On the predictive capabilities of multiphase Darcy flow models

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Outline

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Introduction, subsurface flow models

UQ, pore-scale simulation and upscaling

Model calibration and validation

Conclusions

Motivation
Multiphase flows in porous media

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Applications

Primary and secondary Oil Recovery, Groundwater remediation, Biological flows, Catalysis, Fluidized beds

Upscaled (effective, homogenized, averaged) transport models rely on physical and empirical parameters:

1. Absolute permeability (pure advection)

$$K \propto \frac{V}{\Delta P}$$

2. Dispersivity (diffusion + advection) $D = D(V, D_m)$
3. Relative permeability model

$$K_i = K_i(C) \propto \frac{V_i}{\Delta P_i}$$

4. Capillary pressure model $P_i = P_i(P, C)$

How to quantify the validity of the standard Darcy's models?
How to check their actual predictivity?

Single-phase flow
Decoupled solute transport

Pore-scale model

Steady Navier Stokes equations in the pore space

$$\nabla \cdot \mathbf{u} = 0 \qquad \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\Delta \mathbf{u}$$

Advection Diffusion Reaction:

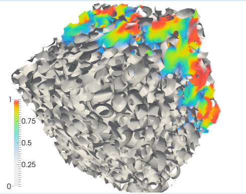
$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c + \mathbf{D}_0 \nabla c) = 0$$

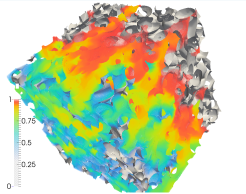
Darcy-scale model

$$\nabla \cdot \mathbf{V} = 0 \qquad \mathbf{V} = -\frac{\mathbf{K}}{\mu}\nabla P$$

Advection-Dispersion-Reaction:

$$\frac{\partial C\phi}{\partial t} + \nabla \cdot (\mathbf{V}C + \mathbf{D}\phi\nabla C) = 0$$





Two phase immiscible flow

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Pore-scale model:

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\rho \frac{\partial}{\partial t}(\mathbf{u}) + \rho \mathbf{u} \cdot \nabla(\mathbf{u}) = -\nabla p + \mu \Delta \mathbf{u} + \kappa \sigma \mathbf{n} \delta(\Gamma)$$

Interface advection:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u} c) = 0$$

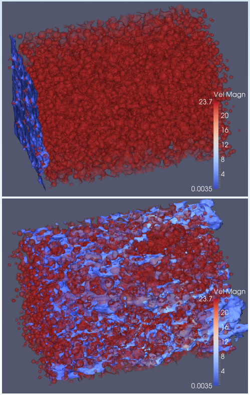
Darcy-scale model

Wang/Beckermann mixture model

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \qquad \mathbf{V} = -\frac{\lambda(K_r)\mathbf{K}}{\mu}(\nabla P - \rho \frac{\partial \mathbf{V}}{\partial t})$$

Advection-Dispersion-Reaction (saturation equation):

$$\frac{\partial C\phi}{\partial t} + \nabla \cdot [\mathbf{V}_c (K_r) C + \mathbf{D}\phi \nabla C] = 0$$



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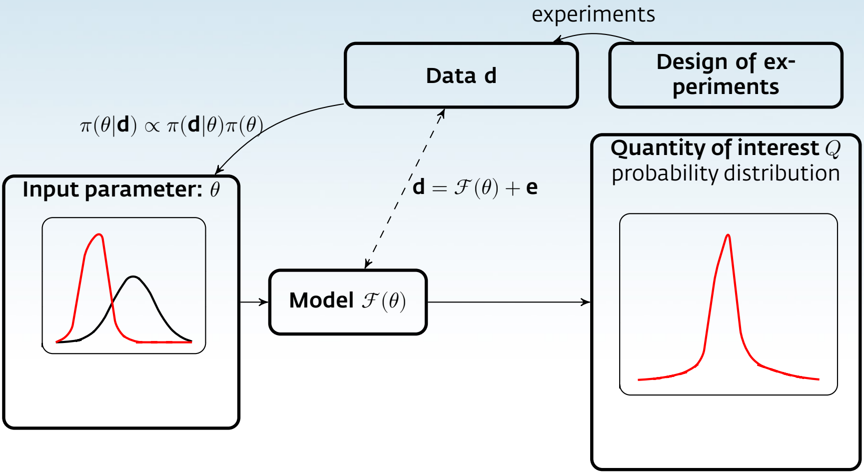
Bayesian UQ

