

# <sup>1</sup> Permeability computation of high resolution $\mu$ CTscan with an <sup>2</sup> unfitted boundary method to improve accuracy

<sup>3</sup> Martin Lesueur<sup>a,\*</sup>, Hadrien Rattez<sup>a</sup> and Oriol Colomés<sup>a</sup>

<sup>4</sup> <sup>a</sup>Civil and Environmental Engineering, Duke University, Durham, NC 27708-0287, USA

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## ABSTRACT

Flow simulations on porous media, reconstructed from Micro-Computerised Tomography ( $\mu$ CT)-scans, is becoming a common tool to compute the permeability of rocks. In order for the value of this homogenised hydraulic property to be representative of the rock at a continuum scale, the sample considered needs to be at least as large as the Representative Elementary Volume. Moreover, the numerical discretisation of the digital rock needs to be fine enough to reach numerical convergence. In the particular case of Finite Elements (FE), studies have shown that simulations should use structured meshes at least two times finer than the original image resolution in order to reach the mesh convergence. These two conditions and the increased resolution of  $\mu$ CT-scans to observe finer details of the microstructure, can lead to extremely computationally expensive numerical simulations. In order to reduce this cost, we couple a FE numerical model for Stokes flow in porous media with an unfitted boundary method, which allows to improve results precision for coarse meshes. Indeed, this method enables to obtain a definition of the pore-grain interface as precise as for a conformal mesh, without a computationally expensive and complex mesh generation for  $\mu$ CT-scans of rocks. From the benchmark of three different rock samples, we observe a clear improvement of the mesh convergence for the permeability value using the unfitted boundary method. An accurate permeability value is obtained for a mesh coarser than the initial image resolution. The method is then applied to a large sample of a high resolution  $\mu$ CT-scan to showcase its advantage.

<sup>27</sup>

## <sup>28</sup> 1. Introduction

<sup>29</sup> Micro-Computerised Tomography ( $\mu$ CT) was first developed to observe the microstructure of dense materials in a  
<sup>30</sup> non-destructive way for applications such as medicine and material sciences (Tuan and Hutmacher, 2005; Salvo et al.,  
<sup>31</sup> 2003). It was later applied to rock materials and has shown to be a very valuable tool for rocks characterization (Mees  
<sup>32</sup> et al., 2003; Cnudde and Boone, 2013). In particular, this technique is at the core of digital rock physics (Andrä et al.,  
<sup>33</sup> 2013; Arns et al., 2005). In this discipline, properties are measured and computed on  $\mu$ CT-scans of rocks such as:  
<sup>34</sup> porosity (Arns et al., 2005; Blunt et al., 2013); mechanical properties (Arns et al., 2002); chemical properties (Godel,  
<sup>35</sup> 2013); hydraulic properties (Arns et al., 2005; Blunt et al., 2013). We will focus on the latter in this contribution and  
<sup>36</sup> compute the permeability based on flow simulations on  $\mu$ CT-scans images.

<sup>37</sup> The concept of permeability was first introduced by Darcy (1856) as a quantification of the hydraulic conductivity  
<sup>38</sup> of soils. This parameter plays a critical role in Darcy's law that is also used in rock mechanics to describe fluid flow at  
<sup>39</sup> the reservoir scale. Permeability is therefore a key parameter to quantify for energy resources engineering (Bjorlykke,  
<sup>40</sup> 2010). For this type of application, the property was previously measured using wireline-log analysis, well testing  
<sup>41</sup> and core flooding experiments on samples collected from drilled wells (Ahmed et al., 1991). However, Darcy's law  
<sup>42</sup> was proven to be a homogenisation of the Stokes formulation (Whitaker, 1986) for a Representative Element Volume  
<sup>43</sup> (REV) of rock. The REV of any property is defined as the minimum sample size above which the value of the property  
<sup>44</sup> assessed has converged to a steady-value. The investigation of the effect of the sample size on the results of simulations  
<sup>45</sup> for Stokes flow simulations in  $\mu$ CT scans has been carried out for many different rock types (Mostaghimi et al., 2012).  
<sup>46</sup> Since the REV of permeability for a rock is usually achieved at the scale of  $\text{mm}^3$  (Guibert et al., 2015; Mostaghimi  
<sup>47</sup> et al., 2012), at which  $\mu$ CT-scanning operates, more interest is building up on computing it directly on  $\mu$ CT-scans of  
<sup>48</sup> the core sample, as being a faster and less expensive method than experimental measurements (Saxena et al., 2018).  
<sup>49</sup> Indeed, the small sample size required for analysis makes it possible to produce multiple measurements on a single

\*Corresponding author

✉ martin.lesueur@duke.edu (M. Lesueur)

ORCID(s): 0000-0001-9535-2268 (M. Lesueur)

50 plug (Arns et al., 2005). Moreover, it enables the computation of hydraulic properties on core materials unsuitable to  
 51 laboratory testing (Arns et al., 2004).

52 To compute the permeability on CT-scan images, several approaches have been used to simulate the fluid flow  
 53 including finite difference (Mostaghimi et al., 2012; Manwart et al., 2002) and finite element-based methods (Borujeni  
 54 et al., 2013; Narváez et al., 2013), vortex and cell centred finite volume method (FVM) (Guibert et al., 2015; Petrasch  
 55 et al., 2008) and lattice Boltzmann method (LBM) (Manwart et al., 2002; Narváez et al., 2013). The FVM and LBM  
 56 are the most common approaches for this application (Song et al., 2019). However, the finite element method has gain  
 57 interest recently as it allows to obtain permeabilities in a good agreement with LBM and FVM but at lower memory  
 58 cost (Yang et al., 2019). Moreover, LBM and FVM are not the most suited methods when the fluid flow is coupled  
 59 with other physical processes like mechanical deformation of the solid matrix. Such deformation can have a major  
 60 effect on permeability evolution (Ghabezloo et al., 2009). In this context, Arbitrary Lagrangian-Eulerian approaches  
 61 in finite elements are more commonly used (Lesueur et al., 2017). For these reasons, we are using the Finite Element  
 62 method in this paper.

63 Resolution of CT-scans have been constantly improving since the technology was developed, obtaining now images  
 64 above  $1000^2$  pixels and with a resolution below a few micrometres (Sarker and Siddiqui, 2009; Soulaine et al., 2016;  
 65 Wang and Fleischmann, 2018). Higher resolutions for the CT-scans are particularly important for porous rocks in  
 66 order to obtain a better characterization of the pore-grain interface like the detailing of grains' shape, which influences  
 67 significantly the value of permeability obtained (Beard and Weyl, 1973; Cox and Budhu, 2008; Torskaya et al., 2013).  
 68 Note that image processing methods also allow to improve on the quality of the microstructure recovered (Iassonov  
 69 et al., 2009; Wang et al., 2019a). In this contribution, we focus on the CT-scan images after segmentation, thus we  
 70 consider that the images present a well-defined pore-grain interface. The higher resolution mentioned comes with the  
 71 constraint of a higher computational effort to run the flow simulation. Indeed, numerical accuracy is obtained when the  
 72 result of the FE simulation converges towards a single value with decreasing size of the mesh elements, called mesh  
 73 convergence. For permeability, the mesh convergence is only obtained with a mesh finer than the image resolution,  
 74 which leads to simulations with a very large number of elements in the case of high resolutions CT-scans. For example,  
 75 the study of Guibert et al. (2015) showed that a mesh size of even twice the resolution of the original image could not be  
 76 enough to reach mesh convergence for permeability. In the case of carbonate rocks, it becomes then extremely difficult  
 77 to get good accuracy on the value of permeability as the REV size can be very large (Mostaghimi et al., 2012; Liu  
 78 et al., 2014). In some instances the size needed for the computation is above the capability of the simulator (Guibert  
 79 et al., 2015) and final permeability value is only computed at the limit of resources.

