_e is defined as the solution of

$$d_{ae}\frac{\partial \tilde{u}_e}{\partial t} + \mathrm{div}_{2\mathrm{D}}(-c_e\nabla\tilde{u}_e + \gamma_e) = 0 \tag{20}$$

on the 3D thin vertical slice $\Omega_e = \Omega \cap S_e$ with $S_e = \{(x,y,z) : R\cos\alpha < x, -e/2 < y < e/2, z^- < z < z^+\}$, where $e = 2(R+h)\sin\alpha$ is the thickness of the slice. The new coefficients are $d_{ae}(x,y,z) = \frac{2\pi x}{e}d_a(r=x,z)$, $c_e(x,y,z) = \frac{2\pi x}{e}c(r=x,z)$, $\gamma_e(x,y,z) = \frac{2\pi x}{e}\gamma(r=x,z)$. The following boundary conditions apply:

$$\partial_y\tilde{u}_e = 0 \qquad \text{for } y = \pm e/2 \tag{21}$$

$$\tilde{u}_e = \tilde{u}_+(R+h,z) \quad \text{for } x = (R+h)\cos\alpha \tag{22}$$

Since the slice and the boundary conditions are invariant with respect to y so is the field $\tilde{u}_e$. In addition, it obviously satisfy

$$\tilde{u}_e(x,y,z) = \tilde{u}_+(r=x,z)$$

Moreover the two solutions being equal we can also show that the related fluxes coincide:

$$q_R = \int_0^{2\pi} c\nabla\tilde{u}_+(R+h)d\theta = 2\pi(R+h)c\partial_r\tilde{u}_+ = ec_e(x=(R+h),y,z)\partial_x u_e = \int_{-e/2}^{e/2} c_e\partial_x u_e dy$$

2.3 Approximate 3D solution on the entire cylinder-slice domain

Combining the two above methods, we can define the approximation solution $\tilde{u}_{he}$ satisfying Equation 1 on a composite domain $\Omega_- \cup S_h \cup \Omega_e$ shown in Figure 1

$$\tilde{u}_{he} = \tilde{u}_- \quad \text{in} \quad \Omega_- \tag{23}$$

$$\tilde{u}_{he} = \tilde{u}_h \quad \text{in} \quad S_h \tag{24}$$

$$\tilde{u}_{he} = \tilde{u}_e \quad \text{in} \quad \Omega_e \tag{25}$$

with the following vanishing flux boundary conditions:

$$\partial_r\tilde{u}_{he} = 0 \quad \text{for} \quad r = R+h, \theta = [\alpha, 2\pi-\alpha] \tag{26}$$

$$\partial_y\tilde{u}_{he} = 0 \quad \text{for} \quad y = \pm e/2, x > (R+h)\cos\alpha \tag{27}$$

$$\partial_z\tilde{u}_{he} = 0 \quad \text{for} \quad z = z^\pm \tag{28}$$

3 NUMERICAL IMPLEMENTATION

The coupled model consists of 3 domains in which the same structure of equations is followed with different coefficients according to the developments in Section 2. The inner zone has a cylindrical mesh, tetrahedral elements are used in the vicinity of the injection well allowing sufficient refining, the totality of inner zone numbers $1.1 \cdot 10^4$ elements. The transition zone S_h is represented by one layer of cylindrical elements (Figure 2). The entire problem is solved for $1.5 \cdot 10^5$ degrees of freedom.

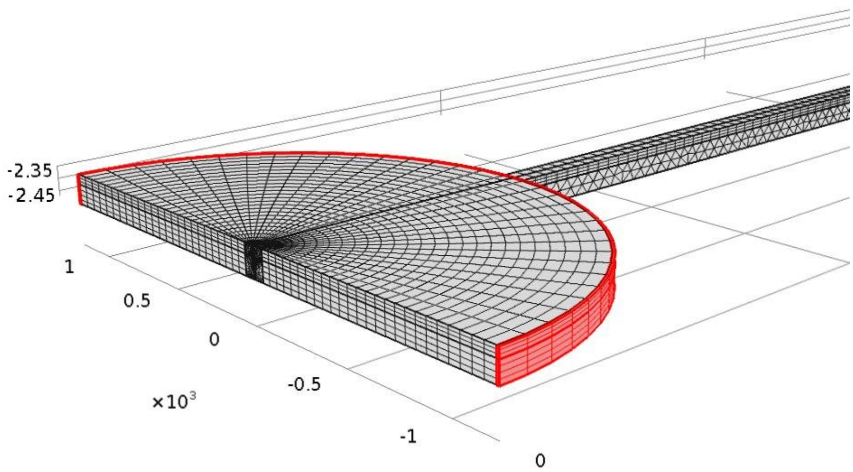

Figure 2: The mesh of the coupled model: 3D zone and rotation-invariant continuation, the transition zone (S_h) is highlighted in red.

A lognormal random field of permeability introduced into the model [5] has the following characteristics: the mean value and standard deviation are 10^{-13} m^2 and $4.9 \cdot 10^{-27}$ m^2 for the horizontal component; 10^{-14} m^2 and $4.9 \cdot 10^{-28}$ m^2 respectively for the vertical component; correlation function in the form of a squared cardinal sine is chosen with correlation lengths (ℓ_x, ℓ_y, ℓ_z) = (50 m, 50 m, 20 m).

