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NUMERICAL ZOOM FOR A MULTI-SCALE PROBLEM

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Abstract.

While working on a complex simulation problem, namely the safety assessment of a nuclear waste repository underground in a clay layer, we observed the necessity of numerical zooms to speed-up the calculations. The problem has several scales du to the geometry, the various geological constants and the time scales.

The domain is decomposed into a large one where the simulations may not be precise and a small one where precision is required; the Chimera method [6] is well adapted to this. In Brezzi et al [1] it was shown to be a particular implementation of Schwarz' method and of Lions'space decomposition method [5] (SDM). The method was analyzed in [1] and in [2] for elliptic problems.

Here we shall present the parabolic case, which occurs for the study of the convection-diffusion of a radionuclide in the clay underground around the repository. The domain is too large and too complex to be discretized in all details. On the other hand the source terms are confined to a small zone. The computations are done in subdomains and the problem is to find a converging strategy for the boundary conditions.

1 Multi-scale Problems

Analysis of results are usually done after the modelling and simulation are completed. Yet with online graphics and interactive development it may be a good idea to make the modelling and the simulations an integrated part of the interactive design. This is particularly useful when the problem is multi-scale because the results are also analyzed usually from a multi-scale view point.

Without loss of generality let us present the problem on which we have applied this paradigm and the solution proposed.

The safety analysis for a nuclear waste repository site is a multi-scale problem because the site extends over several kilometers while the waste is confined by canisters not bigger than a few meters. The time scales are also of a hundred years for the cooling phase, of a few centuries for the leaking phase of the canisters and of up to a million year for the migration phase.

We wish to study a simplified version of the site currently investigated by Andra below the village of Bure, in the west in France, at a depth of 450 m, in a layer of clay, above a layer of dogger-limestone and below a geological layer of limestone and marl.

Water flows slowly through these porous media in a saturated state and convects the radioactive materials after some thousands of years when the canisters have rusted.

The first problem then is to compute accurately the time independent hydrostatic pressure by Darcy's law. The computational domain is $\Omega = (0, 25000) \times (0, 695) \times (0, 300)$. The repository, denoted by R, is in the clay layer. Darcy's law says that the water velocity u is proportional to the gradient of the hydrostatic pressure $\vec{u} = K\nabla H$ and saturation and incompressibility imply $\nabla \cdot u = 0$.

$$K_{marl} = 3.15310^{-5} \quad K_{lim} = 6.3072$$
$$K_{clay} = 3.15310^{-6} \quad K_{dog} = 25.2288$$

Finally H is given on the soil surface and on the lateral boundaries. Homogeneous Neumann conditions are taken on the other boundaries.

In R there are galleries and horizontal holes to store the canisters. Around these the terrain is damaged, and the Darcy constant K is increased ten fold.

The second problem is to study the advection and diffusion of the radio-nucleides. It is governed by a linear convection-diffusion-dissipation equation where the source term is in the initial condition because the time during which the canisters leak is short (2000 years) compared to the time scale of the advection-diffusion.

Such systems are more accurately solved by Discontinuous Galerkin Finite Element Method, but these are an order of magnitude more expensive than standard linear elements for a given number of element (which is the leading factor to describe the geometry).

The paper describes a zooming strategy with a possibility to change the resolution module locally. On Darcy's law, numerical zoom (i.e. neglecting part of the domain in the simulation) is based on Schwarz algorithm or rather on the Chimera version suggested by Lions et al in [4]. On the convection-diffusion-dissipation equation, zooming is based on the fact that the source term is localized in R and because the concentration decays exponentially with the distance to the source. The fact that the resolution module can be changed is more an implementation feast than a theoretical advance.