80 While many solutions to the computational limit existing for high resolution CT-scans are developed with the  
 81 objective to increase the number of elements in a simulation at a lower computational cost (Wang et al., 2019b), we  
 82 opt for a different approach which aims at reducing the number of elements needed to reach mesh convergence. To  
 83 this end, we are looking for a better approximation of the pore-grain interface for a mesh coarser than the CT-scan  
 84 image resolution. Indeed, the magnitude of the approximation on permeability due to a too low resolution image is  
 85 well documented in the literature (Guibert et al., 2015; Borujeni et al., 2013). Here we use an unfitted Finite Element  
 86 Method (FEM) approach in which the geometry of the domain is embedded in a background mesh. Different methods  
 87 can be considered here, typically classified in two main groups: immersed boundary methods or embedded boundary  
 88 methods. The former basically consists on solving the problem in the active and inactive parts of the domain, enforcing  
 89 the boundary condition via a forcing function (see Mittal and Iaccarino, 2005). In the later approach, the equations are  
 90 solved only on the active part of the domain and the boundary conditions are enforced by either modifying the weak  
 91 form of the problem or manipulating the mesh close to the boundary (see e.g. Burman et al., 2015; Rangarajan and  
 92 Lew, 2014). In this work we propose an embedded boundary method for structured quadrilateral/hexahedral meshes  
 93 in which the nodes of the background mesh at the interface between active and inactive elements are displaced in such  
 94 a way that they fit the embedded geometry, see Section 2. Note that one of the main differences with respect to the  
 95 universal meshes approach presented in (Rangarajan and Lew, 2014) is precisely the use of structured grids. By using  
 96 structured grids we can take advantage of octree-based adaptive mesh refinement strategies (see e.g. Lesueur et al.,  
 97 2017). Other advantages of this choice are, for instance, the ability to use spectral approximations or highly efficient  
 98 data-structures.

99 After a first section on the description of this new method, referred as the displaced boundary method, it is bench-  
 100 marked for  $\mu$ CT-scans of three types of rocks presenting different microstructure geometries. We finally showcase the  
 101 method's performance for a high resolution CT-scanned rock sample.

102 **2. Displaced boundary method description**

103 The mesh of the digital rock is constructed using the approach introduced by Lesueur et al. (2017). It relies on the  
 104 image reader capability of the finite element framework MOOSE (Permann et al., 2020) and produces 3D structured  
 105 meshes of the pore space of rock microstructures reconstructed from a stack of segmented µCT-scan images. Our focus  
 106 is when the image is so resolved that one needs to select a mesh coarser than the image resolution in order to restrain  
 107 the computational burden to an acceptable level. In this case, the pore-grain boundary has to be grossly approximated  
 108 in a given way. Specifically in this contribution, it is the pixel value of the element's centroid that dictates whether the  
 109 element should be a pore or a grain. This meshing procedure is showcased for the example of a quarter circle in Fig. 1a  
 110 and the resulting approximation of the boundary can be observed in Fig. 1b.

111 To use our method, we need to mesh the digital rock at its full resolution and extract the pore-grain boundary as a  
 112 STL file. This file contains the geometry of the pore-grain interface that we are trying to match with the lower resolution  
 113 mesh. As a preprocessing step, the distance between the exact interface given by the STL file and the approximated one  
 114 of the mesh is computed. For each node of the meshed pore-grain boundary, we find the closest point on the STL and  
 115 return the distance between the two. The distance is displayed for the example of a quarter circle in Fig. 1c. The nodes  
 116 (and subsequently the integration points) of the mesh are then *displaced* of the computed distance and the pore-grain  
 117 interface now matches the geometry of image at full resolution. The final result is a mesh with a lower resolution than  
 118 the image that still matches closely the pore-grain boundary, as can be observed in the example of a quarter circle in  
 119 Fig. 1d.

120 Note that this technique can be understood as a process to transform the original background mesh to a conforming  
 121 mesh. However, it can also be understood as an unfitted FEM approach in which the mesh is fixed and an additional  
 122 transformation map is applied to the Finite Element reference map. Indeed, this map ( $\varphi_d$ ) can be defined on all the  
 123 mesh nodes as the identity for the interior nodes and the application of the distance field ( $\mathbf{d}$ ) at the boundary ( $\Gamma$ ), i.e.  
 124  $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}^d$  with

$$\hat{\mathbf{x}} = \varphi_d(\mathbf{x}) = \begin{cases} \mathbf{x} + \mathbf{d} & \text{if } \mathbf{x} \in \Gamma, \\ \mathbf{x} & \text{otherwise.} \end{cases} \quad (1)$$

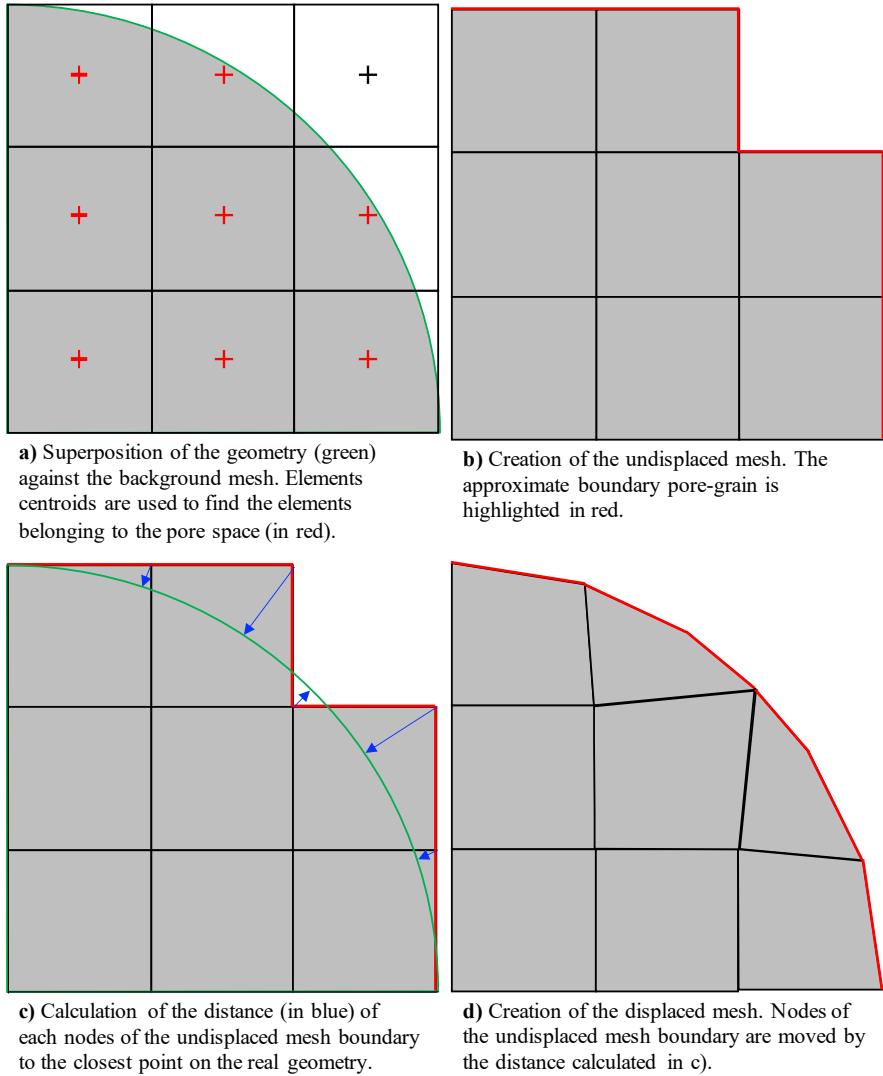
125 In this contribution, the "displaced mesh" refers to the equivalent mesh on which the FE simulations are computed.

