Research field option

CASE STUDY 5
Comparative study of numerical tools to solve closure problems in porous media

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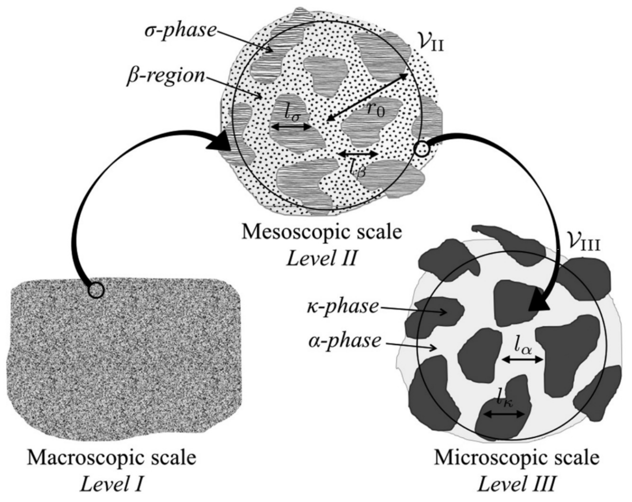
1 Introduction and context

1.1 Description of the problem

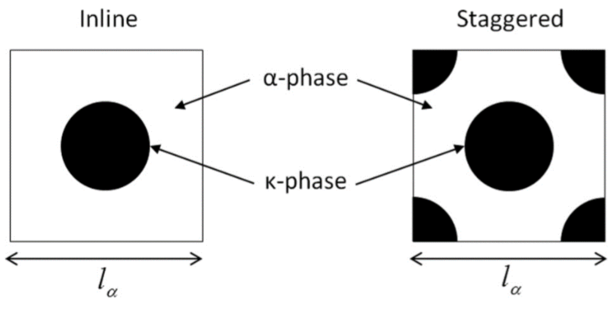
Porous media are composed of empty spaces, called pores (α phase), embedded in a solid or semisolid frame (κ phase), and as such, fluids can flow through them. They are ubiquitous in engineering processes regarding energy and health, from petroleum industry to bio engineering. In such systems, studying the viscous flow mechanism is of great interest. However, the structure is too complex for direct analysis of transport equations within the pores at the macroscopic scale. We can solve transport equations in a pore with numerical tools at the microscopic scale, but deploying such a method at bigger scales would cost lots of computing resources and time. So the homogenization is performed to handle this difficulty. It is based on volume-averaging method which derive the averaged physical properties in a representative volume and extends them to a larger scale.

Figure 1: From microscopic to macroscopic[2]



The reason to use homogenization is to rigorously derive continuum equations for multi phase systems[7]. The key issue is to use local volume averaged equations which are valid everywhere to simplify the calculation. The chosen scale of the average volume must be representative enough to be applied to the whole media. To simplify this process, we take the two elementary volumes as below, as well as performing the homogenization on it. After volume averaging, Darcy's law (3) can be applied to such a scale by solving the closure problem[7].

Figure 2: Simplified elementary volume[2]



The radius of the κ-phase in the center is noted as r_1, and the radius of the corner spheres is noted as r_2.

1.2 Objectives of the study

The objective is to carry out a comparative study of different numerical tools for solving the closure problem. It consists of 3 tasks as below:

- *Get started with different finite elements software programs :* The first objective is to get familiar with OpenFOAM and compare its results with FEnicS, but we also propose another tool: NGSolve.
- *Solve the closure problem :* We apply proper solvers in different pieces of software to solve the same closure problem.
- *Compare their performance :* We rank the different programs depending on the quality of their results, their computation time and their user-friendliness.

2 Methods

2.1 Equation

The velocity field $\underline{v}_\alpha$ in the α phase is determined with incompressible, steady Stokes equations [7]:

$$\begin{cases} \nabla \cdot v_\alpha = 0 \\ 0 = -\nabla p_\alpha + \mu_\alpha \nabla^2 \underline{v}_\alpha \\ \underline{v}_\alpha = 0 & \text{at } \mathcal{A}_{\alpha\kappa} \\ \underline{v}_\alpha = \underline{f}(\underline{r}, t) & \text{at } \mathcal{A}_{\alpha e} \end{cases} \tag{1}$$

p_α and μ_α are the pressure and viscosity in the α-phase, and $\mathcal{A}_{\alpha\kappa}$ and $\mathcal{A}_{\alpha e}$is are respectively the interfaces between the solid and the fluid, and between the fluid and the exterior.

The homogenization based on volume-averaging is then performed as below[7],

$$\langle \psi \rangle = \frac{1}{V_\alpha + V_\kappa} \int_{V_\alpha + V_\kappa} \psi_\alpha dV \tag{2}$$

where ψ is the arbitrary physical quantity which can be v or p. V_α and V_κ are the volume of corresponding phase.

Then we can apply Darcy's law to this volume,

$$\langle v \rangle = -\frac{\underline{\underline{K}}}{\epsilon \mu_\alpha} \nabla \langle p \rangle \tag{3}$$

where $\langle v \rangle$ is the averaged velocity and $\langle p \rangle$ the averaged pressure. ϵ is the porosity defined as

$$\epsilon = \frac{V_\alpha}{V_\alpha + V_\kappa} \tag{4}$$

$\underline{\underline{K}}$ is the permeability tensor, the value of which is uniquely determined by the pore geometry and is independent of the properties of the penetrating fluid[1]. It is a function of closure variables, which lead to the closure problem.

We then characterize the permeability with these two configurations by solving the closure problem with equations[7] in α-phase below,

$$\begin{cases} 0 = -\nabla \underline{b} + \nabla^2 \underline{\underline{B}} + \underline{\underline{I}} \\ \nabla \cdot \underline{\underline{B}} = 0 \end{cases} \tag{5}$$

where $\underline{b}$ and $\underline{\underline{B}}$ are closure variables. The boundary conditions are defined as below :

$$\begin{cases} \underline{\underline{B}} = 0 \text{ at } \partial\Omega_\alpha \bigcap \partial\Omega_\kappa \\ \text{periodic at } \partial\Omega_\alpha \setminus \partial\Omega_\kappa \end{cases} \tag{6}$$

The permeability tensor can then be derived by the equation below,

$$\langle B \rangle^\alpha = \epsilon^{-1} \underline{\underline{K}} \tag{7}$$

where $\langle B \rangle^\alpha$ is the averaged closure variable, averaged on V_α.