2 Chimera and DDM

Consider Darcy's law for saturated stationary flow through porous media

$$-\nabla\cdot(K\nabla H) = f \text{ in } \Omega, \quad H \text{ or } (K\nabla H)\cdot n \text{ given on } \Gamma = \partial\Omega. \tag{1}$$

To make the presentation easier assume that a translation has been made to bring zero Dirichlet conditions on H. Consider the case where $\Omega = \Omega_1 \cup \Omega_2$, with overlapping and denote $\Sigma_i = \partial\Omega_i \cap \Omega_j,\ j = i + 1\%2$ and $S_i = \partial\Omega_i \backslash \Sigma_i$.

The Chimera method presented in [2] is based on the discrete formulation: find $u_{ih} \in V_{ih},\ i = 1, 2$ solution of

$$\int_\Omega K\nabla(u_{1h} + u_{2h})\cdot\nabla(\hat{u}_{1h} + \hat{u}_{2h}) = \int_\Omega f(\hat{u}_{1h} + \hat{u}_{2h}) \quad \forall\hat{u}_{ih} \in V_{ih} \tag{2}$$

where V_{ih} is an approximation of $H^1_0(\Omega_i)$.

The easiest is to solve (2) by a fixed point algorithm wherein u_{ih} is assumed to be known to compute u_{jh} by (2) with $\hat{u}_{ih} = 0,\ j \neq i$; however convergence is guaranteed only if a regularization term $\beta > 0$ is added, so that one finds $u^{m+1}_{ih} \in V_{ih}$ such that $\forall\hat{u}_{ih} \in V_{ih}$

$$\int_\Omega (\beta(u^{m+1}_{ih} - u^m_{ih})\hat{u}_{ih} + K\nabla(u^{m+1}_{ih} + u^m_{jh})\cdot\nabla\hat{u}_{ih}) = \int_\Omega f\hat{u}_{ih} \tag{3}$$

2.1 Numerical Zoom and Mesh Refinement

When $\Omega_1 = \Omega_2$ the method consists in improving the calculation on one mesh by a computation on another mesh. For a preliminary analysis numerical zoom can be framed into this case. The idea is that in some region the mesh is refined (the zoom) and elsewhere it is kept unchanged. In such case we do not want to converge the process (4) but only perform one or two iterations and obtain an improvement over the solution computed on the course mesh.

Usually the algorithm is initialized by $u^0_{kh} = 0$. Then the first 2 iterations are

$$\begin{aligned}
&\int_\Omega (\beta u^1_{1h}\hat{u}_{1h} + K\nabla u^1_{1h}\cdot\nabla\hat{u}_{1h}) = \int_\Omega f\hat{u}_{1h} \ \ \forall\hat{u}_{1h}\\
&\int_\Omega (\beta u^1_{2h}\hat{u}_{2h} + K\nabla u^1_{2h}\cdot\nabla\hat{u}_{2h}) = \int_\Omega f\hat{u}_{2h} \ \ \forall\hat{u}_{2h}\\
&\int_\Omega (\beta(u^2_{1h} - u^1_{1h})\hat{u}_{1h} + K\nabla(u^2_{1h} + u^1_{2h})\cdot\nabla\hat{u}_{1h}) = \int_\Omega f\hat{u}_{1h} \ \ \forall\hat{u}_{1h}\\
&\int_\Omega (\beta(u^2_{2h} - u^1_{2h})\hat{u}_{2h} + K\nabla(u^2_{2h} + u^1_{1h})\cdot\nabla\hat{u}_{2h}) = \int_\Omega f\hat{u}_{2h} \ \ \forall\hat{u}_{2h}
\end{aligned} \tag{4}$$

The Problem. So the problem is to show that u^1_{1h} contains the $O(1)$ part of the solution and that u^2_{2h} is small.

Unless otherwise specified V_{ih} is the P^1 finite element space; the elements are triangles or tetrahedra.