126 The well-posedness of the method is guaranteed if the resulting map leads to transformed elements with a positive  
 127 Jacobian. In that case, the method inherits all the convergence and stability properties of a standard conformal Finite  
 128 Element approach. However, this condition is not satisfied in the general case. Nonetheless, in practice, the method of  
 129 selecting the elements domain (pore or grain) based on the element's centroid (see Fig. 1a) results in an approximated  
 130 pore-grain interface with a distance to the real interface of, at worst, one element's size  $h$ . Therefore, in practice, no  
 131 negative jacobians should be found, which was observed in every simulation of this contribution. However further  
 132 analysis is required to prove theoretical well-posedness. Another drawback of some unfitted FEM approaches is the so  
 133 called *small cut-cell problem*, which results in ill-conditioned matrices caused by the appearance of active elements  
 134 with a measure orders of magnitude smaller than the measure of the neighbouring elements. In the approach presented  
 135 in this work this issue is avoided by only activating the elements whose centroid lies inside the domain. Therefore,  
 136 assuming a sufficiently smooth boundary, the measure of the displaced elements is of the same order as the one of the  
 137 elements from the original background mesh.

138 It is important to highlight that the proposed method does not depend on the way the geometry is characterized.  
 139 That means that it can be used for geometries defined by STL files generated from CT-scanned samples, but also for  
 140 domains defined by continuous distance fields, e.g the level-set method, or domains defined using CAD techniques.  
 141 Furthermore, the proposed approach is suitable for non water-tied geometries, i.e geometries defined by non-contiguous  
 142 parts, as long as a distance field can be provided at the pore-grain interface nodes.

143 Any computation during the simulation is done on the displaced mesh. The FEM simulator used in this contribution  
 144 is MOOSE, in which we can do computations on the displaced mesh. The permeability computation is done following  
 145 the methodology presented in Lesueur et al. (2017), summarised briefly below. Pressure driven stokes flow, expressed  
 146 in dimensionless form as:

$$-\frac{1}{Re} \nabla^2 \vec{v}_f^* + \nabla p_f^* = 0 \quad (2)$$

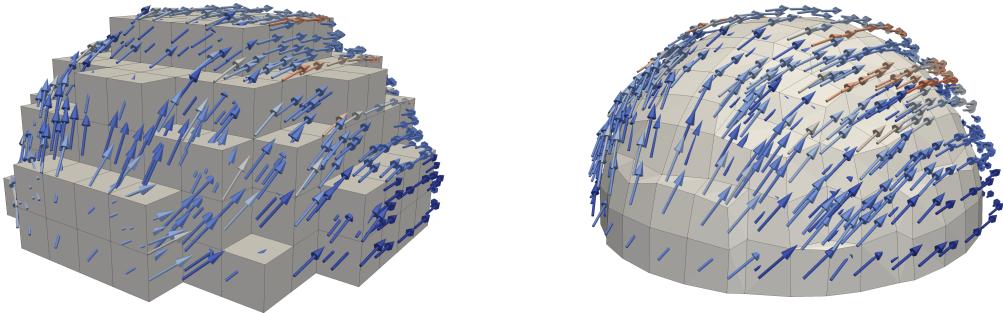


**Figure 1:** Schematic of the meshing procedure of a quarter circle against a 3x3 grid using the displaced boundary method. The displaced mesh (d) results in a better approximation of the real geometry than the undisplaced mesh (b).

$$-\nabla \cdot \vec{v}_f^* = 0 \quad (3)$$

is computed with MOOSE. Following Peterson et al. (2018) the system is stabilised with a Pressure-Stabilizing Petrov-Galerkin formulation, which allows to use simple first order elements instead of the classical Taylor-Hood elements to ensure the InfSup condition. Taking advantage of the solvers of PETSc included in MOOSE, the Schur method is used to precondition the system following Elman et al. (2008). We follow a prescribed solution from Balay et al. (2016) and use a Jacobi preconditioner for the fluid pressure subsystem and the algebraic multigrid method BoomerAMG (Henson and Yang, 2002) from HYPRE for the fluid velocity subsystem. Note that the preconditioning of our system enables to invert rigidity matrix even for elements for not well conditioned elements like in Fig. 1. From the computed flow, the average velocity in the selected direction is post processed on the displaced mesh. The permeability is finally calculated using the formula:

$$k = \mu_f L_{ref} \frac{\phi v_f^*}{\Delta p_f^*} \quad (4)$$



**Figure 2:** Oriented fluid flow vectors coloured with relative magnitude around a demi sphere, traditionally meshed (a) and displaced (b). The sphere is meshed with 10 elements in diameter for both figures.

The method is computationally very light, since the computation of the distances can be particularly efficient (we rely on the libigl library (Jacobson et al., 2018) in this contribution). In fact, for all the simulations presented in this study, using the displaced boundary method did not affect the computation time compared to the undisplaced mesh.

The influence of the method on the value of permeability is showcased conceptually in Fig. 2. A perfect semi sphere is meshed at a lower resolution in Fig. 2a, with 10 elements for the diameter. We use the displaced method to retrieve the smooth geometry of semi-sphere in Fig. 2b. The difference of geometry between the two meshes is reflected in the computed permeability through the porosity first, used in Eq. 4. In addition, this geometrical difference affects in turn the fluid flow. Instead of the fluid flowing through the virtual corners created by the boundary approximations in Fig. 2a, we observe the expected smooth flow around the displaced mesh of the sphere in Fig. 2b. This is the second influence on the permeability, specifically on the average velocity computed, which is used in the permeability formula, Eq. 4.

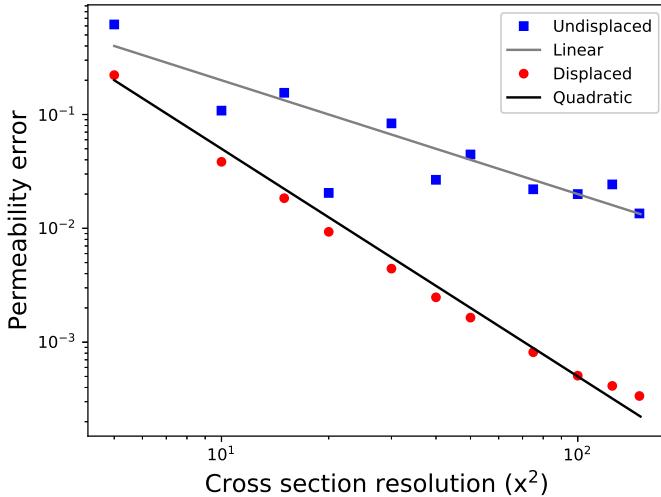
## 2.1. Poiseuille benchmark

We demonstrate the advantage of the method on a benchmark of the analytical solution for the permeability  $k$  of a 3D Poiseuille tube of radius  $R$ ,  $k = \pi R^4 / 8$ . Poiseuille tubes were one of the first models of idealised porous media since their analytical permeability formula helps determining the permeability of the medium based on its porosity, a parameter easily measurable. We can imagine indeed the tubes to represent pore throats. For this reason, this section presents a suitable benchmark of the method for the computation of permeability on CT-scans.