2.2 Protocol

The equations (5) were implemented on OpenFoam and NGSolve, component by component, in order to obtain the permeability tensor with equation (7). First, a grid convergence test was made to check that all three tools converged. Then, the results were compared with FEniCS and [8] to assess the quality of the solution, by plotting the coefficient $C = \frac{2}{9} \frac{r_1^2}{1-\epsilon} \frac{1}{K_{xx}}$ in function of the porosity. Comparisons were made for both geometries of figure 2, in 3D. The execution time was also computed.

2.3 How time execution of the programs is computed ?

All the commands used to compute a single iteration of the program are put into a bash script. For instance, for FEniCS, the script `python_exec.sh` is the following:

```
#!/bin/bash
python3 OLI9_maillage3D.py > /dev/null 2> /dev/null
python3 OLI9_perm3D.py > /dev/null 2> /dev/null
```

The `> /dev/null 2> /dev/null` are there to avoid the log messages from the program. As we cannot see the logs, we must be sure that the program terminates.

This bash script is then called 50 times with the `time` command, to compute the execution time of a single bash script. For instance, for FEniCS, the slurm script is the following:

```
#!/bin/bash
#SBATCH --job-name=testFenics
#SBATCH --output=%x.o%j
#SBATCH --ntasks=1
#SBATCH --mem=32G
#SBATCH --time=01:00:00
#SBATCH --partition=cpu_short

# To clean and load modules defined at the compile and link phases
module purge
module load anaconda3/2021.05/gcc-9.2.0

# To compute in the submission directory
cd ${SLURM_SUBMIT_DIR}
cd TestFenics

source activate fenicsproject

# execution
for i in {0..49}
do
time ./python_exec.sh
done

conda deactivate
```

The resulting log file is then such as this:

```
real 0m28.448s
user 0m6.288s
sys 0m0.848s

real 0m7.753s
user 0m5.695s
sys 0m0.505s

real 0m8.999s
user 0m5.344s
sys 0m0.389s
```

```
real 0m6.302s
user 0m5.454s
sys 0m0.464s
...
```

The `real` time is the important one, and can be easily retrieved with a simple python script, and all the time can be processed to obtain the median and the maximum.

3 Software programs

3.1 OpenFOAM

Presentation

OpenFOAM (Open-source Field Operation And Manipulation) is a Linux software encompassing several 3D numerical solvers for continuum mechanics, and mainly CFD (computational fluid dynamics). These solvers are coded in C++, but OpenFOAM comes with its own programming language, used for three tasks : creating the mesh, choosing the solver (and its options), and the post-processing functions (used here to compute the average over all the grid).

Usage on the Mésocentre

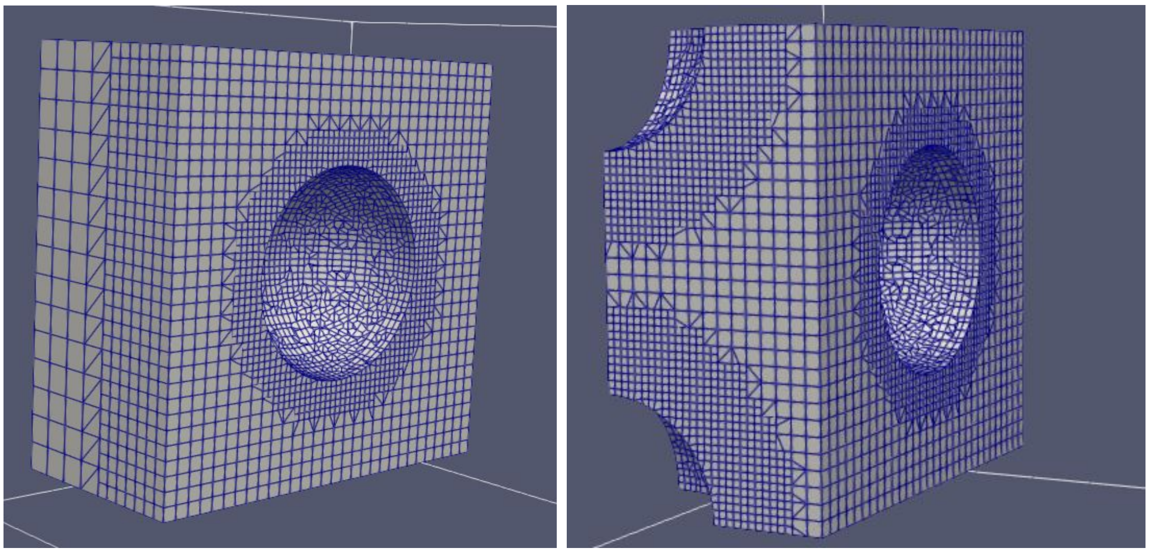
The module `openfoam/2106/gcc-9.2.0-openmpi` must be loaded:
`module load openfoam/2106/gcc-9.2.0-openmpi`.

The version **2106** is important, as tests with the other version *1912* were not successful. In the same way, the opensource version of OpenFOAM (`openfoam/6/intel-19.0.3.199` or `openfoam/8/intel-19.0.3.199`) are not suitable.

