Application of the TRT LB model to simulate pesticide transport in cultivated soils

V. POT, N. ELYEZNASNI

EGC INRA AgroParisTech,Thiverval-Grignon, France

I. GINZBURG

HBAN Cemagref, Antony, France

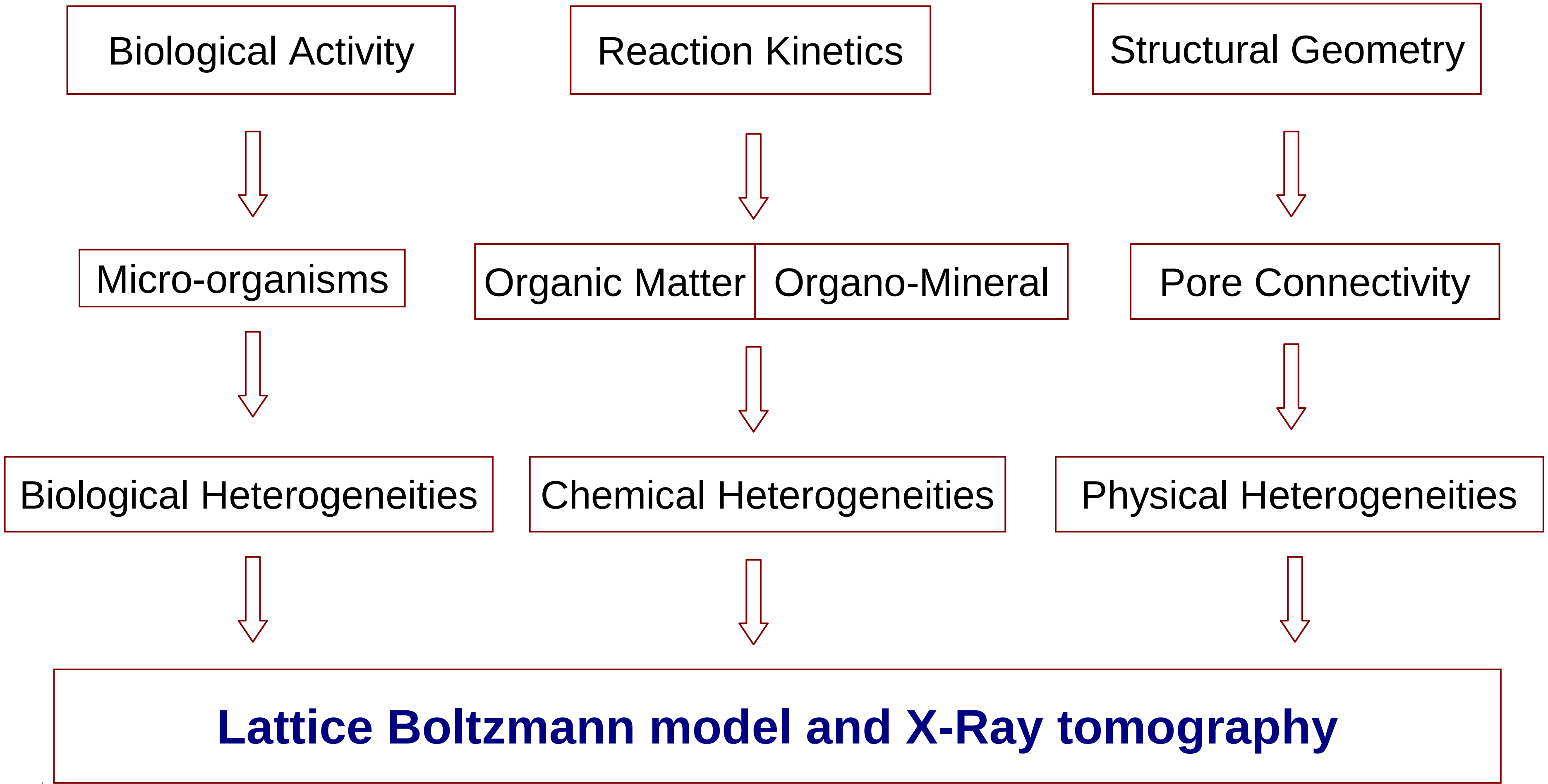
H. HAMMOU

Faculté des Sciences, Université Mohammed Ier, Oujda, Maroc

EGC

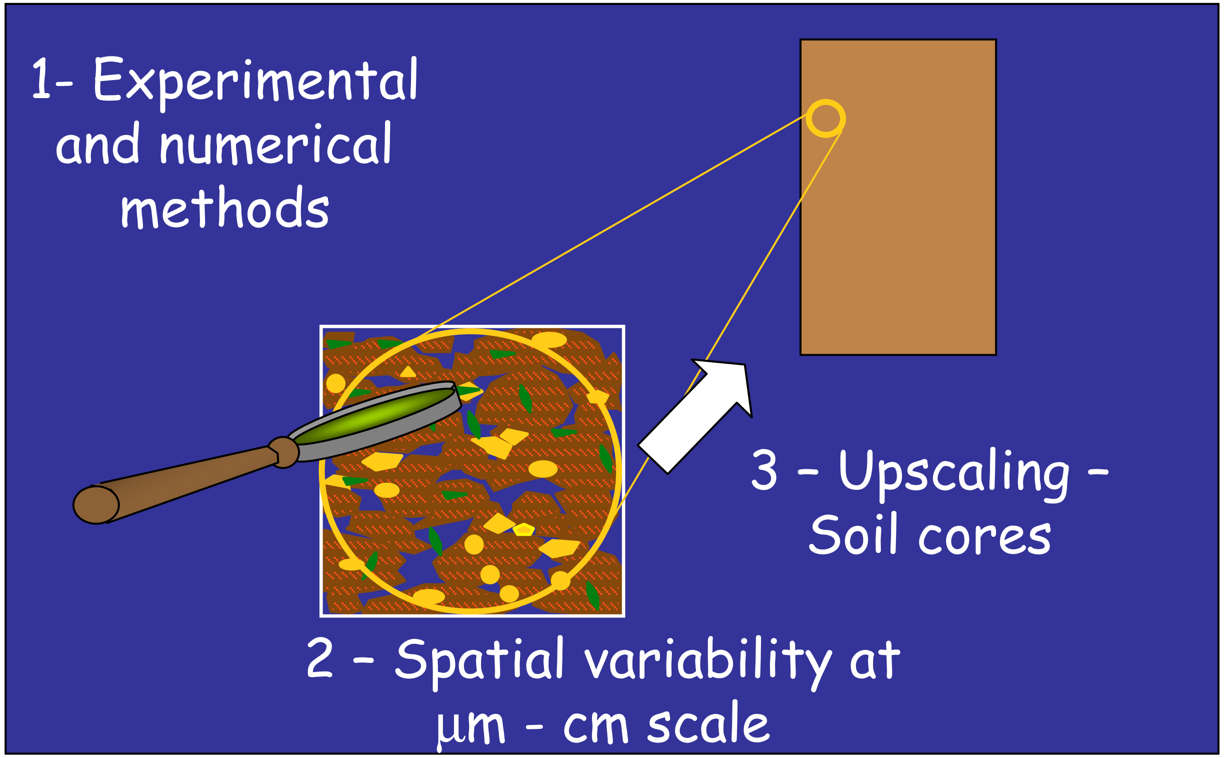
Definition of the problem

Modeling of pesticides (reactive molecules) transport in soil at pore scale



Spatial organization at local scale : infra mm to cm
Objectives & approach

- To explain **macroscopic** sorption and transport parameters as functions of (soil structure, hydrodynamics, spatial distribution and heterogeneity of reactive sites)
- To separate irreversible sorption and biodegradation processes by localizing microbial active sites at the scale of **microbial habitats**



The Studied Soil (1/2)

- The soil is a silty loamy soil:

  19% clay – 75% silt – 6% sand

- Cultivated soil (wheat / maize rotation) with conventional tillage: incorporation of straw residues after harvest, then tillage (28 cm)

- High reactive zones for pesticides in the subsurface layer (0-28cm) can be identified