Mesh Refinement. Assume that V_{1h} is built on a course mesh and that V_{2h} is built on a finer mesh obtained by dividing some elements of the first mesh; then V_{1h} is a subspace of V_{2h} and so u_{1h} belongs to V_{2h} also. Assume $\beta = 0$. With obvious notations,

$$\begin{aligned}&\|u^2_{2h} + u^1_{1h} - u\| \le Ch_2\\ &\|u^1_{1h} - u\| \le Ch_1\\ &\|u^2_{2h}\| \le \|u^2_{2h} + u^1_{1h} - u\| + \|u^1_{1h} - u\| \le C(h_1 + h_2)\end{aligned} \tag{5}$$

which proves that

Proposition 1 *When mesh 2 is a refinement of mesh 1, u^2_{2h} is an $O(h_1)$ correction to u^1_{1h} such that the sum approximates the exact solution with an optimal error of $O(h_2)$.*

Approximated Mesh Refinement. When $\mathcal{T}_{2h}$ is a perturbation of a sub-triangulation of $\mathcal{T}_{1h}$ we can still assert that u^2_{2h} will be a correction to u^1_{1h}.

Assume that each vertex q_i of the triangulation $\mathcal{T}_{2h}$ can be moved to $q_i + \delta q_i$ so that the new triangulation $\mathcal{T}_{2\hbar}$ is a sub-triangulation of $\mathcal{T}_{1h}$. With $\delta q_h(x) := \sum_j \delta q_j w^j(x)$ and w^j the hat functions of $\mathcal{T}_{2\hbar}$, we have (up to higher order terms)

$$\delta w^k = -\nabla w^k \cdot \delta q_h \text{ and } \delta \int_\Omega f = \int_\Omega \nabla \cdot (f \delta q_h) \tag{6}$$

Therefore let $\delta u_{2h} := u_{2\hbar} - u_{2h}$ where u_{2h} is the solution on $\mathcal{T}_{2h}$ and $u_{2\hbar}$ the solution on $\mathcal{T}_{2\hbar}$, then the following can be shown (see [7])

$$\int_\Omega \nabla \delta u_{2h} \nabla w_h = \int_\Omega \nabla u_{2h} (\nabla \delta q_h + \nabla \delta q_h^T - \nabla \cdot \delta q_h) \nabla w_h$$

Thus $\|u_{2h} - u_{2\hbar}\|$ is bounded by $\|\nabla \delta q_h + \nabla \delta q_h^T - \nabla \cdot \delta q_h\|$ which is $O(h_2^\alpha)$, $\alpha = 1, 2$ depending on the smoothness of $\lim_h \delta q_h$. This means that (4) will give $\|u^2_{2h}\| = O(h_1 + h_2^\alpha)$.

When Ω_2 is a sub-domain of $\Omega_1 = \Omega$ then we must use another idea connected with the fact that $u_{2h}|_{\Sigma_2} = 0$ is an approximation of the value it would have had if $\Omega_2 = \Omega$.

3 Darcy's Law: Numerical Implementation and Results

The domain is always a rectangular box, either because it is the physical domain (Figure 1) or because it is the numerical zoom.

The selection of the numerical zoom is done by the user within the public domain visualization software `medit` [9]. A patch to the software has been written for us by P. Frey which allows to select a region with the mouse.

Then the automatic triangulation of the zoom domain is done within the open source tool `freefem3D` [8] and the boundary condition $u_2 = 0$ are applied automatically on the zoom bounding box. Therefore the mesh in the zoom region has nothing to do with the mesh at one level up.

The computation of the integrals in the variational formulations involves products of functions defined on different meshes; quadrature points are used within each element of both triangulations as proposed in [2].

This strategy is applied thrice and the results are shown on Figures 2,3 and 4.

