plotReport

June 19, 2021

1 Velocity and transport report

1.1 Purpose

The present set of geostatistical, flow and trasnport simulations aims to determinate the conditions which trigger non-Fickian transport behaviour for Darcy flow in heterogeneous porous media. Moreover, some additional calibration tests will be carried out in the attempt of relating geostatistical metrics and transport parameters for the most popular upscaled models (e.g. MRMT or CTRW).

1.2 Content

In this report the preliminary results of a small simulation campaign conducted over 28 realizations charcterised by increasing correlation lengths are shown. Boundary conditions are no flow along the lateral boundaries, 1 Pa constant pressure on the inlet boundary and zero pressure gradient on the outlet boundary. The domain dimensions are 2x1x1 meters and the mesh resolution is 0.05 meters which makes the number of total cells summing up to $2 \cdot 10^6$. The domain is populated with a pluri-Gaussian random field which aims to reproduce the high contrast pattern between four permeability facies. Facies permeabilty takes four values equally spaced between $1 \cdot 10^7$ and $1 \cdot 10^{10} m^2/s$.

1.3 Equations

1.3.1 Spectral generation

$$Z(x) = \int_{-\infty}^{+\infty} e^{-2\pi i \mathbf{k} x} \sqrt{S(\mathbf{k})} dW(\mathbf{k}). \tag{1}$$

where $\mathbf{k}$ are frequencies, $dW(\mathbf{k})$ is a complex-valued white noise random measure and $S(\mathbf{k})$ is the amplitude of the spectral measure. This can be rewritten as:

$$Z(x) = \int_{-\infty}^{+\infty} \cos(2\pi \mathbf{k} x) \sqrt{S(\mathbf{k})} dW(\mathbf{k}) + i \int_{-\infty}^{+\infty} \sin(2\pi \mathbf{k} x) \sqrt{S(\mathbf{k})} dW(\mathbf{k}). \tag{2}$$

Periodicity problem:

$$f(x_0) = \sum_{i=1}^{n_{freq}} cos\left(\frac{2\pi i x_0}{L}\right) = \sum_{i=1}^{n_{freq}} cos\left(2\pi i \left(\frac{x_0}{L} + 1\right)\right) = \sum_{i=1}^{n_{freq}} cos\left(2\pi i \frac{x_0 + x_1 - x_0}{L}\right) = f(x_1)$$

- L shold be much longer than the domain length to avoid periodicity;
- item wavelength i/L needs to satisfy $4 \cdot L_{corr} < i/L < L_{corr}/4$.

1.3.2 Darcy

$$\boldsymbol{V} = -\frac{\boldsymbol{k}}{\mu}(\nabla p + \rho g \nabla z) \tag{3}$$

1.3.3 Advection-dispersion-reaction

$$\frac{\partial(\phi c)}{\partial t} + \nabla \cdot (\boldsymbol{V} c) - \phi D \nabla^2 c = c_s R_s. \tag{4}$$

1.3.4 Péclet number

$$Pe = \frac{advective transport rate}{diffusive transport rate} = \frac{L \cdot u}{D} \tag{5}$$

where u is the flow velocity, D is the hydraulic dispersion coefficient and L is a characteristic length. At different length scales correspond different Péclet numbers: - micro-Péclet for L in the range of pore scale; - meso-Péclet for L in the range of the correlation length; - macro-Péclet for L in the range of the domain size.

1.4 Breaktrough curve fitting

The analytical solution of the advection-dispersion eqution is a cumulative Inverse Gaussian distribution. In this section we assume that the transport is Fickian hence the breakthrough curve (BTC) is well described by a cumulative Inverse Gaussian distribution. To prove or reject this hypothesis we estimate the parameters μ and λ using the experimental BTC data, as if the population of the recorded concentration in time was sorted from a real Inverse Gaussian distribution. We then visually compare the empirical BTC with the analytical one for which the parameters μ and λ were estimated using the experimental data. If the curves coincide the hypothesis is accepted otherwise it is rejected.