The permeability is computed on both the approximately meshed tube and the displaced mesh. A mesh convergence is performed and we plot in Fig. 3 the error of the permeability compared to the analytical solution for both methods. We can see that the displaced method, in red, reaches below 1% of error very quickly, after only 20 elements in diameter, whereas the undisplaced mesh still is not under this value of 1% of error even at 150 elements in diameter. A similar magnitude of the error was observed by Yang et al. (2019). The reason why the permeability convergence of the undisplaced method is not smooth is that the volume on integration changes randomly for each mesh refinement step, as seen in the comparison of Fig 4 top and bottom left. We can also see in Fig. 3 the different orders of convergence between the undispersed and displaced methods, linear and quadratic respectively. Note that in the undisplaced case, since we do not capture properly the boundary, the solution will be subject to an error at least of the order of the element size. Therefore, since we use stabilized linear Finite Elements with optimal quadratic convergence rate, see for instance Burman and Fernández (2011), the convergence rate of the solution will be at most linear. On the contrary, the proposed displaced approach results in a conformal discretization of the boundary, leading to the expected optimal convergence rate (quadratic). Such a smooth convergence allows to be more predictive on the extrapolation of the converged value.

## 3. Method performance

In order to showcase the method's performance on rock permeability computation, we compare the mesh convergence with and without the displaced boundary method for three completely different rock samples. We select the LV60A sandpack Imperial College Consortium On Pore-Scale Modelling (2014a), the S1 sandstone Imperial College



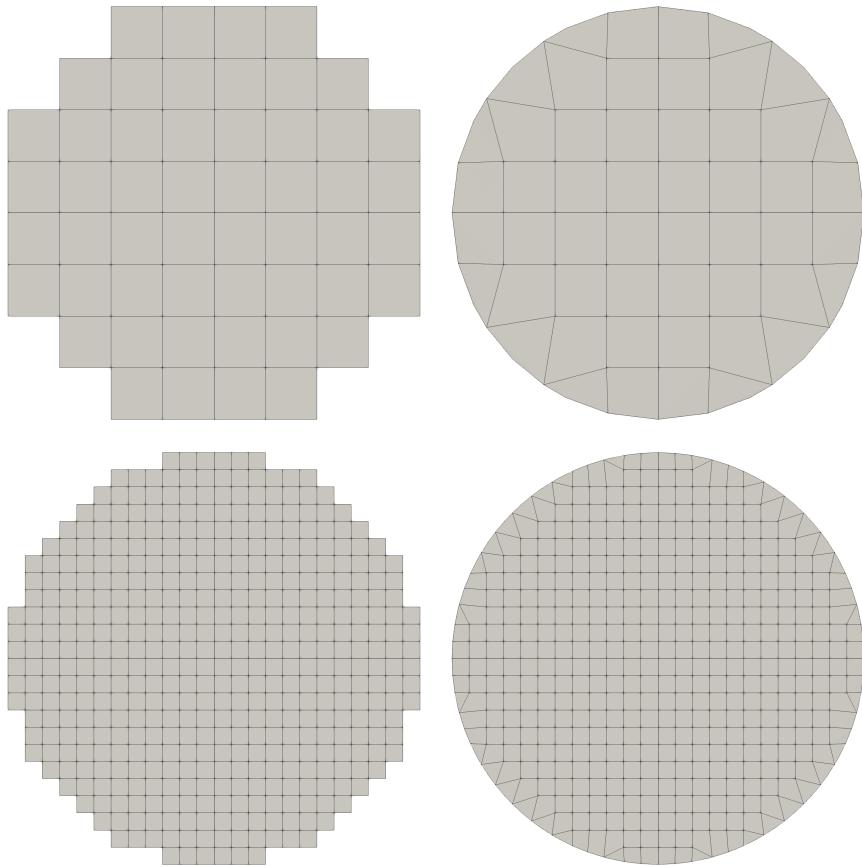
**Figure 3:** Permeability error compared to the analytical value for a tube of Poiseuille flow using both the undisplaced and displaced boundary method. Quadratic convergence of the error can be appreciated with the displaced boundary method (fitted with  $5x^{-2}$  in black) while the undisplaced method has only a linear convergence (fitted with  $2x^{-1}$  in grey).

191 Consortium On Pore-Scale Modelling (2014b) and finally, the Ketton limestone. As observed in Fig. 5, the nature of  
 192 the rock studied changes its microstructure. In addition, the CT-scanning process influences the digitisation of said  
 193 microstructure. The differences between the samples are listed below:

- 194 • **Granularity** The sandpack and the limestone are granular. It is harder to distinguish the grains in the sandstone  
 195 as they are heavily cemented to each other. The rock matrix forms instead an interconnected skeleton.
- 196 • **Consolidation** A sandpack is known for being unconsolidated sand. We expect the sandstone to be more con-  
 197 solidated than the limestone as the porosity is a bit lower.
- 198 • **Texture** The sandpack grains are quite coarse; The sandstone has a fairly smooth interface; The limestone grains  
 199 are extremely smooth.
- 200 • **Roundness** The sandpack and sandstone have grains that can be of various shapes, elongated or compact. The  
 201 limestone instead have very round grains.
- 202 • **Grain size** The sandpack is known for having a very homogeneous grain size distribution. It differs from the  
 203 limestone where a big contrast of size exists between some grains.
- 204 • **Resolution** The limestone has been CT-scanned at a much higher resolution than the other two rocks. We can  
 205 almost visualise the pixels in Fig. 5a. The exact resolutions are listed in the caption of Fig. 5.

206 By selecting such a diverse array of samples, we aim at emphasising on the generic nature of the method, that can be  
 207 applied to any rock's CT-scan.

208 The permeability is computed on 3D subsets of the samples of Fig. 5 using the flow simulator and permeability  
 209 postprocessing of Sec. 2. For each sample, the mesh convergence of permeability is established with and without the  
 210 displaced boundary method and the results are plotted in Fig. 6,7,8. We note that our method has no impact at the  
 211 CT-scan original resolution because the distance computed would then be zero. However, a difference in resolution of  
 212 one element is sufficient to fall back on the mesh convergence curve of the displaced method. The phenomenon is also  
 213 present at half of the resolution of the CT-scan but is less impactful. In addition to the absolute value of permeability  
 214 we also plot the error compared to the final value, computed respectively for each method. The two method are not  
 215 evaluated against the same final value because our method converges to a different value than the undisplaced mesh,  
 216 by a few %. This small difference can be explained by the fact that the displaced mesh is always smooth, i.e. not



**Figure 4:** Visualisation of the mesh undisplaced (left) and displaced (right) for a higher resolution top to bottom.

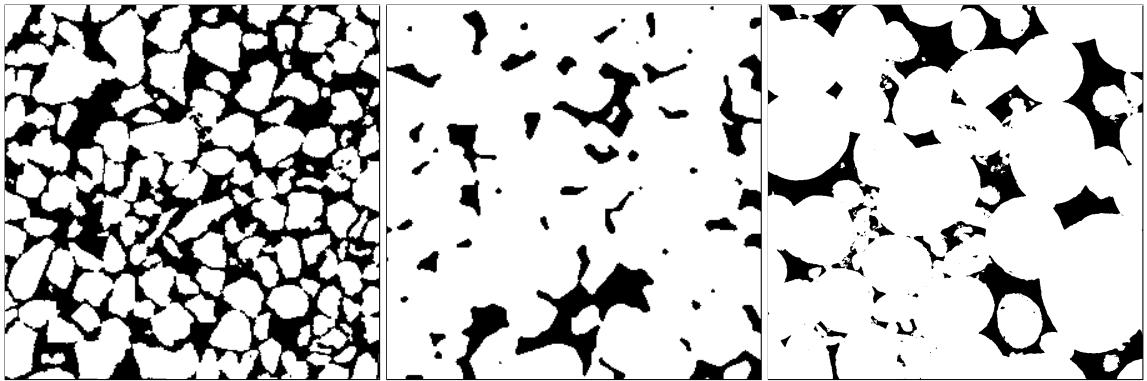
217 pixelated, unlike the undisplaced mesh. This can be observed for example in Fig. 2,4. As shown in Fig. 3, this  
 218 smoothness influences the results of permeability. Interestingly in the case of low resolution CT-scans, this difference  
 219 could be considered an improvement considering that our method is able to retrieve the original smoothness of a rock,  
 220 artificially pixelated during the CT-scanning process.