In our predictions there exist many sources of error/uncertainty:
numerics, model, randomness, parameters



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Heterogeneous and Multiscale data assimilation

- Data come from Experiments at different scales
- Accurate physical models exists for pore-scale (Navier-Stokes) flow
- How to combine all these data?
- Development of stochastic models for upscaling and modelling errors

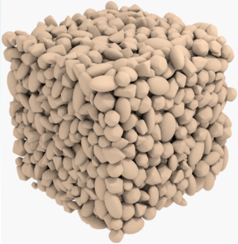
Propagation across scales

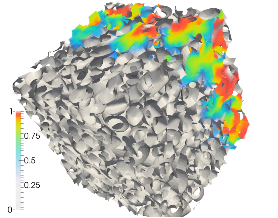
- Variability starts at the Navier-Stokes scale with random geometry
- It propagates to stochastic effective transport parameters of phenomenological or homogenized models[a]
- With the help of spatial statistical model assumptions we can link to the macro-scale stochastic models

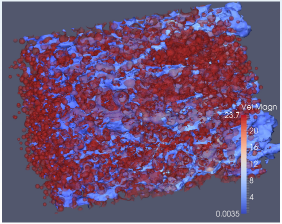
[a] Random and periodic homogenization can be used only for global quantities with specific norms

Pore-scale simulation videos

+ Promising tool for model development, calibration and validation
− Still not fully predictive for complex flow problems due to numerical and geometrical approximations, sample size and physical assumptions







Pore-scale simulation of solute transport (Icardi et. al, 2014)

Pore-scale simulation of CO_2 injection (Icardi et. al, in preparation)

Monte Carlo and Multilevel MC

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Given a random variable X and a quantity of interest Q

$$E[Q(X)] = \frac{1}{M}\sum_{i=1}^{M} Q(X_i) + e \qquad \text{with} \quad e \sim \mathcal{N}\left(0, \frac{Var(Q)}{M}\right)$$

Multilevel Monte Carlo Giles, 2008

Given different accuracy levels ℓ and solution $Q_\ell^{(i)} = Q_\ell(X_i)$, the multilevel estimator is defined as

$$\mathcal{A}_{ML} = \sum_{\ell=0}^{L}\sum_{i=1}^{M_\ell} \frac{Q_\ell^{(i)} - Q_{\ell-1}^{(i)}}{M_\ell}$$

with M_ℓ number of samples on level ℓ and $Q_{-1} = 0$.

- WEAK (mean) ERROR: $|E[Q - Q_\ell]| \approx 2^{-\alpha\ell}$
- MULTILEVEL VARIANCES: $Var(Q_\ell - Q_{\ell-1}) \approx 2^{-\beta\ell}$
- COMPUTATIONAL WORK: $E[\text{Cost}\,(Q_\ell - Q_{\ell-1})] \approx 2^{\gamma\ell}$

Improving MLMC

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Icardi, Boccardo, Tempone (2015, Adv Water Res)
Hoel, Icardi, Tempone (in preparation)
Diffusion and Navier-Stokes equations in random perforated domains

Multiscale MLMC

- Using models at different scales via averaging/homogenization (e.g., Navier-Stokes/Darcy)
- Upscaled model should be fast $\Rightarrow$ approximate/reduced model

High-order MLMC

- Differences with high-order stencils
- Richardson extrapolation for reducing bias (Giles, 2008; Lemaire, Pagés, 2013)
- Multi-Index Monte Carlo (MIMC, Haji-Ali, Nobile, Tempone, 2014)
- Weighted MLMC for reducing variance

$$C_\ell Q_\ell - C_{\ell-1} Q_{\ell-1} + C_{\ell-2} Q_{\ell-2}$$

where C_i can be optimized to minimize the total variance of the estimator

These improvements are particularly important for complex black-box solvers when the convergence properties (α, β) are not guaranteed or non asymptotic

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Bayesian model validation

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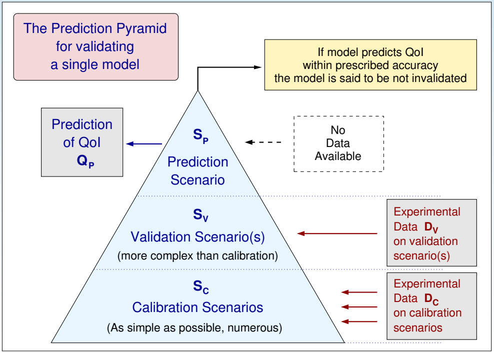
The validation pyramid[1]