1.4.1 Cumulative Inverse Gaussian distributions

$$F(x;\mu,\lambda) = \Phi\left(\sqrt{\frac{\lambda}{x}}\left(\frac{x}{\mu} - 1\right)\right) + \mathrm{e}^{\frac{2\lambda}{\mu}} \Phi\left(-\sqrt{\frac{\lambda}{x}}\left(\frac{x}{\mu} + 1\right)\right) \tag{6}$$

1.4.2 Parameters estimation

$E[X] = \mu_1$

$Var[X] = \mu_2 - \mu_1^2 = \frac{\mu_1^3}{\lambda}$

$\mu_1 = \int_0^{+\infty} f(t)tdt = \int_0^{+\infty} F'(t)tdt = -\int_0^{+\infty} Fdt + [Ft]_0^{+\infty} = -\sum_{i=0}^{+\infty} F_i(t)\Delta t + F(t_{+\infty})t_{+\infty}$

$$\mu_2 = \int_0^{+\infty} f(t)t^2dt = \int_0^{+\infty} F'(t)t^2dt = -2\int_0^{+\infty} Ftdt + \left[Ft^2\right]_0^{+\infty} = -2\sum_{i=0}^{+\infty} F_i(t)t_i\Delta t + F(t_{+\infty})t_{+\infty}^2$$

1.5 Velocity and mechanical dispersion from BTC moments

Following the paper of *Yu et al. 1999*, we computed the velocity and the mechanical dispersion coefficient from the statistical moments μ_1 and μ_2. According to the aforementioned paper, the flow velocity is

$$v = \frac{x}{\mu_1}$$

while the hydraulic dispersion is

$$D_{mec} = \frac{Var[X]v^3}{2x} = \frac{x^2}{2\lambda}.$$

Mechanical dispersion and correlation lengths in the longitudinal direction show a positive trend while in the transversal directions no relevant trend appears. The average velocity from the stastical moments falls within one magnitude order if compared with the average velocity computed thorugh OpenFOAM. The hydrodynamic dispersion is given by the sum of the molecular diffusion with the mechanical dispersion:

$$D = D_{mol} + D_{mec} \tag{7}$$

1.5.1 Mechanical dispersion index (alpha)

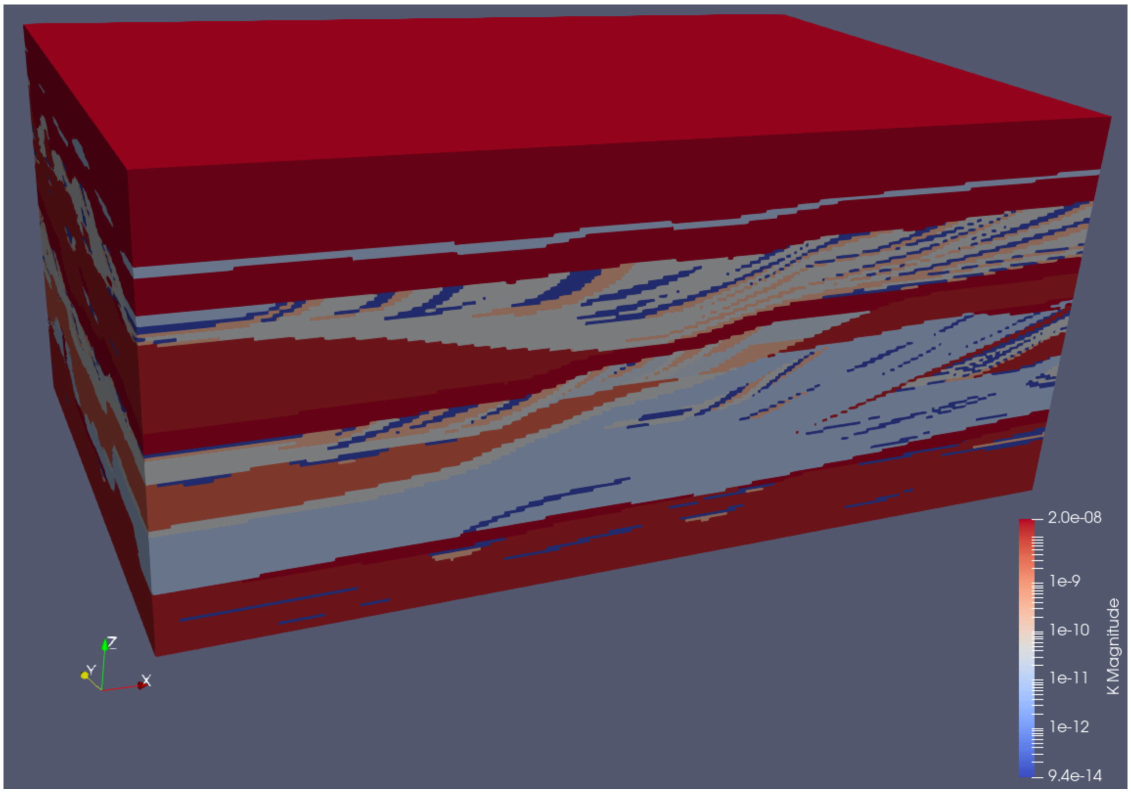
$$\alpha = \frac{D_{mec}}{v} \tag{8}$$

[14]:

```
from IPython.display import Image
Herten = Image(filename="/data/PGSFlowTransport/tutorials/RESULTS/Herten/
 ↪Herten9/images/Herten10facies.png")
print("Herten_10_facies")
display(Herten)

#k1Field = Image(filename="/home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/
 ↪tutorials/RESULTS/stopConcAdapTmstp_3/images/K1field.png")
#k2Field = Image(filename="/home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/
 ↪tutorials/RESULTS/stopConcAdapTmstp_3/images/K2field.png")
#print("TS1")
#display(k1Field)
#print("TS2")
#display(k2Field)

#ts1 = Image(filename="/home/pmxep5/OneDrive/Nottingham/Write/VIVA/
 ↪VIVA_2nd_year/images/veLcorr/ts1K.png", width=500, height=500)
#ts10 = Image(filename="/home/pmxep5/OneDrive/Nottingham/Write/VIVA/
 ↪VIVA_2nd_year/images/veLcorr/ts10K.png", width=500, height=500)
#ts20 = Image(filename="/home/pmxep5/OneDrive/Nottingham/Write/VIVA/
 ↪VIVA_2nd_year/images/veLcorr/ts20K.png", width=500, height=500)
```

```
#ts30 = Image(filename="/home/pmxep5/OneDrive/Nottingham/Write/VIVA/
↪VIVA_2nd_year/images/veLcorr/ts30K.png", width=500, height=500)
#display(ts1)
#display(ts10)
#display(ts20)
#display(ts30)
```