Mesh

The two geometries below have been created :

Figure 3: Meshes created by OpenFoam and visualized with Paraview

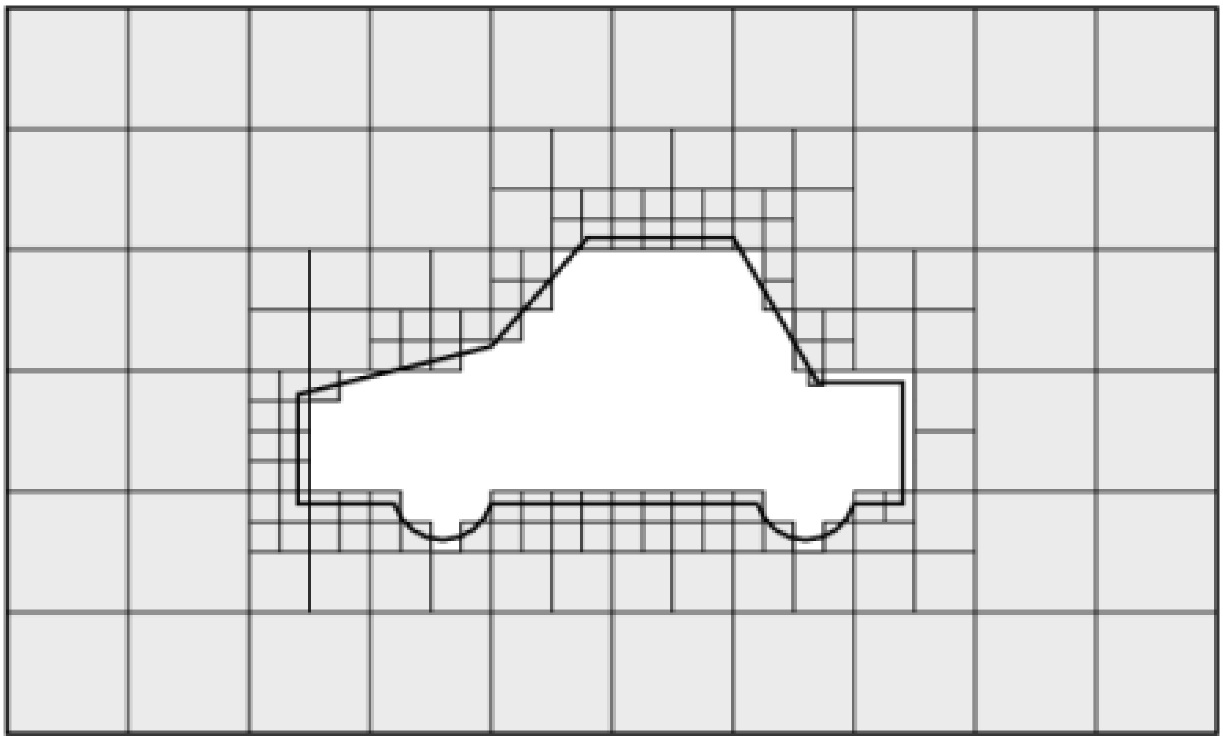


Several tools are available in OpenFoam to create a mesh ; the built-in utility `blockMesh` allows creating simple geometries and was used for the background cube.

To create a mesh with this utility, the geometry must first be split into different blocks, each one with exactly 8 vertices. Then, each block is meshed, and the user can choose the form (hexahedron, prism, wedge...), the number and expansion ratio of the elements for each direction.

For more sophisticated geometries, the utility `snappyHexMesh` can be used. A user-specified volume, defined for instance in an STL file (in our case, a sphere) is "removed" from the background mesh (defined with `blockMesh`). The cells that intersect the surface of the volume are refined, and all the elements that do not have at least 50 % of their volume outside the geometry are removed, as shown below :

Figure 4: Example of cell removal with snappyHexMesh



Solvers

Five solvers are available to solve Navier-Stokes equations for incompressible flow : `boundaryFoam`, `icoFoam`, `pimpleFoam`, `pisoFoam` and `simpleFoam`. `icoFoam` doesn't allow for a source term in the equation, so it was discarded. Since `simpleFoam` is one of the few solvers specialized for the steady-state equation, it was privileged. It does not solve exactly the equation we want, taking into account the inertial term $\nabla \cdot (\underline{u} \times \underline{u})$. However, this term should be of minor importance, since we are working with very low Reynolds numbers. This solver is based upon the SIMPLE algorithm. This algorithm seeks to solve the equation :

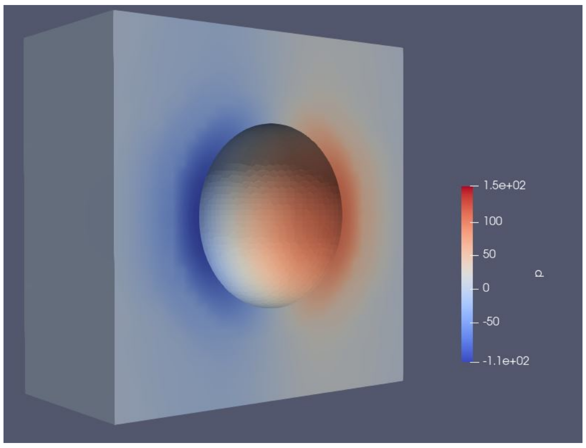
$$\begin{cases} \nabla \cdot (\underline{u} \times \underline{u}) - \nabla \cdot \underline{\underline{R}} = -\nabla p + \underline{S} \\ \nabla \cdot \underline{u} = 0 \end{cases} \tag{8}$$

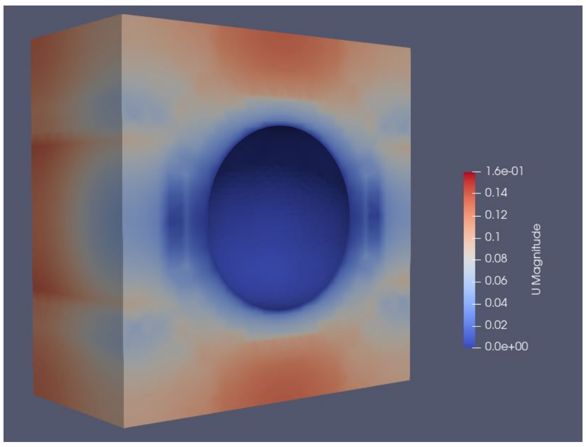
where $\underline{\mathrm{u}}$ is the velocity, p the pressure, $\underline{\underline{\mathrm{R}}}$ the stress tensor and $\underline{\mathrm{S}}$ the source term.
The algorithm works as follows :