221 For all rock samples, we can observe that the mesh convergence is not reached at the image resolution with the  
 222 undisplaced method, as confirmed by Guibert et al. (2015). We only manage to fall under 2% of error at twice the  
 223 initial image resolution. Still, Guibert et al. (2015) showed that an even more accurate value can be reached at four times  
 224 the resolution of the initial image.

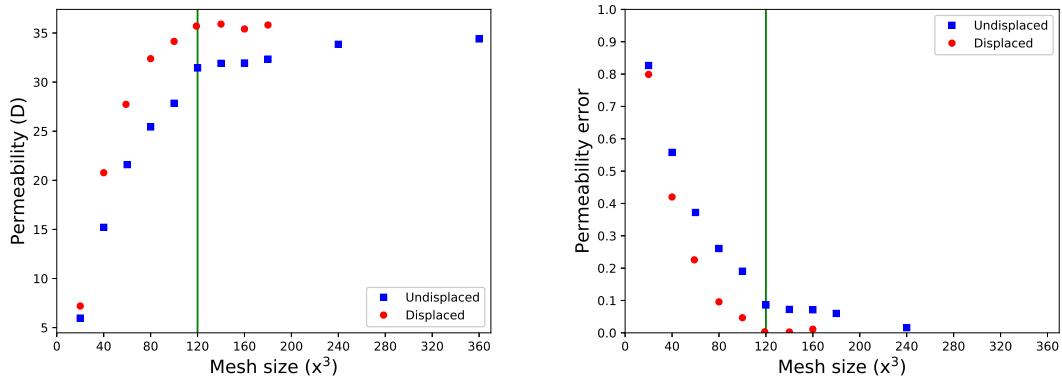
225 Using the displaced boundary method, we reach the mesh convergence (below 2% error) for each sample, always  
 226 earlier than with the undisplaced method. Interestingly though, the convergence isn't reached for the same relative  
 227 resolution. For the sandpack and the sandstone that have a similarly low resolution, respectively 10.002  $\mu$ m and  
 228 8.683  $\mu$ m, the convergence is achieved around the initial image resolution. However, it is for the limestone that has a  
 229 high resolution of 3.00006  $\mu$ m that our method performs the best. Mesh convergence is achieved at half of the image  
 230 resolution.

231 By comparing the displaced boundary method with the undisplaced method, we expose that there exists actually  
 232 two different convergences when running a mesh convergence of permeability.

233 The displaced boundary method exposes two different influences on the mesh convergence of permeability for  
 234 regular meshing. The first one is the convergence of the geometry of the pore-grain boundary. Indeed with the undis-  
 235 placed method, a matching geometry of the interface is only achieved at image resolution or one of its multiples. This  
 236 could explain why Guibert et al. (2015) could not obtain a mesh convergence below the the image resolution, because  
 237 the geometry would always be approximated under this resolution. The advantage of using our method is to be able to



**Figure 5:** Visualisation of grains (white) and pore space (black) on a segmented slice of the samples studied. (a) The LV60A sandpack Imperial College Consortium On Pore-Scale Modelling (2014a) with a resolution of  $10.002 \mu\text{m}$  (sample size of  $(3\text{mm})^2$ ). (b) The S1 sandstone Imperial College Consortium On Pore-Scale Modelling (2014b) with a resolution of  $8.683 \mu\text{m}$  (sample size of  $(2.6\text{mm})^2$ ). (c) The Ketton limestone with a resolution of  $3.00006 \mu\text{m}$  (sample size of  $(3\text{mm})^2$ ).

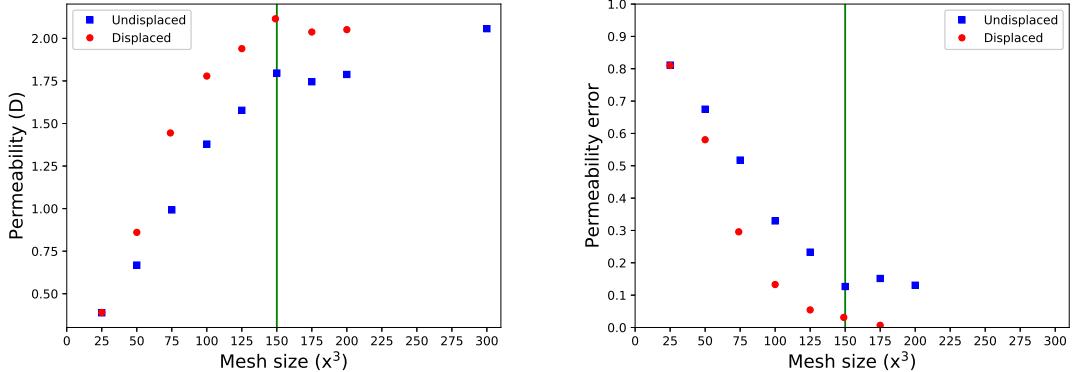


**Figure 6:** Mesh convergence of the permeability of a sample of the LV60A sandpack of size  $(1.2\text{mm})^3$ , with and without the displaced boundary method. The resolution of the original scan is  $120^3$  voxels. (a) shows absolute permeability computation and (b) the evolution of the permeability error compared to the final value.

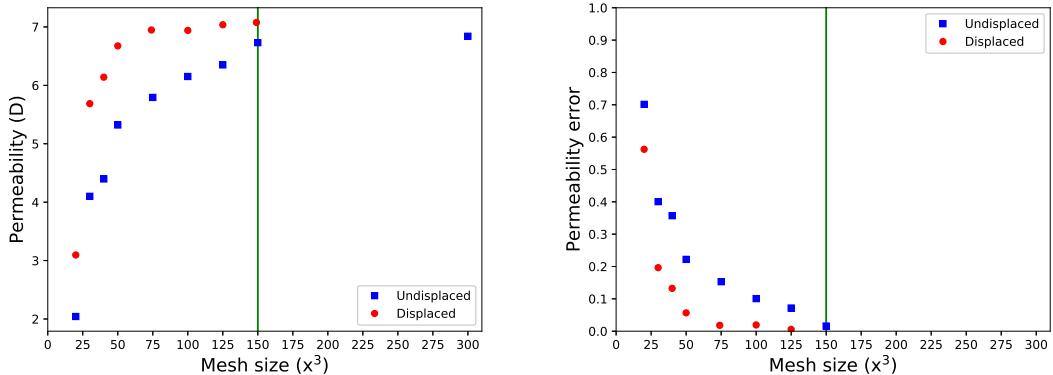
have a good approximation of the interface very early. The second is the numerical mesh convergence itself. This one is achieved independently of the image resolution at a specific absolute value of mesh size  $h$ . High resolution images seems to be the most interesting application of our method because, in that case, the numerical mesh convergence is reached much earlier than the convergence of the geometry. Since our method is not affected by the convergence of the geometry, we therefore obtain a global mesh convergence much earlier than with the undisplaced method, as shown for the limestone sample in Fig. 8.

