# Second order deviation of absolute permeability due to unresolved morphological features at the pore scale

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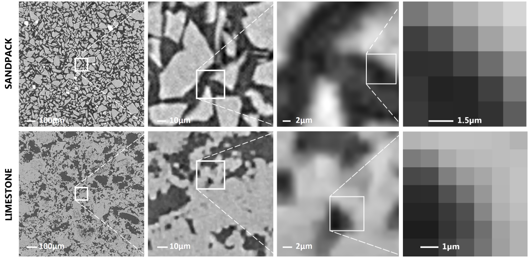
# Summary

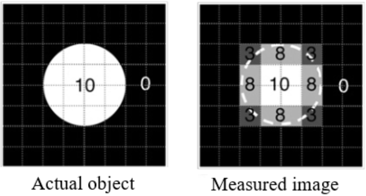
## Table of contents:

# From X-ray $\mu$CT uncertainties...

- Rock X-ray scans and related pore space geometry up to the voxel scale
- Compromise between sample volume and scan resolution,
- Partial-Volume effect,
- Blurred rock matrix interfaces, unresolved features
- **Morphological uncertainties**




M. Soret and al (2007)

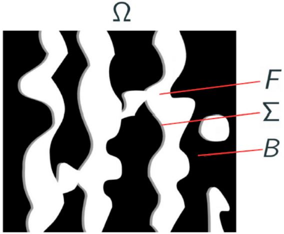



**Quantify the deviation of computed absolute permeability accounting these uncertainties in real rock geometries**

# ...to slip length formalism in Stokes problem

## One-phase flow of Newtonian fluid in an impermeable rock matrix

- Relation between these features uncertainties and slip condition
- Isotropic permeability case : $\mathbf{K}_\beta = \kappa_\beta \mathbf{I}$ with $\kappa_\beta$ scalar




- Quantify the impact of slip length $\beta$ on the upscaled absolute permeability :

$$\kappa_\beta = \phi\mu < \boldsymbol{u}_\beta >_F / < \mathbf{f} >_F, \qquad (1)$$

where $\phi =< \varepsilon >_\Omega$ is the macro-porosity and $\boldsymbol{u}_\beta$ the pore-scale velocity

D. Lasseux, F.J. Valdés-Parada, J.A.O. Ochoa Tapia and B. Goyeau, *A macroscopic model for slightly compressible gas slip flow in homogeneous porous media*, Phys. Fluids (2014).

D. Lasseux, F.J. Valdés-Parada and M.L. Porter, *An improved macroscale model for gas slip flow in porous media*, J. Fluid Mech. (2016)

# ...to slip length formalism in Stokes problem

## One-phase flow of Newtonian fluid in an impermeable rock matrix

One has $\kappa_\beta = \phi\mu < u_\beta >_F / < f >_F$ where $(u_\beta, p_\beta)$ solution of the Stokes problem

$$\begin{cases} -\Delta u + \nabla p = f & \text{in} \quad F, \\ \nabla \cdot u = 0 & \text{in} \quad F, \\ u - \beta T D(u) n = 0 & \text{on} \quad \Sigma, \\ u \text{ and } p \text{ periodic} & \text{on} \quad \Gamma_F = \partial\Omega \cap \partial F \end{cases} \tag{2}$$

with

- $n$ the unit inward normal field at $\Sigma$,
- $T = I - n \otimes n$ the projector on tangential components,
- $D(u) = (\nabla u + \nabla u^T)/2$
- B.C. imply $u \cdot n = 0$ no-slip-through on $\Sigma$.

**Two strategies:** full deviation $[\kappa_0, \kappa_\beta]$ with interface B.C.
or higher-order deviations with $\kappa_\beta = \kappa_0 + \beta L_0 + \frac{\beta^2}{2} L_1 + \mathcal{O}(\beta^3)$


Y. Achdou, O. Pironneau, F. Valentin, *Effective boundary conditions for laminar flows over periodic rough boundaries*, J. Comput. Phys. (1998).
M. Bonnivard, A.-L. Dalibard, D. Gérard-Varet, *Computation of the effective slip of rough hydrophobic surfaces via homogenization*, Math. Models Methods Appl. Sci. (2014)

# First order linear deviation

## Asymptotic expansion with $\kappa_\beta = \kappa_0 + \beta L_0 + \mathcal{O}(\beta^2)$ with $\beta \ll L$

Look for formal development of $u_\beta$ and $p_\beta$ w.r.t $\beta$ :

$$u_\beta = U^0 + \beta U^1 + \beta^2 r_\beta \quad \text{and} \quad p_\beta = P^0 + \beta P^1 + \beta^2 q_\beta$$