Calibration, Validation, Prediction

1. start with priors on unknown parameters $\pi(\theta)$
2. compute posterior $\pi(\theta|d_c)$ given data d_c in the calibration scenario
3. forward propagation $\pi(\theta|d_c)$ in a new validation scenario to obtain $\pi(Q_c)$
4. incorporate new data d_v and recompute $\pi(\theta|d_c, d_v)$ and $\pi(Q_d)$
5. compute a "distance" Δ (e.g., KL divergence) between $\pi(Q_d)$ and $\pi(Q_c)$
6. if $\Delta < TOL$ model is valid
7. prediction and forward propagation to obtain final QoI $\pi(Q_v)$

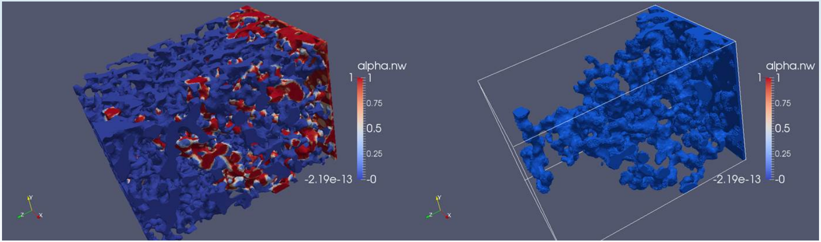


Ingredients: prior, data, error models
Strongly depends on: choice of measurements, choice of QoI

[1] Babuska, Nobile, Tempone; Oden, Moser, Ghattas

Calibration experiment

Let us focus on an simple virtual experiment condition:
Pore-scale results are exactup to a small Gaussian uncorrelated error
One single sample



- surfactant flooding experiment studied by Landry et al (2014)
- Low density and viscosity ratio (≈ 1)
- Quasi-neutral wetting (95 degrees contact angle)
- 5 imposed pressure gradients $10^3 - 10^7$ Pa/m
- Measured mean saturation in the volume

Models to calibrate

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Darcy-scale model

Wang/Beckermann mixture model

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0 \qquad V = -\frac{\lambda(K_r)K}{\mu}(\nabla P - \rho \frac{\partial V}{\partial t})$$

Advection-Dispersion-Reaction (saturation equation):

$$\frac{\partial C\phi}{\partial t} + \nabla \cdot [V_c\,(K_r)\,C + D\phi\nabla C] = 0$$

- 1D Advection-Diffusion Equation

$$K_r = 1$$

$$\theta = \{K, D/\Delta P\}$$

- 1D ADE with Corey-Brook relative permeability

$$K_r \propto (1 - C)^\gamma$$

$$\theta = \{K, D/\Delta P, \gamma\}$$

Implementation

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- Geometry (random packing): Blender + random packing code (Python)
- Pore-scale DNS: **OpenFOAM** (Algebraic VOF)

2-parameters model

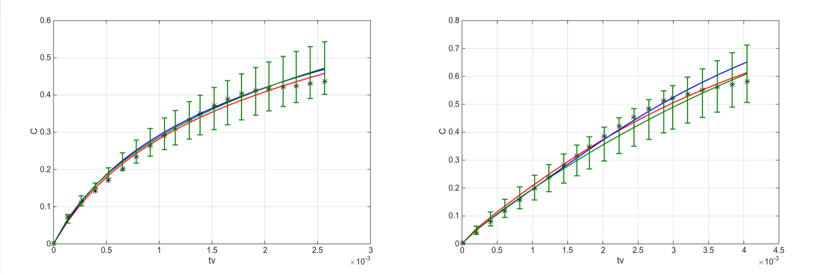
- Forward problem: analytical solution of Advection-Diffusion in semi-infinite domain
- Bayesian inversion: **Chebfun** with full representation of 2D prior and posterior PDF
- Resampling: **Chebfun** to compute marginals and acceptance-rejection probabilities
- Surrogate: **Chebfun** (expensive)