#### 4. Application to high resolution CT-scan

After demonstrating the efficiency of the displaced boundary method for permeability computation on rocks'  $\mu$ CT-scan in the previous section, we apply it in the case where it is the most advantageous, for a high resolution CT-scan. We select again the Ketton carbonate on which our method has shown an impactful improvement on the cost of permeability computation (Fig. 8). However in this section, we select a larger sample, of  $500^3$  voxels in size, visualised in Fig. 10a. Since mesh convergence with the undisplaced method can only be reached at around two times the resolution of the original image, permeability should be computed on a sample of at least  $1000^3$  voxels. Since our system solves for the pressure and the velocity variables in each direction, this corresponds to solving for  $4 \times 10^9$  Degrees Of Freedom (DOF). Running a flow simulation for such size requires obviously to be run on a supercomputer on which enormous



**Figure 7:** Mesh convergence of the permeability of a sample of the S1 sandstone of size  $(1.3\text{mm})^3$ , with and without the displaced boundary method. The resolution of the original scan is  $150^3$  voxels. (a) shows absolute permeability computation and (b) the evolution of the permeability error compared to the final value.



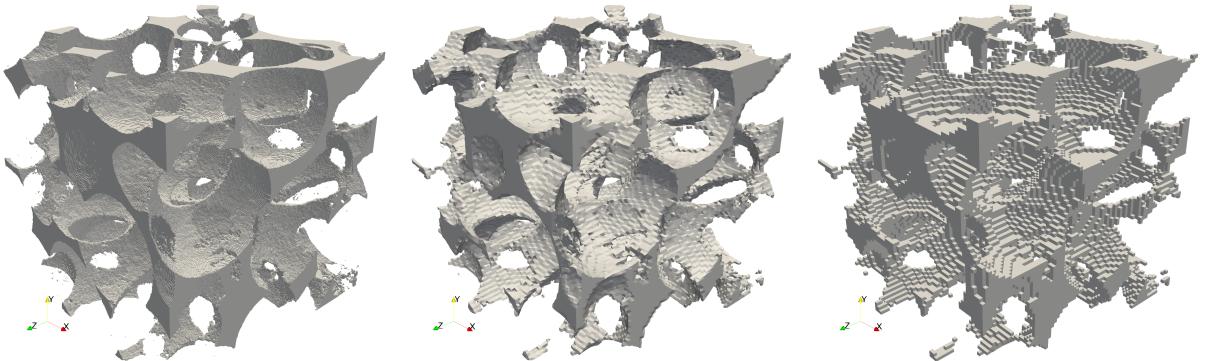
**Figure 8:** Mesh convergence of the permeability of a sample of the Ketton carbonate of size  $(0.45\text{mm})^3$ , with and without the displaced boundary method. The resolution of the original scan is  $150^3$  voxels. (a) shows absolute permeability computation and (b) the evolution of the permeability error compared to the final value.

253 memory allocation is needed. In our case, this size surpasses our solving capabilities. Yet we show in this section that  
 254 the permeability of such a large sample can be retrieved easily with the displaced boundary method. In comparison,  
 255 we also show how much error the undisplaced method still has at the limit of our resources.

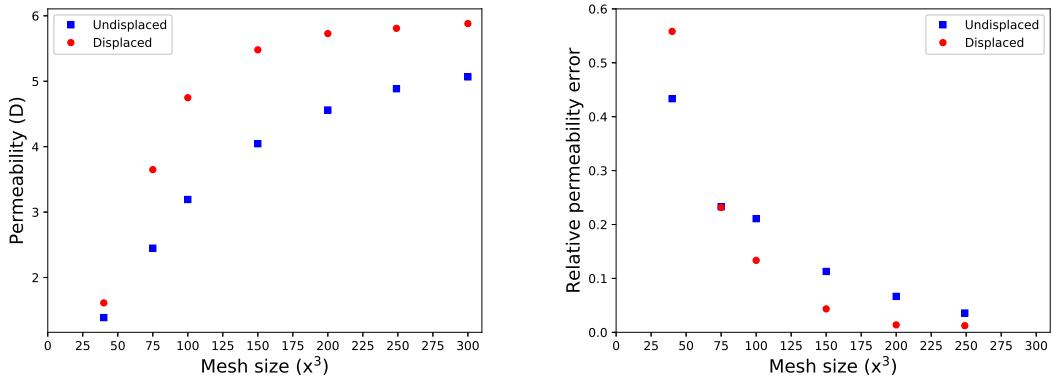
256 The mesh convergence of the two methods is plotted in Fig. 9, in absolute values and with the relative error. Contrary to the previous benchmarking section, we simulate a real application of the method. Therefore the convergence  
 257 is assessed at each increment of size by evaluating the relative error compared to the previous size selected, unlike the  
 258 previous section where the absolute error is computed. Convergence is deemed reached under 2% error. It is achieved  
 259 with the displaced boundary method at less than half the image resolution, similarly to Fig. 8. The improvement  
 260 can be seen two ways. At the converged size of  $200^3$  voxels, it corresponds to a gain of 5% accuracy compared to  
 261 the undisplaced method. On the other hand, if we expect the mesh convergence of this sample would normally be  
 262 reached at  $1000^3$  voxels with the undisplaced method, using the displaced boundary method corresponds to saving  
 263  $4 \times (1000 - 200)^3 \approx 2 \times 10^9$  DOF of computation, which is a consequent amount.  
 264

## 265 5. Conclusions

266 In this contribution, we have presented a method to improve the mesh convergence of permeability computations  
 267 on  $\mu$ CT-scan. We have managed to do so by approximating the pore-grain geometry of the digital microstructure



**Figure 9:** Visualisation of meshed pore space of the Ketton sample of size  $(1.5\text{mm})^3$ . (a) is the original scan composed of  $500^3$  voxels ; (b) is meshed with  $75^3$  elements with the boundary displaced to fit (a) ; (c) is meshed undisplaced with  $75^3$  elements.



**Figure 10:** Mesh convergence of the permeability of a sample of the Ketton carbonate of size  $(1.5\text{mm})^3$ , with and without the displaced boundary method. The resolution of the original scan is  $150^3$  voxels. (a) shows absolute permeability computation and (b) the evolution of the permeability error compared to the consecutive value.

more accurately than regular meshing techniques. The unfitted boundary method used is implemented in the MOOSE simulation platform. The simulations are performed for an equivalent mesh, in which the nodes of the regular mesh close to the boundary are displaced to the closest point on the exact interface. The method has been benchmarked on the analytical solution of the Poiseuille tube (Sec. 2.1), shown to improve mesh convergence of permeability on three different digital rock samples of a sandpack, a sandstone and a limestone (Sec. 3) and finally applied to a high resolution CT-scan of a limestone (Sec. 4).