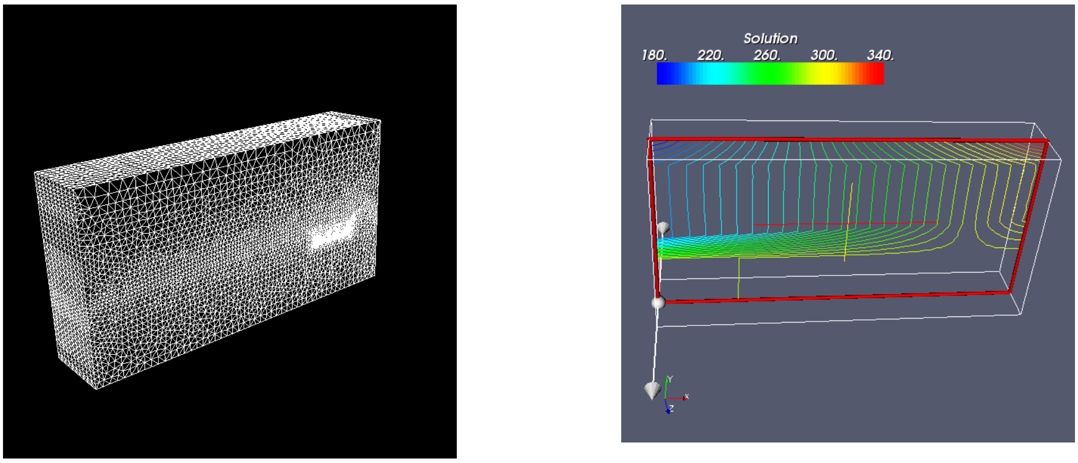

Figure 1: Mesh and solution u_{1h}^1 of Darcy's equation in the entire domain. The triangulation is too coarse to account for all the details in the repository.

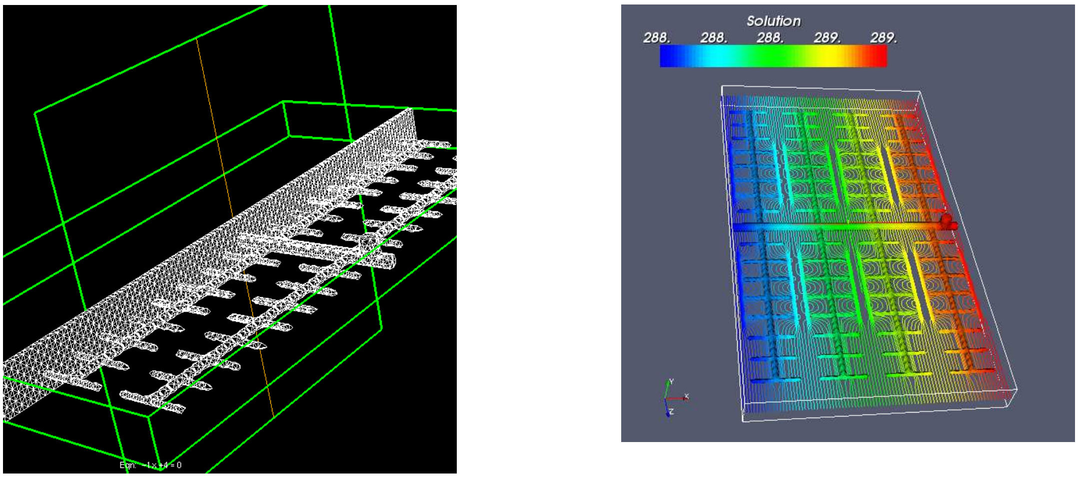

Figure 2: First zoom: triangulation and solution $u_{1h}^1 + u_{2h}^2$ of Darcy's equation in the clay layer around the repository Ω_2. Here u_{1h}^1 is the one shown on Figure 1 and it is not recomputed.

Perspectives

The method proposed raises several questions:

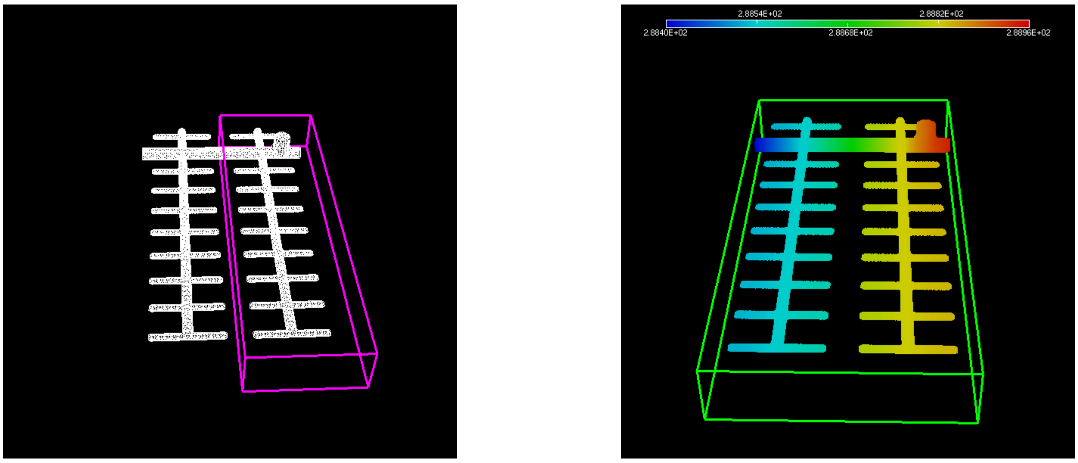

Figure 3: Second zoom: triangulation and Solution of Darcy's equation in a region which is smaller than the entire site. Only a u^3_{2h} is computed in Ω_2 shown on the left with $u^2_{1h} = u^1_{1h} + u^2_{2h}$.

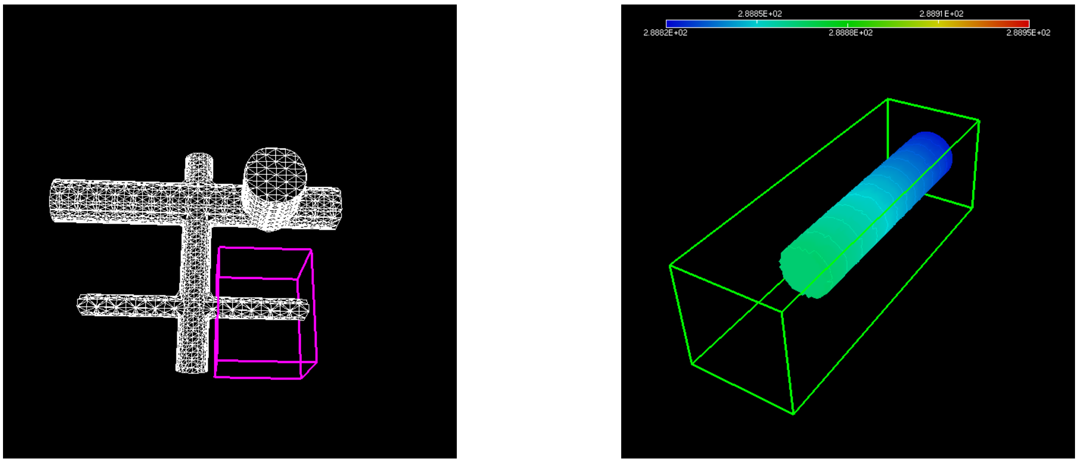

Figure 4: Third zoom: triangulation and solution of Darcy's equation in a region near a single gallery. As above only a u^4_{2h} is computed in Ω_2 shown on the left with $u^3_{1h} = u^1_{1h} + u^2_{2h} + u^3_{2h}$.

- It seems to work even though it is justified only in very special cases and with two levels only.
- A natural method for numerical zooms would be to use Schwarz algorithm and apply on the zoom bounding box Dirichlet conditions from one course level up. The drawback is that the computations are no longer corrections to the solution, but still it seems to perform just as well. We know of counter examples for convergence, but these seems not to occur in practice, so are we doing better?
- The method is very sensitive to the position of the quadrature points which should not be too close to any of the vertices. Can we live with that?

The same strategy can be applied to the convection diffusion part with even greater success because the source terms are confined to a very small region. The results will be shown at the time of the conference and in the proceedings. We will also report on a good behavior of the interpolation operators on the method when we switch from a P^1 finite element method on a coarse level to a Discontinuous - Galerkin method on the lower level.

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