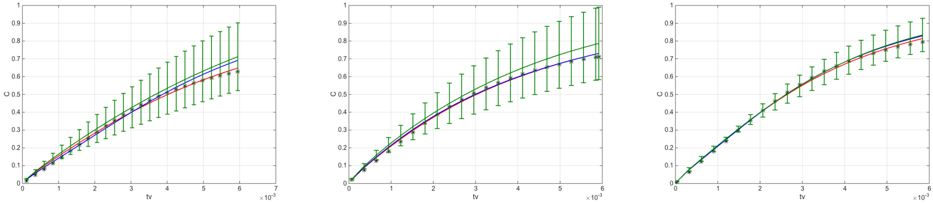
3-parameters model

- Forward problem: **Chebfun** with `pde15s`
- Bayesian inversion: Matlab **MCMC** toolbox
- Surrogate: ??

Advection Dispersion Equation

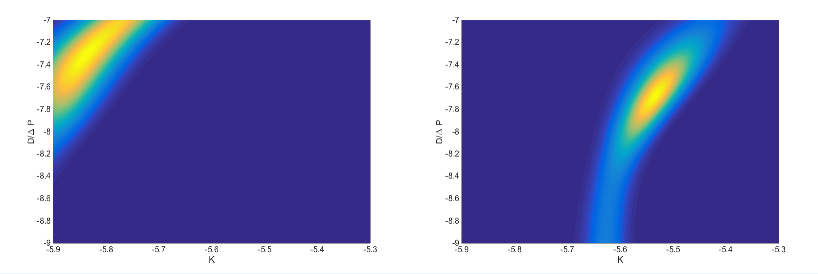
Assimilation of single data sets

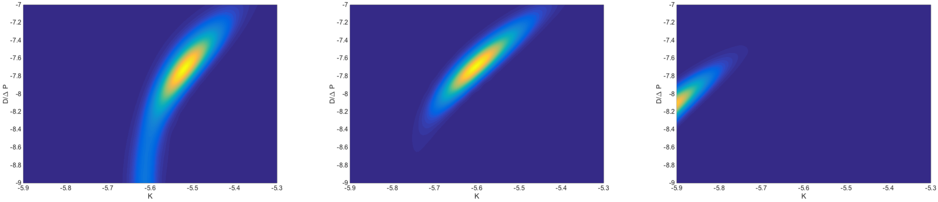




Advection Dispersion Equation

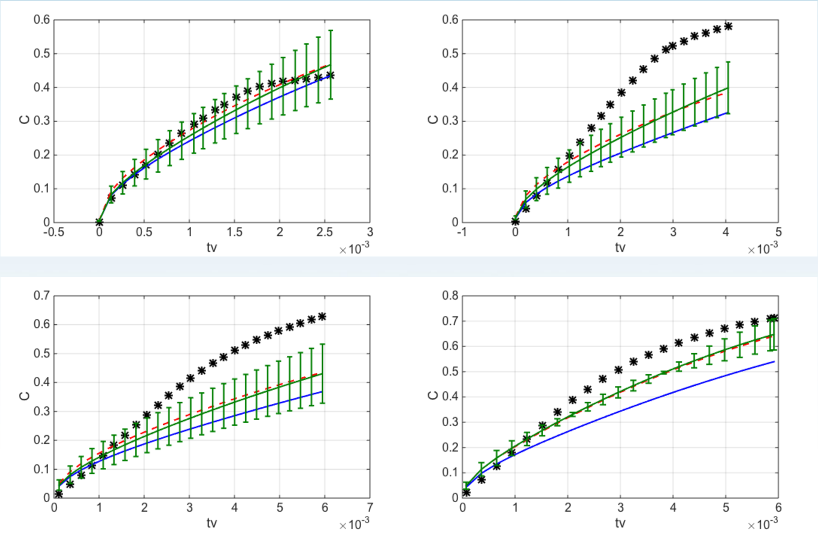
Assimilation of single data sets





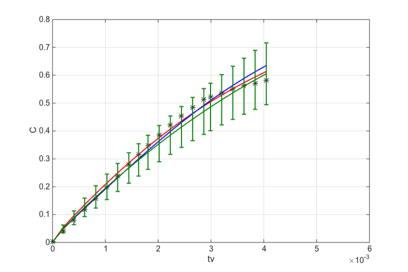
Advection Dispersion Equation

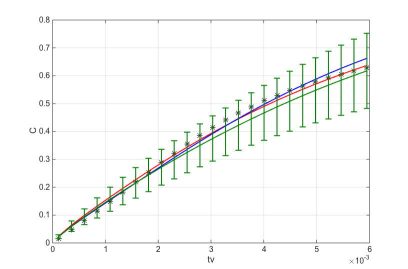
Sequential assimilation of data sets 1 to 5