Our method allows to obtain a geometrical accuracy of the pore-grain boundary for very coarse meshes. In order to obtain global mesh convergence of the permeability, we only need to satisfy the absolute numerical mesh convergence. For this reason, our method is expected to perform better for high resolution CT-scans where the numerical mesh convergence is reached even for meshes coarser than the image resolution. Still, the unfitted boundary finite element method has been applied in this contribution to  $\mu$ CT images of digital rocks obtained after relatively coarse voxelised segmentation. However, the recent development of Super Resolution Convolutional Neural Networks (Wang et al., 2019a; Janssens et al., 2020) enable to produce high quality, high resolution images that are optimised for further segmentation and grey scale analysis of large samples. This unfitted boundary method would prove particularly useful by taking profit of the very high resolution pore-grain boundary resulting from more complex segmentation.

Finally, this method has only been applied here in the case of a static interface. However, multi-physical processes like mechanical deformations of the solid matrix (Lesueur et al., 2017) or dissolution-precipitation mechanisms (Lesueur et al., 2020; Rattez et al., 2019; Guevel et al., 2019) induce a displacement of the interface, which cannot

remain static during a simulation. The unfitted boundary method applied to flow coupled to these processes would allow to track accurately and in a continuous way the interface without at the same time requiring a very fine mesh.

## References

- Ahmed, U., Crary, S.F., Coates, G.R., 1991. Permeability estimation. The various sources and their interrelationships. *Journal of Petroleum Technology* 43, 578–587. doi:10.2118/19604-PA.
- Andrä, H., Combaret, N., Dvorkin, J., Glatt, E., Han, J., Kabel, M., Keehm, Y., Krzikalla, F., Lee, M., Madonna, C., Marsh, M., Mukerji, T., Saenger, E.H., Sain, R., Saxena, N., Ricker, S., Wiegmann, A., Zhan, X., 2013. Digital rock physics benchmarks—part i: Imaging and segmentation. *Computers & Geosciences* 50, 25–32. doi:10.1016/j.cageo.2012.09.005.
- Arns, C.H., Bauget, F., Limaye, A., Sakellariou, A., Senden, T., Sheppard, A., Sok, R.M., Pinczewski, V., Bakke, S., Berge, L.I., Oren, P.E., Knackstedt, M.A., 2005. Pore scale characterization of carbonates using x-ray microtomography. *SPE Journal* 10, 475–484. doi:10.2118/90368-pa.
- Arns, C.H., Knackstedt, M.A., Pinczewski, W.V., Garboczi, E.J., 2002. Computation of linear elastic properties from microtomographic images: Methodology and agreement between theory and experiment. *GEOPHYSICS* 67, 1396–1405. doi:10.1190/1.1512785.
- Arns, C.H., Knackstedt, M.A., Pinczewski, W.V., Martys, N.S., 2004. Virtual permeametry on microtomographic images. *Journal of Petroleum Science and Engineering* 45, 41–46.
- Balay, S., Abhyankar, S., Adams, M.F., Brown, J., Brune, P., Buschelman, K., Dalcin, L., Eijkhout, V., Gropp, W.D., Kaushik, D., Knepley, M.G., McInnes, L.C., Rupp, K., Smith, B.F., Zampini, S., Zhang, H., 2016. PETSc Users Manual. Technical Report ANL-95/11 - Revision 3.7. Argonne National Laboratory.
- Beard, D.C., Weyl, P.K., 1973. Influence of texture on porosity and permeability of unconsolidated sand. *AAPG Bulletin* 57. doi:10.1306/819a4272-16c5-11d7-8645000102c1865d.
- Bjorlykke, K., 2010. Petroleum Geoscience: from Sedimentary Environments to Rock Physics. doi:10.1007/978-3-642-02332-3, arXiv:arXiv:1011.1669v3.
- Blunt, M.J., Bijeljic, B., Dong, H., Gharbi, O., Iglesias, S., Mostaghimi, P., Paluszny, A., Pentland, C., 2013. Pore-scale imaging and modelling. *Advances in Water Resources* 51, 197–216. doi:10.1016/j.advwatres.2012.03.003.
- Borujeni, A.T., Lane, N., Thompson, K., Tyagi, M., 2013. Effects of image resolution and numerical resolution on computed permeability of consolidated packing using LB and FEM pore-scale simulations. *Computers & Fluids* 88, 753–763. doi:10.1016/j.compfluid.2013.05.019.
- Burman, E., Claus, S., Hansbo, P., Larson, M.G., Massing, A., 2015. Cutfem: discretizing geometry and partial differential equations. *International Journal for Numerical Methods in Engineering* 104, 472–501.
- Burman, E., Fernández, M.A., 2011. Analysis of the pspg method for the transient stokes' problem. *Computer methods in applied mechanics and engineering* 200, 2882–2890.
- Cnudde, V., Boone, M., 2013. High-resolution x-ray computed tomography in geosciences: A review of the current technology and applications. *Earth-Science Reviews* 123, 1–17. doi:10.1016/j.earscirev.2013.04.003.
- Cox, M.R., Budhu, M., 2008. A practical approach to grain shape quantification. *Engineering Geology* 96, 1–16. doi:10.1016/j.enggeo.2007.05.005.
- Darcy, H.P.G., 1856. Détermination des lois d'écoulement de l'eau à travers le sable, in: *Les fontaines publiques de la ville de Dijon*. V. Dalamont, pp. 590–594.
- Elman, H., Howle, V.E., Shadid, J., Shuttleworth, R., Tuminaro, R., 2008. A taxonomy and comparison of parallel block multi-level preconditioners for the incompressible navier–stokes equations. *J. Comput. Phys.* 227, 1790–1808. doi:10.1016/j.jcp.2007.09.026.
- Ghabezloo, S., Sulem, J., Saint-Marc, J., 2009. Evaluation of a permeability–porosity relationship in a low-permeability creeping material using a single transient test. *International Journal of Rock Mechanics and Mining Sciences* 46, 761–768. doi:10.1016/j.ijrmms.2008.10.003.
- Godel, B., 2013. High-resolution x-ray computed tomography and its application to ore deposits: From data acquisition to quantitative three-dimensional measurements with case studies from ni-cu-PGE deposits. *Economic Geology* 108, 2005–2019. doi:10.2113/econgeo.108.8.2005.
- Guevel, A., Rattez, H., Veveakis, M., 2019. Contact phase-field modeling for chemo-mechanical degradation processes. Part II: Numerical applications with focus on pressure solution. Preprint arXiv doi:arXiv:1907.00698.
- Guibert, R., Nazarov, M., Horgue, P., Hamon, G., Creux, P., Debenest, G., 2015. Computational permeability determination from pore-scale imaging: Sample size, mesh and method sensitivities. *Transport in Porous Media* 107, 641–656. doi:10.1007/s11242-015-0458-0.
- Henson, V.E., Yang, U.M., 2002. BoomerAMG: A parallel algebraic multigrid solver and preconditioner. *Applied Numerical Mathematics* 41, 155–177. doi:10.1016/s0168-9274(01)00115-5.
- Iassonov, P., Gebreleges, T., Tuller, M., 2009. Segmentation of x-ray computed tomography images of porous materials: A crucial step for characterization and quantitative analysis of pore structures. *Water Resources Research* 45. doi:10.1029/2009wr008087.
- Imperial College Consortium On Pore-Scale Modelling, 2014a. Lv60a sandpack. doi:10.6084/m9.figshare.1153795.
- Imperial College Consortium On Pore-Scale Modelling, 2014b. S1 sandstone. doi:10.6084/m9.figshare.1189274.v1.
- Jacobson, A., Panizzo, D., et al., 2018. libigl: A simple C++ geometry processing library. [Https://libigl.github.io/](https://libigl.github.io/).
- Janssens, N., Huysmans, M., Swennen, R., 2020. Computed tomography 3D super-resolution with generative adversarial neural networks: Implications on unsaturated and two-phase fluid flow. *Materials* 13. doi:10.3390/ma13061397.
- Lesueur, M., Casadiego, M.C., Veveakis, M., Poulet, T., 2017. Modelling fluid-microstructure interaction on elasto-visco-plastic digital rocks. *Geomechanics for Energy and the Environment* 12, 1–13. doi:10.1016/j.gete.2017.08.001.
- Lesueur, M., Poulet, T., Veveakis, M., 2020. Three-scale multiphysics finite element framework (FE3) modelling fault reactivation. *Computer*