In the context of Risk Assessment the quantity of interest considered in this study is the probability that the maximal extent of the carbon dioxide (r_{max}) exceeds a certain radius r_0. The performed 100 simulations are insufficient to obtain maximal extent statistics for a fixed angle θ. Nevertheless, we define an estimator of the cumulative density function of the maximum radius using angular averaging. To do so, an indicator function *h* which equals to 0 for radius exceeding r_0 is considered:

$$h(\omega, r_0 - r_{max}(\theta)) = \begin{cases} 1, & r_{\max} \le r_0 \\ 0, & r_{\max} > r_0 \end{cases} \tag{29}$$

The statistical quantity $\overline{h}(r_0)$ representing the ensemble average of the function $h(r_0)$ would give the cumulative probability at radius r_0:

$$\overline{h}(r_0) = \mathbb{E}(h(\omega, r_0 - r_{\max})) = \int_\Omega h(\omega, r_0 - r_{\max}) dP(\omega) = \tag{30}$$
$$= \int_0^{+\infty} h(r_0 - r) p_{r_{\max}}(r) dr = P(r_{\max} < r_0),$$

where $\omega = \{\omega_i\}$, i=1,...100 is the number of the sample.

Introducing the spatial average $H(\omega, r_0)$ allows an estimate of the cumulative probability in the following way:

$$P(r_{max} < r_0) = \overline{H}(r_0) \approx \widehat{H}(r_0) = \frac{1}{N} \sum_{i=1}^{N} H(\omega_i, r_0) \tag{31}$$

Computing P($r_{max} <$ r_0) for each r_0 gives the whole CDF curve of the maximal lateral spread r_{max}. The resulting complementary cumulative distribution function (1-$\widehat{H}(r_0)$) is shown in Figure 3 together with the N=100 samples of 1-$H(\omega_i, r_0)$.

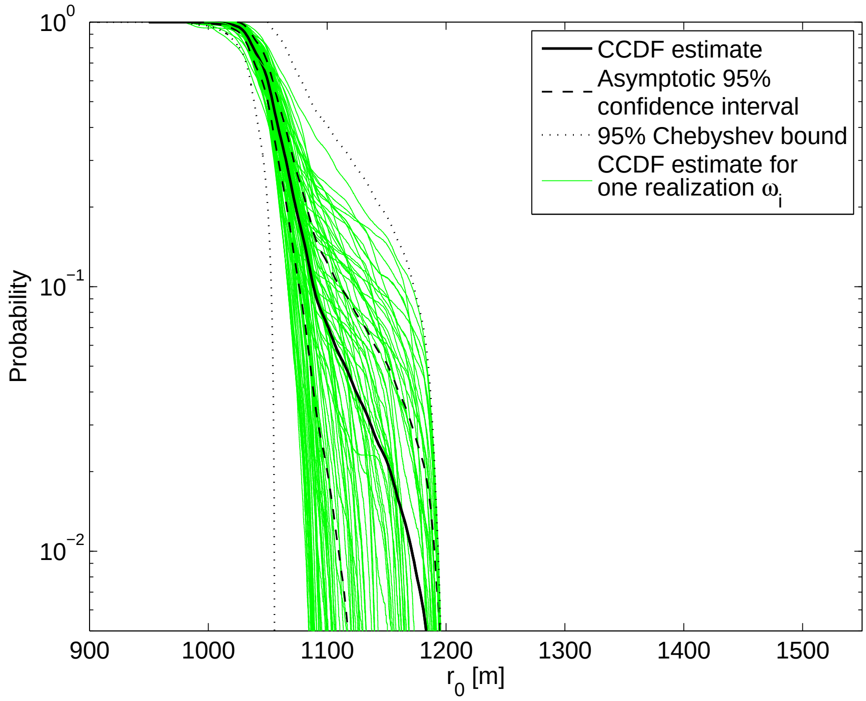

Figure 3: Estimate of the complementary cumulative density function (CCDF) of the maximal lateral spread (in black) for the case of heterogeneous permeability; the curves 1-$H(\omega_i, r_0)$ for each model output: 100 samples (in green), the theoretical 95% confidence interval is computed as $\sqrt{P(1-P)/100}$ and Chebyshev 95% bound is computed as $\pm k\sigma$, where $k = 1/\sqrt{1-0.95}$ and σ is the standard deviation of the values 1-$H(\omega_i, r_0)$ for each given r_0.

The asymptotic standard deviation of the estimator $\widehat{H}(r_0)$ is expressed as [6]:

$$\sigma_{\widehat{H}} = \sqrt{\frac{1}{N} \overline{H}(r_0)(1 - \overline{H}(r_0))} \approx \sqrt{\frac{1}{N} \widehat{H}(r_0)(1 - \widehat{H}(r_0))}.$$

4 CONCLUSIONS

The main contributions of the work are:

- A theoretical framework for a coupling of 3D and rotation invariant models is proposed for diffusion-type problems
- The coupling is implemented in a 3D Finite Element model. The model predicts the underground fluxes during and after CO_2 injection in a deep saline aquifer.
- Developed statistical estimator gives access to probabilistic quantities of interest such as threshold exceedence probability for the maximal extent of the carbon dioxide after 10 years of injection.

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