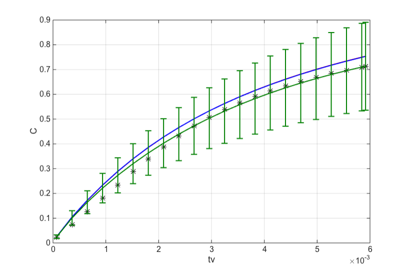


Advection Dispersion Equation

Sequential assimilation of data sets 2 to 4







Advection Dispersion Equation

Sequential assimilation of data sets 2 to 4

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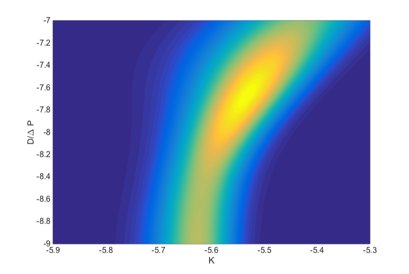
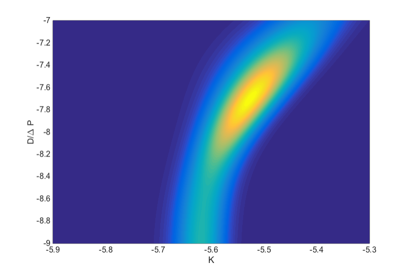
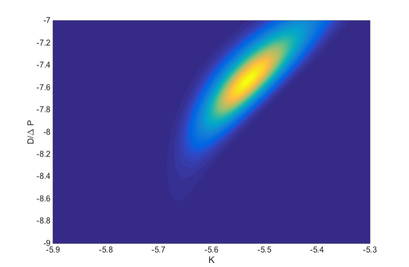
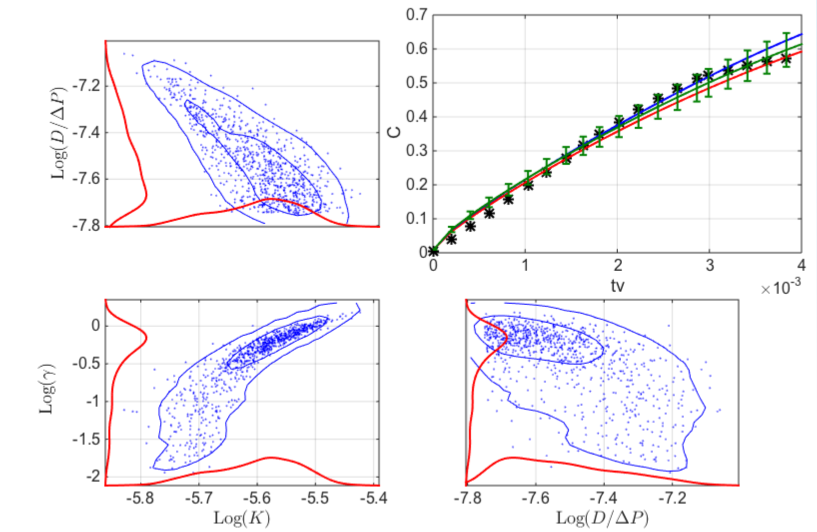