1. Advance to the next time step t^{n+1}
2. Initialize $\underline{u}^{n+1}$ and p^{n+1} using the latest available values
3. Discretize the momentum equation in the form $\underline{\underline{M}}\underline{u} = -\nabla p$, and write $\underline{\underline{M}}\underline{u} = \underline{\underline{A}}\underline{u} - \underline{H}$ with $\underline{\underline{A}}$ the matrix containing only the diagonal elements of $\underline{\underline{M}}$
4. Use the new expression $\underline{u} = \underline{\underline{A}}^{-1}\underline{H} - \underline{\underline{A}}^{-1}\nabla p$ in the continuity equation, which becomes $\nabla \cdot (\underline{\underline{A}}^{-1}\underline{H}) = \nabla \cdot (\underline{\underline{A}}^{-1}\nabla p)$
5. Solve the continuity equation for p, and update the value for $\underline{u}$ with the expression $\underline{u} = \underline{\underline{A}}^{-1}\underline{H} - \underline{\underline{A}}^{-1}\nabla p$
6. Go back to step 2 if the algorithm has not converged

The user can choose the value of the viscosity ν and the source term, the discretization schemes used by the solver to compute the derivatives, the tolerance value for the residuals below which the algorithm considers there is convergence and stops the loop, the boundary conditions (cyclic, Neumann-type, Dirichlet-type, etc.), the turbulence model (it was deactivated in our case)... Cyclic conditions were enforced on the external boundaries for both pressure and velocity, and the conditions $\underline{u} = 0$ and $\nabla p = 0$ were imposed at the interface between the two phases. Since p is defined up to an additive constant, the user must select a reference cell, that will be set to a reference value (also chosen by the user).
The results obtained with the source term (1 0 0) are shown below :

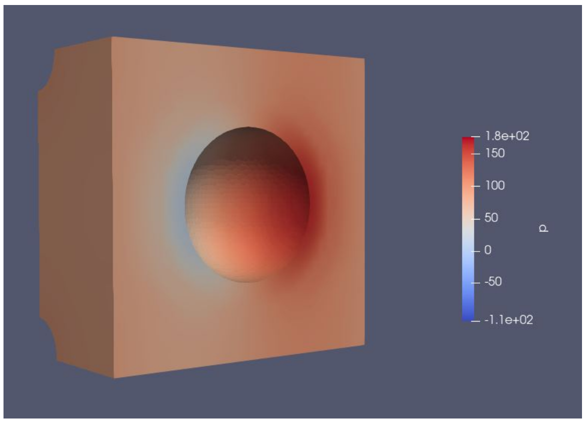
Figure 5: Fields obtained with simpleFoam, with $r_1 = 0.25$, and $r_2 \in \{0, 0.125\}$

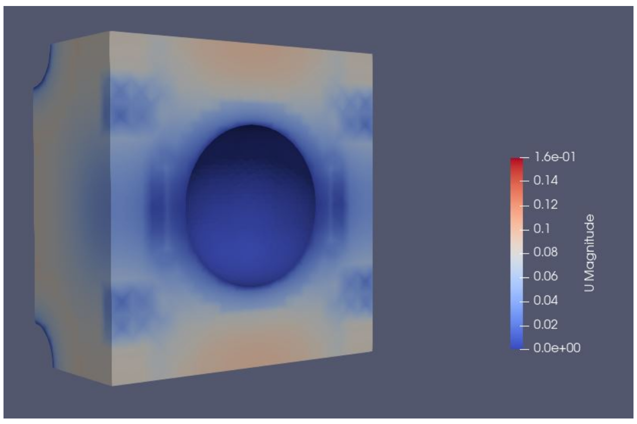




Pseudo-pressure field

Magnitude of pseudo-velocity field





3.2 NGS-Py Finite Element Tool

Presentation

Netgen [4] is an automatic 2D and 3D tetrahedral mesh generator. NGSolve [3, 5] is a finite element library which can be linked to Netgen and contains arbitrary order finite elements of all standard element geometries, scalar, vector-valued, hybrid DG finite element spaces. Program flow as well as geometry description and equation setup can be controlled from Python. Together they offer a rich Python interface inspired by the FEniCS project.

Installation

You first need to create a conda environment for NGSolve:
`conda create --name ngsolveprojets`
Then you need to activate it: `conda activate ngsolveprojets`.
Then, instructions can be found on the NGSolve website:

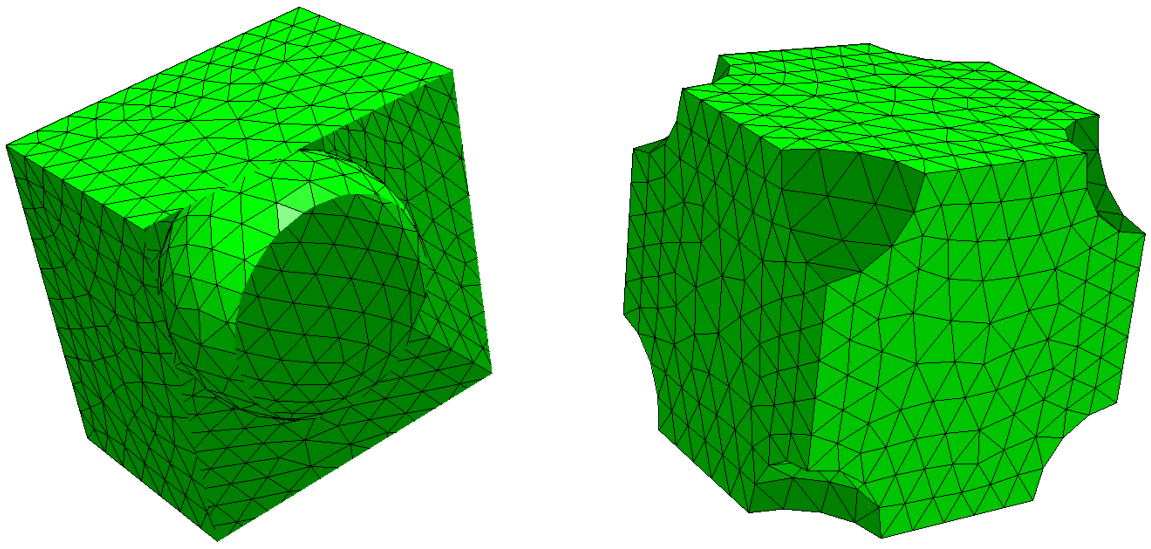
- Add conda-forge and ngsolve channels:
  ```
  conda config --add channels conda-forge
  conda config --add channels ngsolve
  ```
- Install NGSolve: `conda install ngsolve`

The anaconda environment must be activated every time NGSolve will be used:
`conda activate ngsolveprojets`
Once the environment loaded, a simple `python3 program.py` runs the python program with NGSolve.