- 346 Methods in Applied Mechanics and Engineering 365, 112988. URL: <https://doi.org/10.1016/j.cma.2020.112988>, doi:10.1016/j.cma.2020.112988.
- 347 Liu, J., Pereira, G.G., Regenauer-Lieb, K., 2014. From characterisation of pore-structures to simulations of pore-scale fluid flow and the upscaling  
348 of permeability using microtomography: A case study of heterogeneous carbonates. Journal of Geochemical Exploration 144, 84–96. doi:10.  
349 1016/j.gexplo.2014.01.021.
- 350 Manwart, C., Aaltosalmi, U., Koponen, A., Hilfer, R., Timonen, J., 2002. Lattice-boltzmann and finite-difference simulations for the permeability  
351 for three-dimensional porous media. Physical Review E 66. doi:10.1103/physreve.66.016702.
- 352 Mees, F., Swennen, R., Geet, M.V., Jacobs, P., 2003. Applications of x-ray computed tomography in the geosciences. Geological Society, London,  
353 Special Publications 215, 1–6. doi:10.1144/gsl.sp.2003.215.01.01.
- 354 Mittal, R., Iaccarino, G., 2005. Immersed boundary methods. Annu. Rev. Fluid Mech. 37, 239–261.
- 355 Mostaghimi, P., Blunt, M.J., Bijeljic, B., 2012. Computations of absolute permeability on micro-CT images. Mathematical Geosciences 45,  
356 103–125. doi:10.1007/s11004-012-9431-4.
- 357 Narváez, A., Yazdchi, K., Luding, S., Harting, J., 2013. From creeping to inertial flow in porous media: a lattice boltzmann–finite element study. J.  
358 Stat. Mech: Theory Exp. 2013, 2–38. doi:10.1088/1742-5468/2013/02/p02038.
- 359 Permann, C.J., Gaston, D.R., Andriš, D., Carlsen, R.W., Kong, F., Lindsay, A.D., Miller, J.M., Peterson, J.W., Slaughter, A.E., Stogner, R.H.,  
360 Martineau, R.C., 2020. MOOSE: Enabling massively parallel multiphysics simulation. SoftwareX 11, 100430. URL: <http://www.sciencedirect.com/science/article/pii/S2352711019302973>, doi:<https://doi.org/10.1016/j.softx.2020.100430>.
- 361 Peterson, J.W., Lindsay, A.D., Kong, F., 2018. Overview of the incompressible navier–stokes simulation capabilities in the MOOSE framework.  
362 Adv. Eng. Software 119, 68–92. doi:10.1016/j.advengsoft.2018.02.004.
- 363 Petrasch, J., Meier, F., Friess, H., Steinfield, A., 2008. Tomography based determination of permeability, dupuit–forchheimer coefficient, and  
364 interfacial heat transfer coefficient in reticulate porous ceramics. Int. J. Heat Fluid Flow 29, 315–326. doi:10.1016/j.ijheatfluidflow.  
365 2007.09.001.
- 366 Rangarajan, R., Lew, A.J., 2014. Universal meshes: A method for triangulating planar curved domains immersed in nonconforming meshes.  
367 International Journal for Numerical Methods in Engineering 98, 236–264. doi:10.1002/nme.4624.
- 368 Rattez, H., Disidoro, F., Sulem, J., Veveakis, M., 2019. Influence of dissolution on the frictional properties of carbonate faults. Preprint EarthArXiv  
369 doi:10.31223/osf.io/b8xuh.
- 370 Salvo, L., Cloetens, P., Maire, E., Zabler, S., Blandin, J.J., Buffière, J.Y., Ludwig, W., Boller, E., Bellet, D., Josserond, C., 2003. X-ray micro-  
371 tomography an attractive characterisation technique in materials science. Nuclear Instruments and Methods in Physics Research, Section B:  
372 Beam Interactions with Materials and Atoms 200, 273–286. doi:10.1016/S0168-583X(02)01689-0.
- 373 Sarker, M., Siddiqui, S., 2009. Advances in micro-CT based evaluation of reservoir rocks, in: SPE Saudi Arabia Section Technical Symposium,  
374 Society of Petroleum Engineers. doi:10.2118/126039-ms.
- 375 Saxena, N., Hows, A., Hofmann, R., O. Alpak, F., Freeman, J., Hunter, S., Appel, M., 2018. Imaging and computational considerations for  
376 image computed permeability: Operating envelope of Digital Rock Physics. Advances in Water Resources 116, 127–144. URL: <https://doi.org/10.1016/j.advwatres.2018.04.001>.
- 377 Song, R., Wang, Y., Liu, J., Cui, M., Lei, Y., 2019. Comparative analysis on pore-scale permeability prediction on micro-CT images of rock using  
378 numerical and empirical approaches. Energy Science and Engineering 7, 2842–2854. doi:10.1002/ese3.465.
- 379 Soulaine, C., Gjetvaj, F., Garing, C., Roman, S., Russian, A., Gouze, P., Tchelepi, H.A., 2016. The impact of sub-resolution porosity of x-ray  
380 microtomography images on the permeability. Transport in Porous Media 113, 227–243. doi:10.1007/s11242-016-0690-2.
- 381 Torskaya, T., Shabro, V., Torres-Verdín, C., Salazar-Tio, R., Revil, A., 2013. Grain shape effects on permeability, formation factor, and capillary  
382 pressure from pore-scale modeling. Transp. Porous Media 102, 71–90. doi:10.1007/s11242-013-0262-7.
- 383 Tuan, H.S., Hutmacher, D.W., 2005. Application of micro CT and computation modeling in bone tissue engineering. Computer-Aided Design 37,  
384 1151–1161. doi:10.1016/j.cad.2005.02.006.
- 385 Wang, J., Fleischmann, D., 2018. Improving spatial resolution at CT: Development, benefits, and pitfalls. Radiology 289, 261–262. doi:10.1148/  
386 radiol.2018181156.
- 387 Wang, Y.D., Armstrong, R.T., Mostaghimi, P., 2019a. Enhancing resolution of digital rock images with super resolution convolutional neural  
388 networks. Journal of Petroleum Science and Engineering 182, 106261. doi:10.1016/j.petrol.2019.106261.
- 389 Wang, Y.D., Chung, T., Armstrong, R.T., McClure, J.E., Mostaghimi, P., 2019b. Computations of permeability of large rock images by dual grid  
390 domain decomposition. Advances in Water Resources 126, 1–14. doi:10.1016/j.advwatres.2019.02.002.
- 391 Whitaker, S., 1986. Flow in porous media i: A theoretical derivation of darcy's law. Transp. Porous Media 1, 3–25. doi:10.1007/bf01036523.
- 392 Yang, L., Yang, J., Boek, E., Sakai, M., Pain, C., 2019. Image-based simulations of absolute permeability with massively parallel pseudo-  
393 compressible stabilised finite element solver. Computational Geosciences 23, 881–893. doi:10.1007/s10596-019-09837-4.