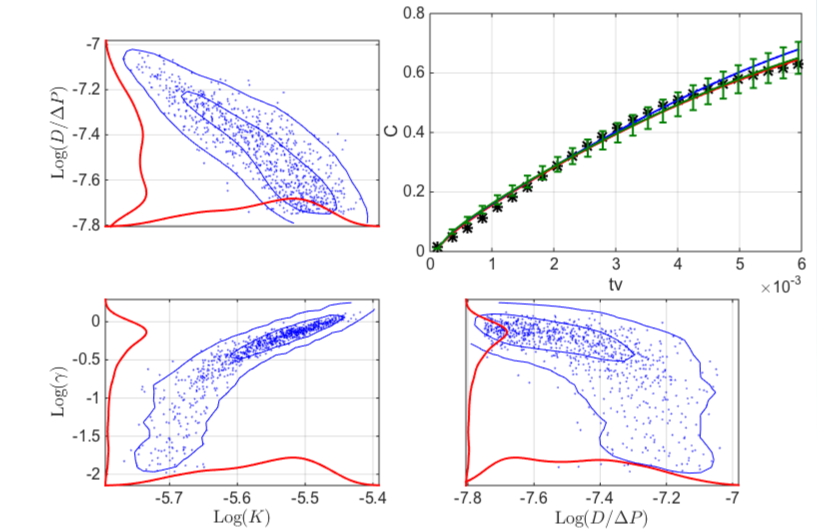
Brooks-Corey relative permeability

Second data set



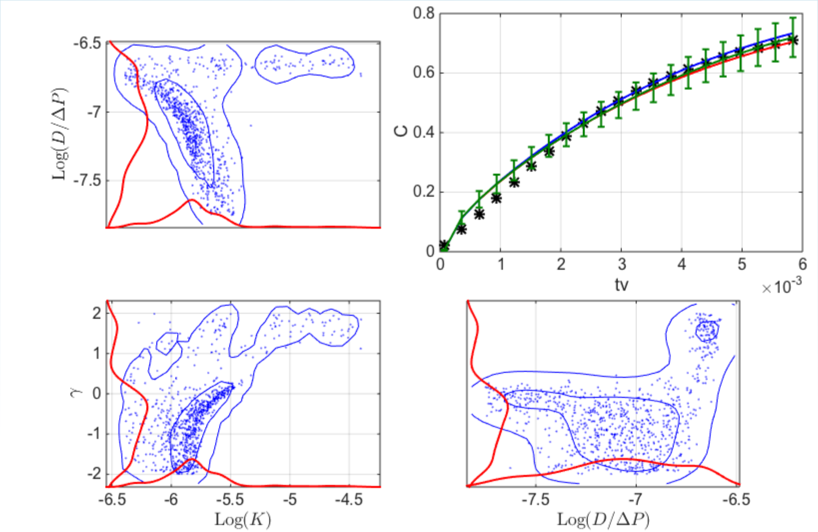
Brooks-Corey relative permeability WARWICK

Second+third data set



Brooks-Corey relative permeability

Second+third+fourth data set



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Achievements

Usage of few global measurements and simple models for complex phenomena leads to

- Surprisingly good fit of simple ADE for single data sets though with large uncertainties
- Improvement with relative permeability models but affected by overfitting

More efforts are needed for:

- Better error models and uncertainty for pore-scale data (ongoing)
- Adding wetting and higher-order (Forchheimer) terms to capture the whole range of flow rate (ongoing)

Future works

- Choose different validation and prediction scenarios
- Study influence of measurements and quantity of interest
- Modelling error for Darcy's scale models
- Assimilate data computed on different samples

Research overview I

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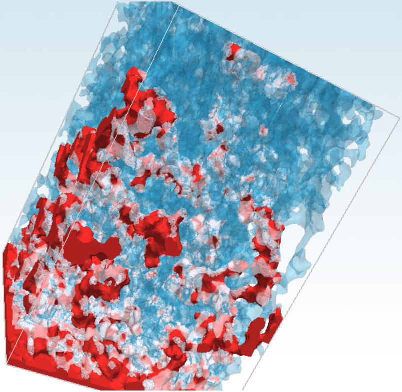
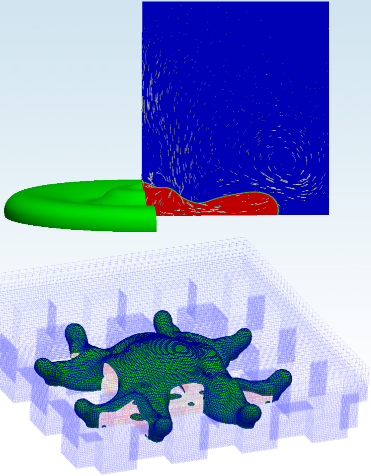
Multiphase flows simulation

Interphase tracking in unsaturated porous media



Drop impacts on random micro-surfaces



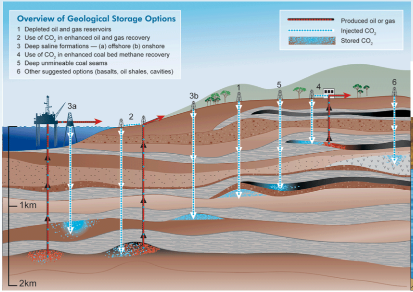
Adaptive Mesh Refinement, Numerical validation, Sensitivity to discretization parameters and convergence properties