Mesh

Netgen allows for precise control of the meshing process while still providing automatic options. The geometry can be constructed either using a point-edge-shape system alike GMSH either using shapes primitives and Boolean operators.

Figure 6: Mesh created and visualized using Netgen for the two cell geometry



Algorithm 1: How to create a mesh in 2D using Netgen

```
1. Define the geometry object : geo = SplineGeometry()
2. Define the vertex of the geometry : geo.AppendPoint(x,y) $\rightarrow$ PointObject
3. Define the edges of the geometry :
   geo.Append(["'line",PointObjA,PointObjB],leftdomain=(int),rightdomain=(int),
   bc="name" ) $\rightarrow$ EdgeObject
     Or for curved edges
   /* Some primitives also exist in 2D for rectangles and circles.      */
   :
   geo.Append(["spline3",PointObjA,PointObjB,PointObjC],leftdomain=(int),rightdomain=(int),
   bc="name" ) $\rightarrow$ EdgeObject
     • For periodic conditions, just add copy=OtherEdge when defining the second edge.
     • Some good practice :
         – Renaming the domains with str-type name with : geo.SetMaterial(DomainId,name)
         – Setting a max mesh size for each domain with :
           geo.SetDomainMaxH(DomainId,size)
4. Generate the mesh :
   geo.GenerateMesh(maxh=defaultSize) $\rightarrow$ NetgenMeshObject
5. Convert it to an NGSolve mesh :
   geo.GenerateMesh(maxh=defaultSize) $\rightarrow$ NGSolveMeshObject
```

Algorithm 2: How to create a mesh in 3D using Netgen (using CSG)

```
1. Create the geometry object : geo = CSGGeometry()
2. Add primitives : Sphere, Cube, Plane, etc.
3. Define the final geometry with boolean operation : Union (+), Intersection (*), etc.
4. Generate the mesh : geo.GenerateMesh(maxh=defaultSize) $\rightarrow$ NetgenMeshObject
5. Convert it to an NGSolve mesh :
   geo.GenerateMesh(maxh=defaultSize) $\rightarrow$ NGSolveMeshObject
```

Solvers

In NGSolve, no physics solver is provided. The type of spaces (H1,L2,P1, etc), the weak form of the physics equations have to be defined. For linear problems on standard space, only matrix inversion is needed, though tools like Newton solver for non-linear equations are provided. Below is described the procedure for setting up a general problem :

$$\text{Find u that satisfies} \quad K(u,v) = f(v), \quad \forall v \in I_{\text{trial functions}} \tag{9}$$

Algorithm 3: How to solve an equation using NGSolve

```
1. Setup the finite element space :
   H1(mesh,order=(int),dirichlet="boundName1|boundName2") → space
Other type exist like P1,L2, etc.
FE-spaces can have spacial periodicity with Periodic(Space) → PeriodicSpace
Product space are constructed using the (*) operator.
2. Extract the test and trial function : u = FESpace.TrialFunction()
3. Create the bilinear form object and add the left part of (9) :
   K=BilinearForm(FEspace,symmetric=True)
Note : grad, rot, InnerProduct, OuterProduct, dx(integrator), etc are already defined
   accordingly to the spaces used
4. Do the same for the linear form and add the source term using the command :
f =LinearForm(FEspace)
5. Assemble the form (load them into RAM) using the .Assemble() method
6. Prepare the space for the solution using gfu =GridFunction(FESpace)
And (optionally display it with Draw(gfu)
7. Solve the problem with
gfu.vec.data = K.mat.Inverse(FESpace.FreeDofs()) * f.vec
8. Do some postprocessing with Integrate(gfu,mesh) for example
```

Figure 7: Magnitude of the pseudo-velocity and pseudo-pressure field with $r_1 = 0.25$, $r_2 = 0$ for the permeability closure problem for the x-component

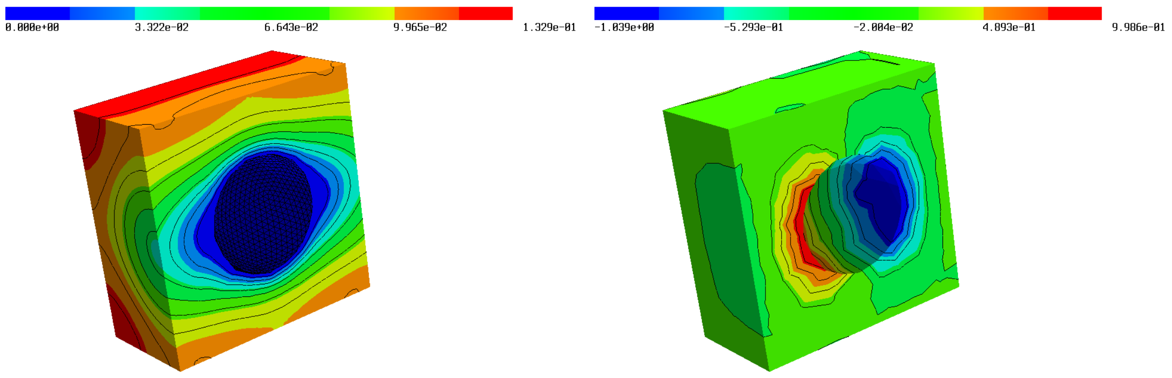
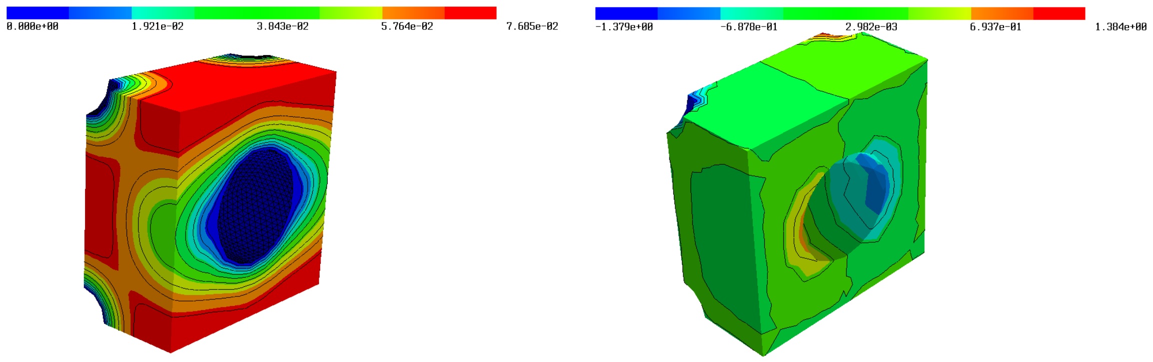