The profiles $(U^0, P^0)$ and $(U^1, P^1)$ respectively satisfy :

$$\begin{cases} -\Delta U^0 + \nabla P^0 = f & \text{in } F, \\ \nabla \cdot U^0 = 0 & \text{in } F, \\ U^0 = 0 & \text{on } \Sigma, \end{cases} \qquad \begin{cases} -\Delta U^1 + \nabla P^1 = 0 & \text{in } F, \\ \nabla \cdot U^1 = 0 & \text{in } F, \\ U^1 = TD(U^0)n & \text{on } \Sigma, \end{cases}$$

- Compute directly the linear deviation

$$L_0 = \phi\mu < U^1 >_F / < f >_F \quad \text{and} \quad \kappa_0 = \phi\mu < U^0 >_F / < f >_F$$

- Non-homogeneous Dirichlet B.C. on $U^1$ for linear deviation (prescribed slip velocity) vs Robin one on $u_\beta$ for full deviation
- First order uncertainty interval $[\kappa_0, \kappa_0 + \beta L_0]$



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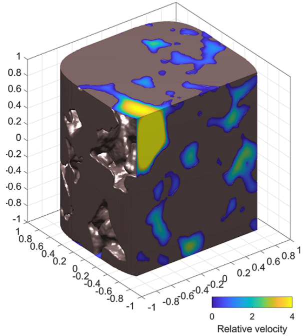
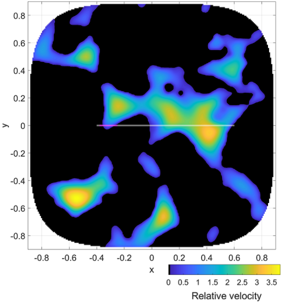
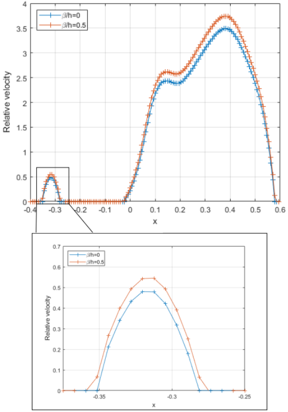
# Non representative samples

Bentheimer ($\mathbf{256^3}$) with large pore structure and voxel size $\boldsymbol{h = 2.2\mu m}$
& Cylindrical pore of radius $\boldsymbol{R}$ in domain of length $\boldsymbol{L}$




Analytical solution for the Stokes flow in a cylindrical pore:

Porosity $\phi = \dfrac{\pi R^2}{L^2}$, Specific area $\boldsymbol{As} = \dfrac{2\pi R}{L^2}$,

First order linear deviation $\kappa_\beta = \dfrac{\pi R^4}{8L^2} + \beta \dfrac{\pi R^3}{2L^2}$ and dimensionless

ratio $\dfrac{L_0}{\kappa_0 A_s} = \dfrac{2L^2}{\pi R^2} \simeq \mathbf{2.9}$

Bentheimer : $\phi = \mathbf{28.75\%}$ and $\boldsymbol{As} = \boldsymbol{25mm^{-1}}$

Relative permeability deviation about **8%**


Permeability uncertainty up to second order deviation

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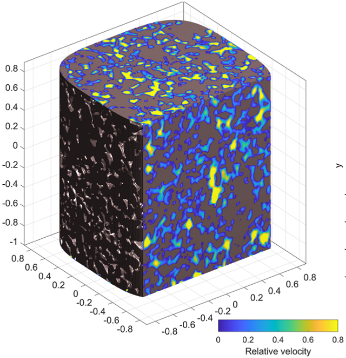
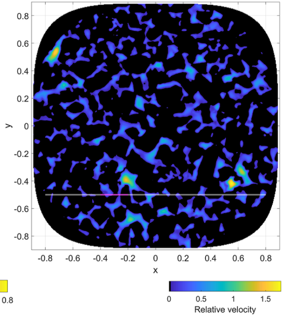
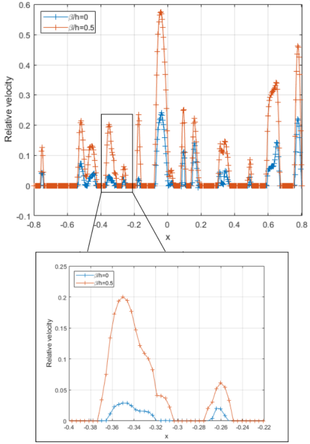
# Slip flow of Newtonian fluid in Castlegate

Representative sample ($512^3$) with **25.1%** porosity, $\boldsymbol{A_s = 15.7mm^{-1}}$ and $\boldsymbol{h = 5.6\mu m}$




$$\kappa_0 = 15.9\mu m^2 \text{ and } \kappa_\beta = 25.7\mu m^2 \text{ for } \beta/h = 0.5$$