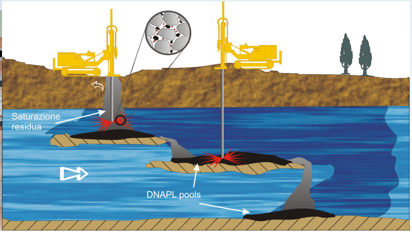
Research overview II

Groundwater flows

Carbon storage and groundwater remediation

Pictures courtesy of IPCC (left) and Groundwater Engineering group at Politecnico di Torino (right)





Multi-scale models, stochastic PDEs, data assimilation, HPC implementation, Numerical and analytical upscaling (homogenization, volume averaging)

Research overview III

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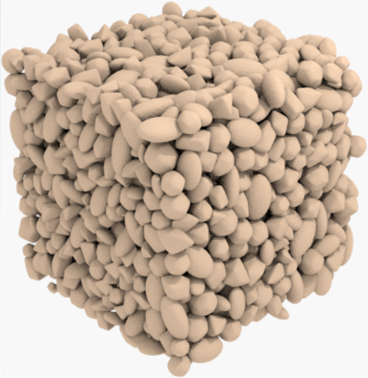
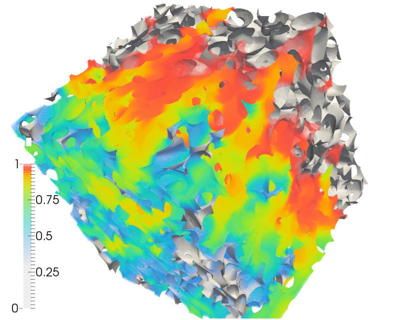
Random heterogeneous materials





Granular random packings, PDE discretisation in large complex geometry,
Anomalous transport and mixing properties

Research overview IV

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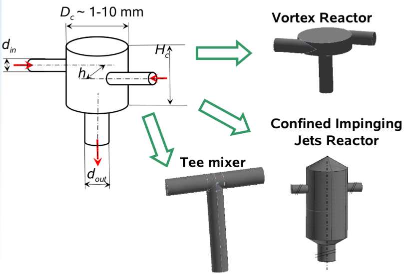
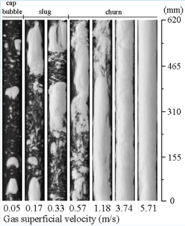
Turbulent multiphase systems

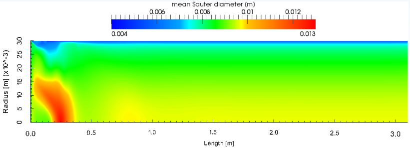
Micro-reactors modelling



Population balance for gas-liquid flows

Icardi, Ronco, Marchisio, Labois, 2014





Turbulence and LES, Nano-scale non-equilibrium fluids, Coagulation and transport of inertial particles, Micro-mixing models, Kinetic (Boltzmann, PDF) models

Mesoscale and kinetic models

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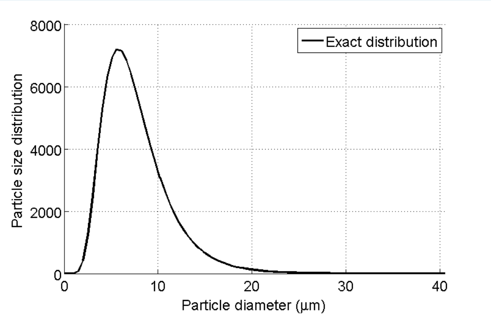
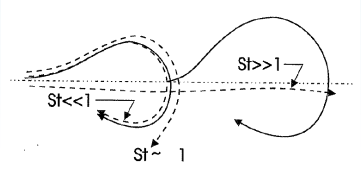
Retain micro-scale and fluctuating properties through statistical description
(Generalised Population Balance Model / Fokker-Planck)

e.g., Particle Size Distribution $$f(L;x,t) = \int_{\mathcal{R}^3} f(L,U_p;x,t)\,dU_p$$



$$\mathrm{St} = \frac{\tau_p}{\tau_f}$$



Particles of different size behave very differently according to their Stokes number.

Example: particle-laden flow

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Quadrature-based moment methods