Figure 8: Magnitude of the pseudo-velocity and pseudo-pressure field with $r_1 = 0.25$, $r_2 = 0.125$ for the permeability closure problem for the x-component



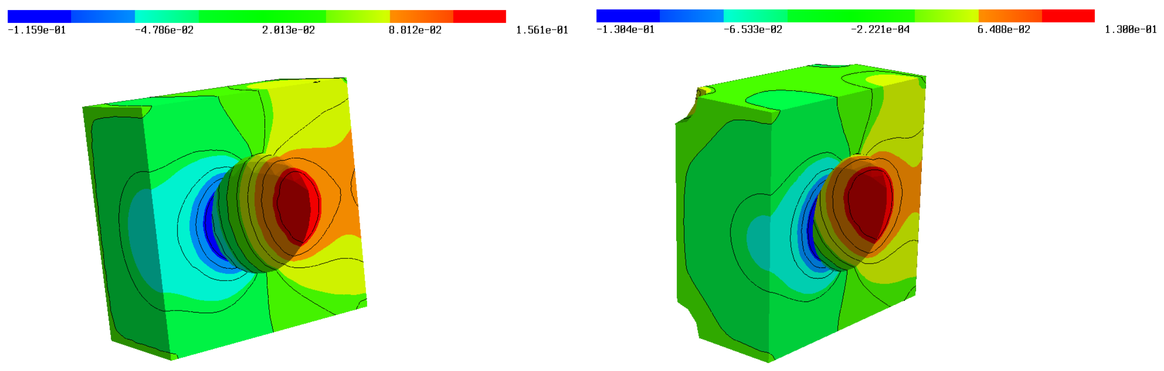


Figure 9: Pseudo-potential fields with $r_1 = 0.25$, $r_2 = 0$ and with $r_1 = 0.25$, $r_2 = 0$ for the diffusive closure problem for the x-component

3.3 FEniCS project

Presentation

FEniCS is a popular open-source computing platform for solving partial differential equations (PDEs). It enables users to quickly translate scientific models into efficient finite element code. With the high-level Python and C++ interfaces to FEniCS, it is easy to get started, but FEniCS offers also powerful capabilities for more experienced programmers. This software runs on a multitude of platforms, ranging from laptops to high-performance clusters.h

Installation

Instructions can be found on the FEniCS project website:

- Download the anaconda environment:
  `conda create -n fenicsproject -c conda-forge fenics`
- Activate the anaconda environment: `source activate fenicsproject`
- Install matplotlib: `conda install matplotlib`

The anaconda environment must be activated every time FEniCS will be used:
`source activate fenicsproject`
Once the environment loaded, a simple `python3 program.py` runs the python program with FEniCS.

Mesh

FEniCS has its own best built-in. It works very well on simple geometries, but has trouble adapting when they become complex. This software program also allows to manually build a mesh.

Both of these methods are not used here. Not efficient for the first one, complicated for the second. It is more relevant to use GMSH to settle this meshing task. This open source 3D finite element mesh generator offers, like Netgen, 2 modes of operation : choose to define the geometry by points, edges and surfaces or by primitives to get curved edges.

Solvers

DOLFIN it how FEniCS' solver is named. As NGsolve it is an adaptive finite element solver for PDEs, but there are two differences between them. DOLFIN mainly uses a functional approach in its coding, while NGsolve uses Object-Oriented Programming. The most important difference in our application is that DOLFIN uses Taylor-Hood's elements, whereas NGsolve uses H^1 x H^1 x H^1 x L^2 elements.

Algorithm 4: How to solve an equation using DOLFIN

```
1. Setup the finite element space
2. Extract the test and trial function
3. Define bilinear and linear form of the weak equations
4. Assemble the form
5. Prepare the space for the solution
6. Solve problem
```

4 Results

4.1 Mésocentre

The EM2C Mésocentre is used because it is a reliable way to compute and compare programs. Moreover, it will be used to run those programs as it allows running long scripts on a distant computer, with high memory capacity compared to a standard desktop PC or laptop.

Mésocentre hardware:

Nb of nodes	192
Nb of CPU	2
CPU reference	Intel Xeon Gold 6230 20C @ 2.1 GHz
CPU gen	Cascade Lake
Max memory	192 GB
Max allocable memory	180 GB

Nb of nodes	14
Nb of CPU	4
CPU reference	Intel Xeon Gold 6230 20C @ 2.1 GHz
CPU gen	Cascade Lake
Max memory	1.5 TB
Max allocable memory	1540 GB
SSD disk space (tmp)	870 GB

4.2 Comparison

The porosity curves are plotted below, for both geometries. For $r_2 = 0$, the three tools are compared with the data from [8]. NGSolve and OpenFoam have trouble dealing with extreme values of r_1, but mainly follow the benchmark from the literature for more reasonable values of r_1. FEniCS seems to provide the most reliable results. For the second figure, only OpenFoam and NGSolve are compared, and the two curves follow the same trend and are mainly in agreement.