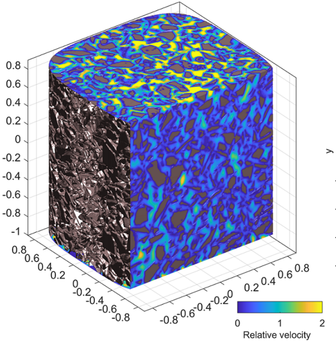
Relative permeability deviation of **61.63%**

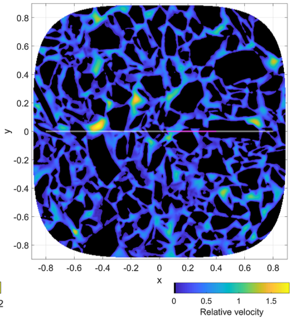
S.Perez, P. Moonen, P.Poncet, *On the Deviation of Computed Permeability Induced by Unresolved Morphological Features of the Pore Space*, Transp Porous Med 141, 151–184 (2022)

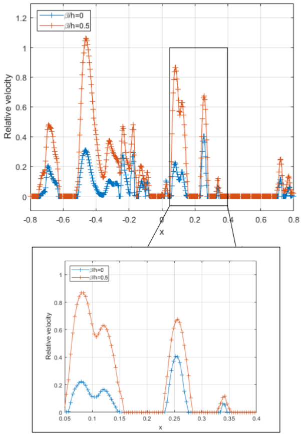
Castlegate $\boldsymbol{\mu CT}$ from the Digital Rock data portal - sampled in Utah, USA

# Slip flow of Newtonian fluid in sand pack

Representative sample ($512^3$) with higher porosity **45.4%**, $\boldsymbol{A_s = 93mm^{-1}}$ and $\boldsymbol{h = 1.5\mu m}$




$$\kappa_0 = 10.2\mu m^2 \text{ and } \kappa_\beta = 24.8\mu m^2 \text{ for } \beta/h = 0.5$$

Relative permeability deviation of **143%**

S.Perez, P. Moonen, P.Poncet, *On the Deviation of Computed Permeability Induced by Unresolved Morphological Features of the Pore Space*, Transp Porous Med 141, 151–184 (2022)

Sand pack $\mu$**CT** provided by P. Moonen - DMEX Centre for X-ray Imaging (UPPA)

# Results Summary

## Absolute permeability ranges and comparison of relative deviations

- Full deviation $[\kappa_0, \kappa_\beta]$ and linear deviation $[\kappa_0, \kappa_0 + \beta L_0]$ comparison
- Non linear effects with $\kappa_\beta = \kappa_0 + \beta L_0 + \mathcal{O}(\beta^2)$
- Two dimensionless ratios : $K'/\kappa_0 A_s$ with $K' = (\kappa_\beta - \kappa_0)/\beta$ and $L_0/\kappa_0 A_s$

| Sample | Porosity | $A_s$ | β | $\kappa_0$ | Full deviation | | |
|---|---|---|---|---|---|---|---|
| | | | | | Relative deviation $K'/\kappa_0$ | $(\kappa_\beta - \kappa_0)/\kappa_0$ | $K'/\kappa_0 A_s$ |
| **Unit** | _ | $mm^{-1}$ | $\mu m$ | $\mu m^2$ | $mm^{-1}$ | _ | _ |
| *Cyl. Pore* | $\pi R^2/L^2$ | $2\pi R/L^2$ | _ | $\pi R^4/8L^2$ | $4/R$ | $\beta\pi R^3/2L^2\kappa_0$ | $2L^2/\pi R^2$ |
| *Bentheimer* | 28,75 % | 25 | 1,1 | 28,7 | 78 | 8,36 % | 3,1 |
| *Castlegate* | 25,1 % | 15,7 | 4,26 | 15,9 | 215,5 | 91,82 % | 13,7 |
| *Sandpack* | 45,4 % | 93 | 1,14 | 10,2 | 1684 | 192,15 % | 18,1 |

- Significant deviation due to geometrical uncertainty
- Sensitivity to the pore space structure
- Similar dimensionless ratios for the representative vs non representative samples