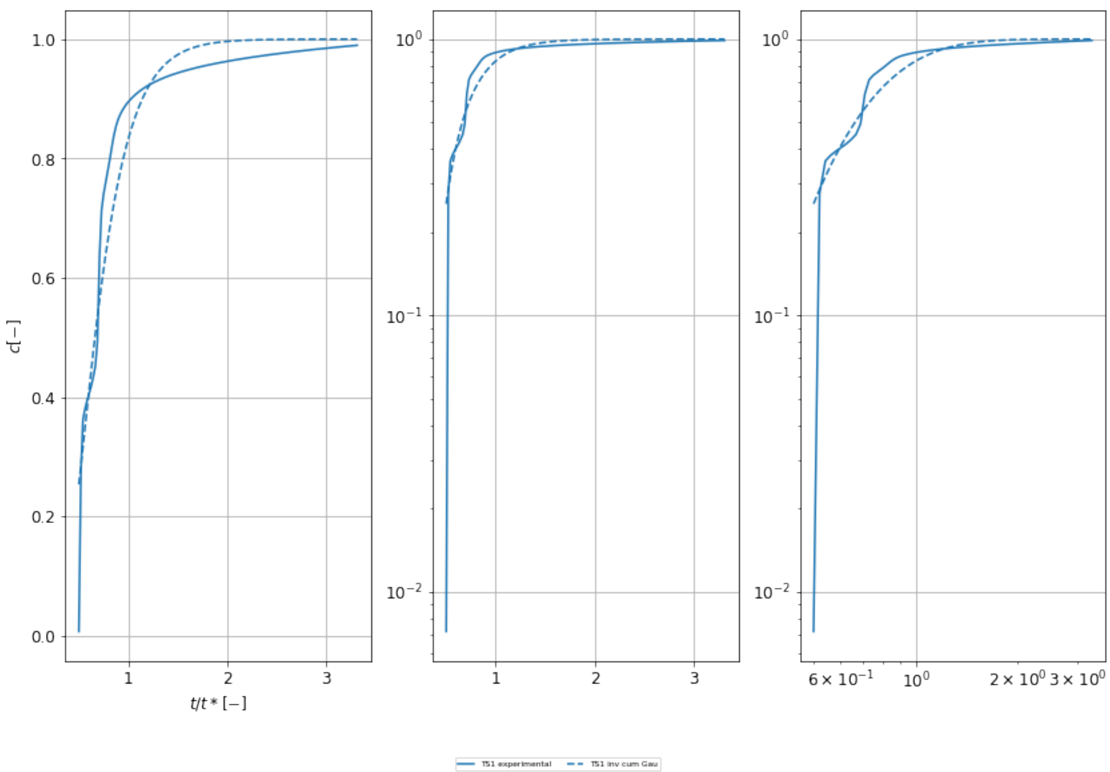
Herten_10_facies

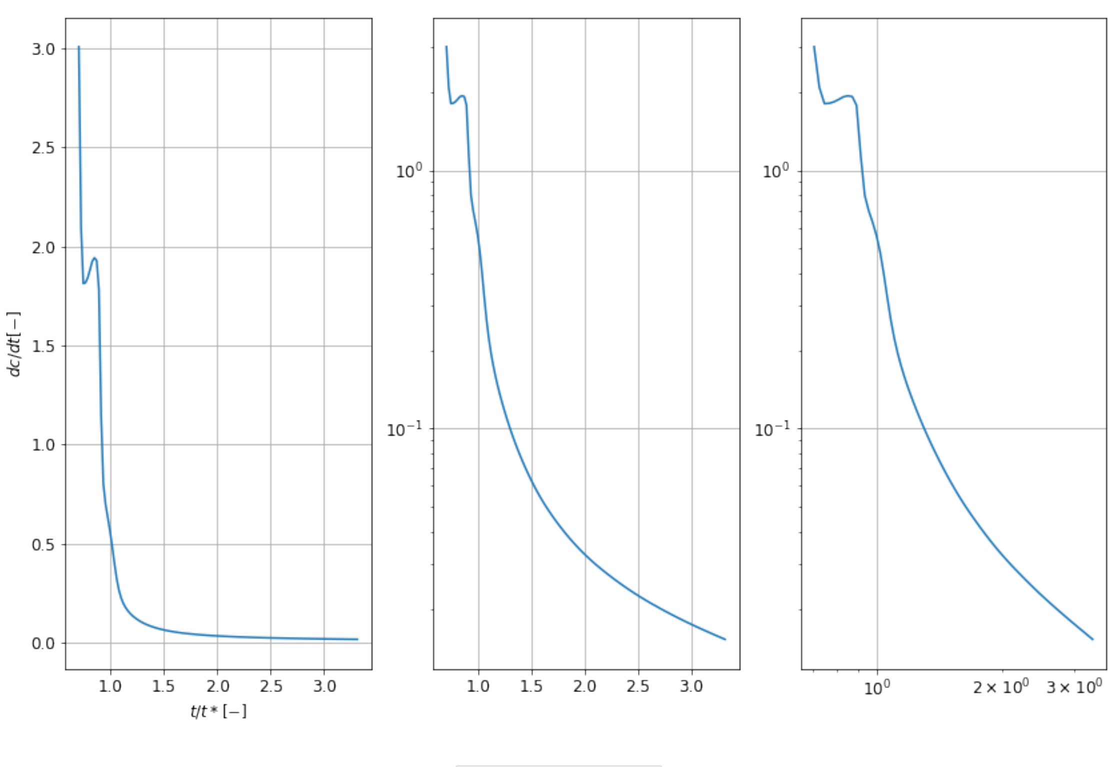


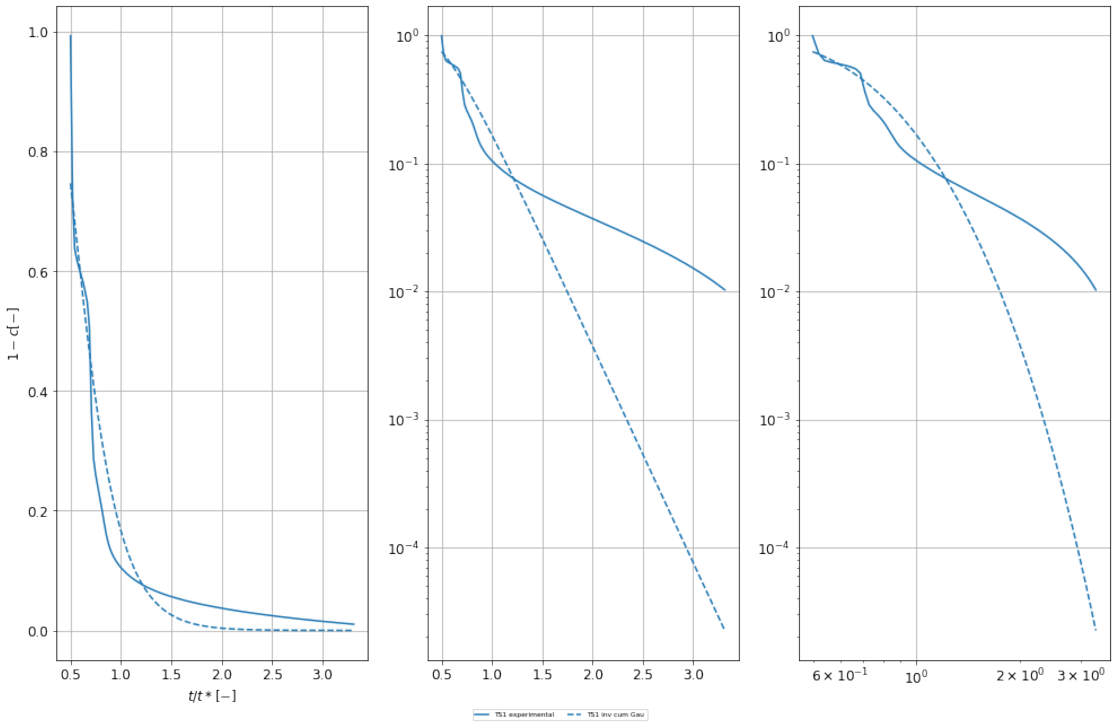
[3]:
```
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/
↪plotKVsLcorr.py
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/simAnalyser.
↪py
%run -i /data/PGSFlowTransport/etc/Python/simAnalyserHoriz.py
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/
↪corrFunction.py
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/
↪plotVvsLcorr.py
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/plotMDvsCL.
↪py
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/plotMDvsV.py
```

```
#%run -i /home/pmxep5/OpenFOAM/pmxep5-8/PGSFlowTransport/etc/Python/
↪plotALPHAvsCLvsPECLET.py
#%run -i /data/PGSFlowTransport/etc/Python/corrFunction.py

# Paths
# luin67272: /home/pmxep5/OpenFOAM/pmxep5-7/PGSFlowTransport/etc/Python
# gercphd: /data/PGSFlowTransport/etc/Python/
```

```
FLOW METRICS
Mean Vx Vy Vz = 0.000000342 0.000000000 0.000000001
Estimated mean Vx = 0.000000417

Péclet:
  Macro = (5466.48 1.88 9.90)
  Meso = (0.00 0.00 0.00)

TRANSPORT METRICS
mu_1 = 38381873.047204
mu_2 = 19577866050315212.000000
Inv Gau lambda = 3123109.505021
alpha_estimatedMeanVx = 98.317073
alpha_meanVx = 119.959591

Dispersion:
  Molecular = 0.000000001
  Estimated mechanical = 0.000041
  Estimated hydrodynamic = 0.000041

Computed ||c|| = 10.688194
Estimated ||c|| = 10.790565
```


$c[-]$
$t/t*[-]$
TS1 experimental
TS1 inv cum Gau


$dc/dt[-]$
$t/t*[-]$
TS1 experimental
TS1 inv cum Gau


1 − c[−]
t/t * [−]
TS1 experimental
TS1 inv cum Gau

```
[ ]:
```