Figure 10: Porosity curves with $r_2 = 0$

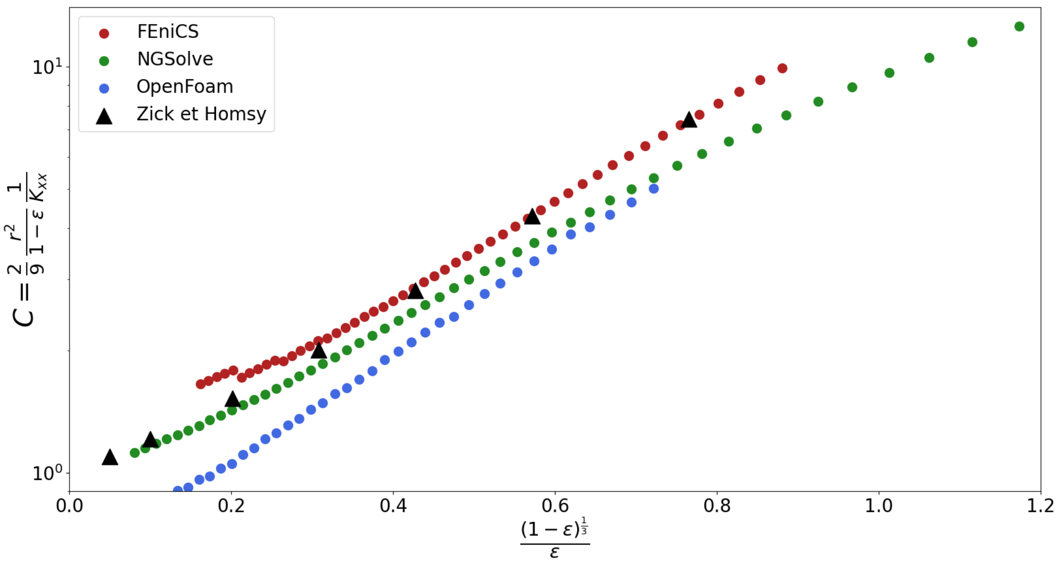
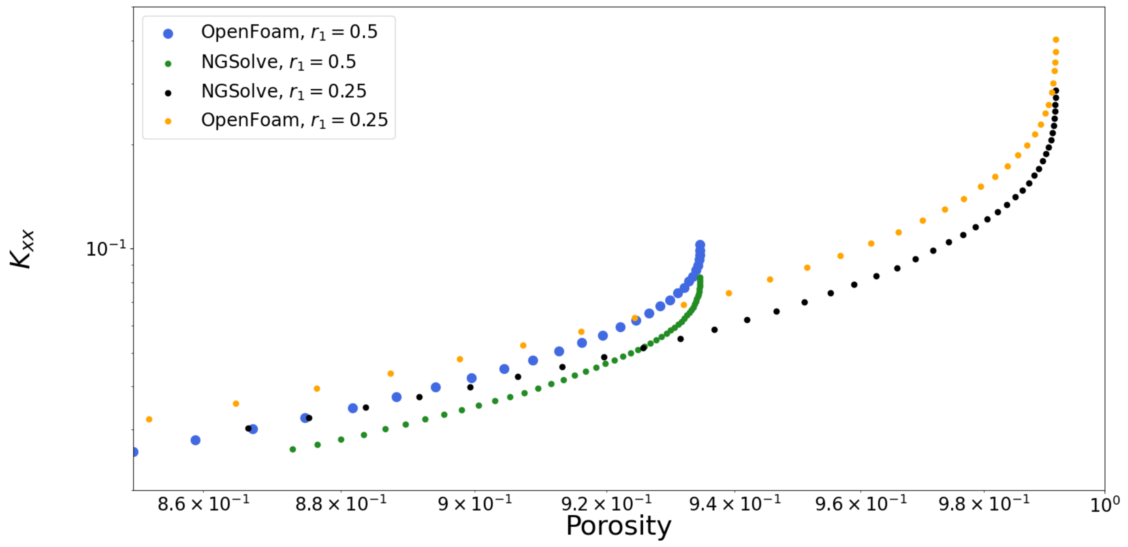


Figure 11: Porosity curves obtained with a fixed r_1 and varying r_2



The diffusion problem

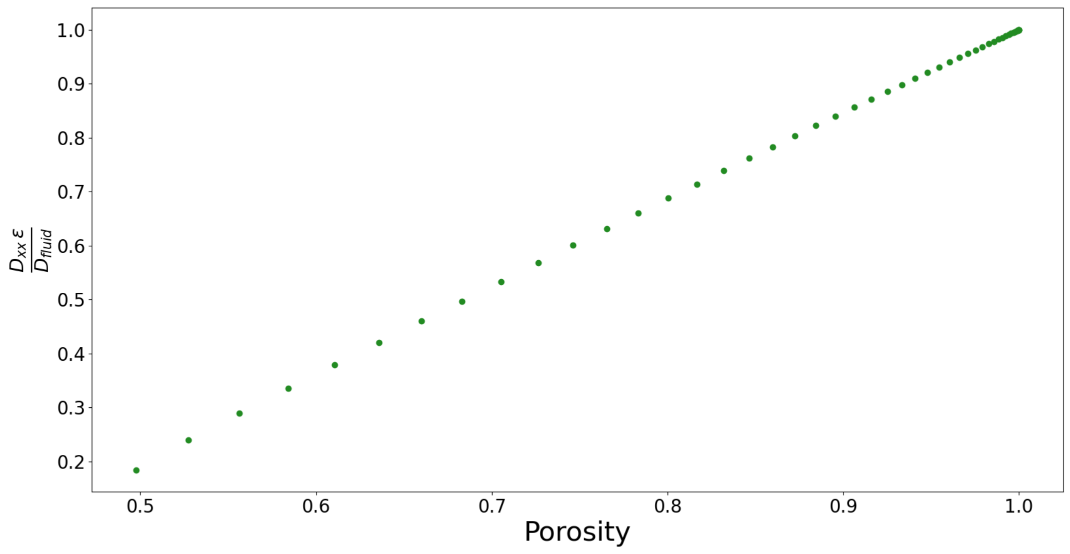
$$\begin{cases} \nabla^2 \underline{b} = 0 \\ -\underline{n} \cdot \nabla \underline{b} = \underline{n} \text{ at } \partial\Omega_\alpha \bigcap \partial\Omega_\kappa \\ \text{periodic at } \Omega_\alpha \setminus \partial\Omega_\kappa \end{cases} \tag{10}$$

was solved on NGSolve.