# Results Summary

## Absolute permeability ranges and comparison of relative deviations

- Full deviation $[\kappa_0, \kappa_\beta]$ and linear deviation $[\kappa_0, \kappa_0 + \beta L_0]$ comparison
- Non linear effects with $\kappa_\beta = \kappa_0 + \beta L_0 + \mathcal{O}(\beta^2)$
- Two dimensionless ratios : $K'/\kappa_0 A_s$ with $K' = (\kappa_\beta - \kappa_0)/\beta$ and $L_0/\kappa_0 A_s$

| Sample | Porosity | $A_s$ | β | $\kappa_0$ | Linear deviation | | |
|---|---|---|---|---|---|---|---|
| | | | | | Relative deviation $L_0/\kappa_0$ | $\beta L_0/\kappa_0$ | $L_0/\kappa_0 A_s$ |
| *Unit* | _ | $mm^{-1}$ | $\mu m$ | $\mu m^2$ | $mm^{-1}$ | _ | _ |
| *Cyl. Pore* | $\pi R^2/L^2$ | $2\pi R/L^2$ | _ | $\pi R^4/8L^2$ | $4/R$ | $\beta\pi R^3/2L^2\kappa_0$ | $2L^2/\pi R^2$ |
| *Bentheimer* | 28,75 % | 25 | 1,1 | 28,7 | 63,7 | 6,97 % | 2,5 |
| *Castlegate* | 25,1 % | 15,7 | 4,26 | 15,9 | 186 | 79,25 % | 11,9 |
| *Sandpack* | 45,4 % | 93 | 1,14 | 10,2 | 1561 | 179,22 % | 16,8 |

- Significant deviation due to geometrical uncertainty
- Sensitivity to the pore space structure
- Similar dimensionless ratios for the representative vs non representative samples



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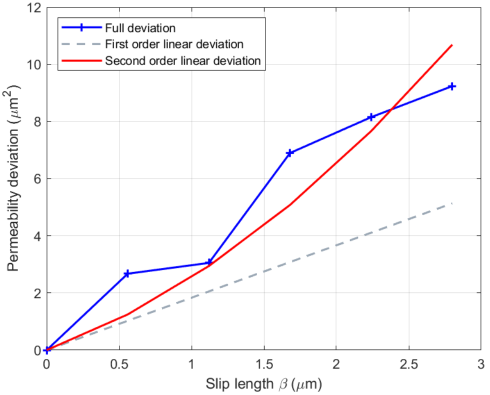
# Second order deviation on the Castlegate

$\kappa_\beta = \kappa_0 + \beta L_0 + \frac{\beta^2}{2} L_1 + \mathcal{O}(\beta^3)$

Generalisation to

$$u_\beta = \sum_{j=0}^{2} \beta^j U^j + \beta^3 r_\beta \quad \text{and} \quad p_\beta = \sum_{j=0}^{2} \beta^j P^j + \beta^3 q_\beta$$

with an intrinsic slip-flow correction for the second order profile $(U^2, P^2)$




- Full permeability deviation $\kappa_\beta$
- First and second order deviation $\beta L_0$ and $\beta L_0 + \frac{\beta^2}{2} L_1$
- Macroscopic effect due to second order deviation
- Real geometry applications in agreement with what was developed by D. Lasseux, F.J. Valdés-Parada and al

D. Lasseux, F.J. Valdés-Parada and M.L. Porter, *An improved macroscale model for gas slip flow in porous media*, J. Fluid Mech. (2016)

# Conclusion and prospects

- Permeability uncertainty coming from X-ray $\mu CT$ in 3D geometries
- Comparison of full deviation and first order linear deviation coming from expansion of $\kappa_\beta$
- Second order deviation is relevant to explain the apparent permeability macroscopic effects
- Quantifying uncertainties on permeability for evolving fluid/solid interface under reactive processes

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Thank You

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S. Perez, F. J. Valdés-Parada, D. Lasseux, P. Poncet



LMAP Pau (FR), UMR CNRS 5142, E2S-UPPA

# Part I

# Appendix

# Representative slip length $\beta$

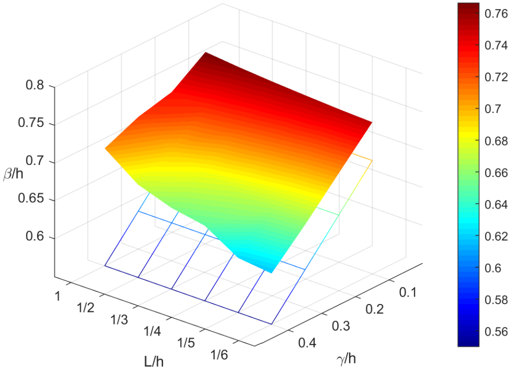
- Choice of $\beta$ related to $\mu$CT image uncertainties
- Based on the voxel size $h$ with $0 \leq \beta \leq h$ and adjusted to deal with pore roughness
- Sinusoidal roughness pattern on a voxel

$$\varphi(x, y) = \delta + \frac{\gamma}{2} \sin(2\pi x/L) \sin(2\pi y/L)$$

Mean solid position at $\delta/h = 0.25$

Representative slip length for both under-resolved roughness and blurred interface

$\beta/h = 0.5$ to $0.76$ in real rock applications




Permeability uncertainty up to second order deviation

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