The tensor $\underline{\underline{D}}$ defined by :

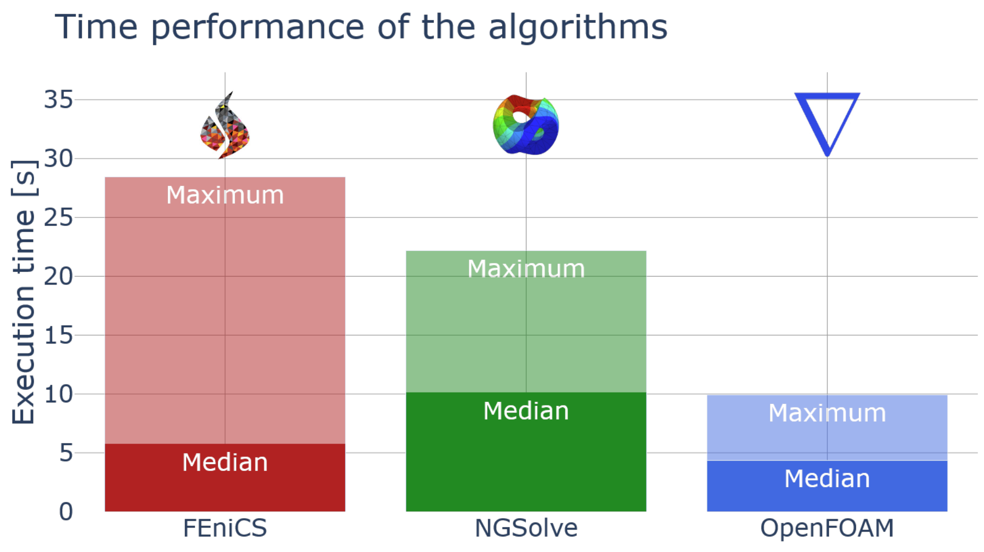
$$\underline{\underline{D}} = D_{fluid}(\underline{\underline{I}} + \frac{1}{V_\alpha}\int_{\partial\Omega_\alpha \bigcap \partial\Omega_\kappa} \underline{n}\,\underline{b}\,dS) \tag{11}$$

was computed and the curve below was plotted :



Duration of each program

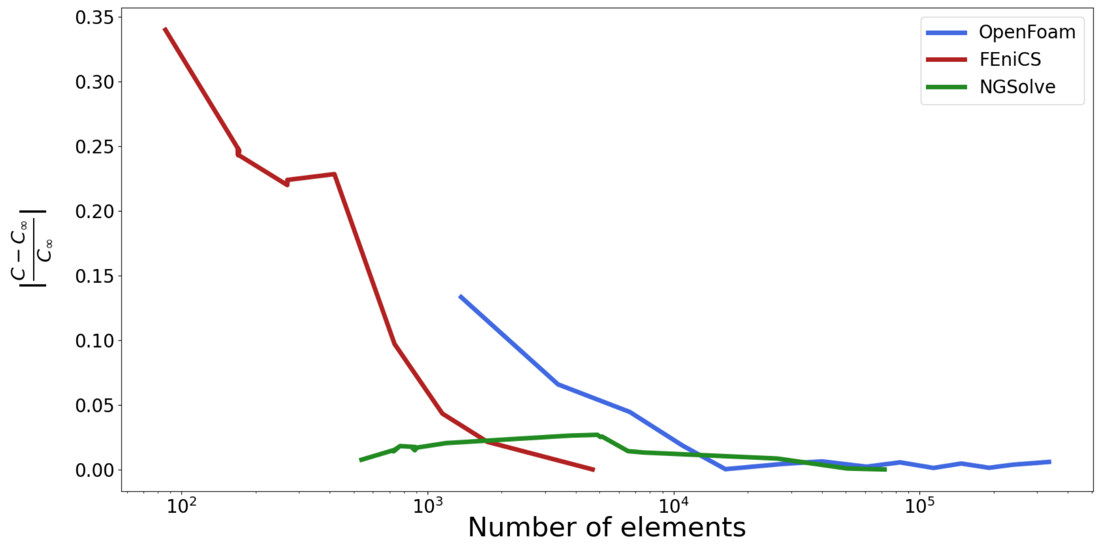
Figure 12: Time execution of each piece of software



OpenFOAM is the quickest to run the study, with a relative consistency. A few iterations are about 2 times longer, and correspond to the maximum time. FEniCS is the second quickest. It is really consistent, but the first execution takes a very long time, about 5 times longer. NGSolve is the slowest, but is relatively consistent. The first iteration is also a lot longer, but less than FEniCS' first one.

To check grid convergence and compare speeds of convergence, the relative error $|\frac{C-C_{infty}}{C_\infty}|$ is plotted for each software, for a unique value of r_1.

We check that the error goes to zero when the number of elements is increased, and we see that NGSolve converges almost immediately, while FEniCS and OpenFoam need respectively 10^3 and 10^4 elements to reach their asymptotical value.



5 Conclusion

Three numerical tools; FEniCS, NGSolve and OpenFoam, were compared in order to solve a closure problem, and to compute the permeability tensor. All three pieces of software give a permeability tensor in the same order of magnitude than the literature and mainly follow the same trend. FEniCS seems to be the better fit to the benchmark data; however NGSolve performs better for very low radii. OpenFoam gives the most inaccurate results, especially for extreme values of r_1.

OpenFoam is the only tool specialized for 3D problems, hence it was naturally the quickest to run, followed by FEniCS and then NGSolve. OpenFoam is the slowest software to converge in mesh, the quickest being NGSolve.

OpenFoam is not user-friendly, as `blockMesh` requires the user to manually input all vertices, and custom boundary conditions and solvers need to be entirely coded. Therefore, this software is only recommended if the geometry and boundary conditions are very simple, and if a solver for the equation we seek to solve is already available. Fenics and NGSolve tend to be more users friendly, or at least offer a smoother workflow and less frustrating experience if one is accustomed to concepts like weak formulation.

References

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