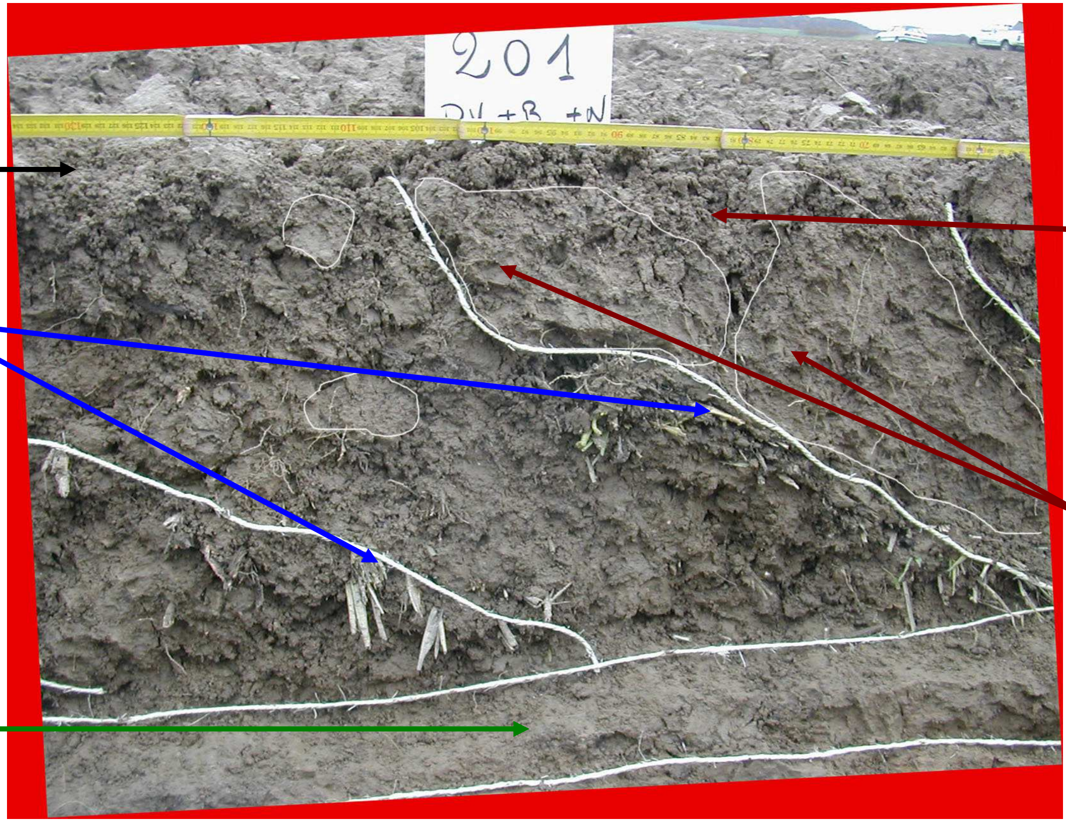
The Studied Soil (2/2)

Vertical soil profile after tillage

Soil surface

Furrows:
. Accumulation of straw residues
. High content of fresh Organic Matter

Plough layer (compacted soil)



Interfurrows: Loose soil zones

Interfurrows: Compacted soil

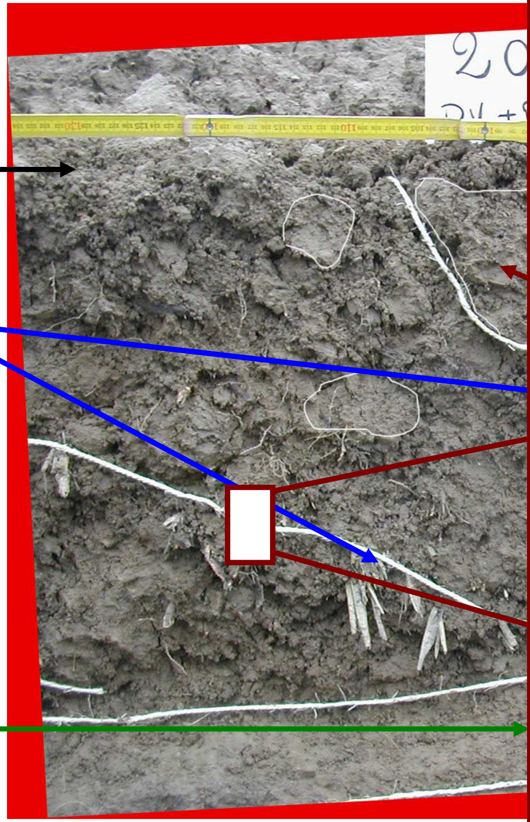
The Studied Soil (2/2)

Vertical soil profile after tillage

Soil surface

Furrows:
. Accumulation of straw residues
. High content of fresh Organic Matter

Plough layer
(compacted soil)



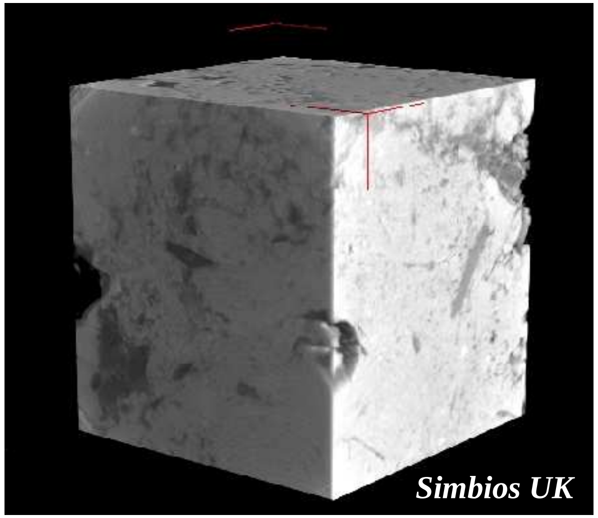
Soil column sampling in the furrows:

5 cm diameter
6 cm height

3D CT images of soil sample (1/4)

3D reconstructed image of soil CT scan

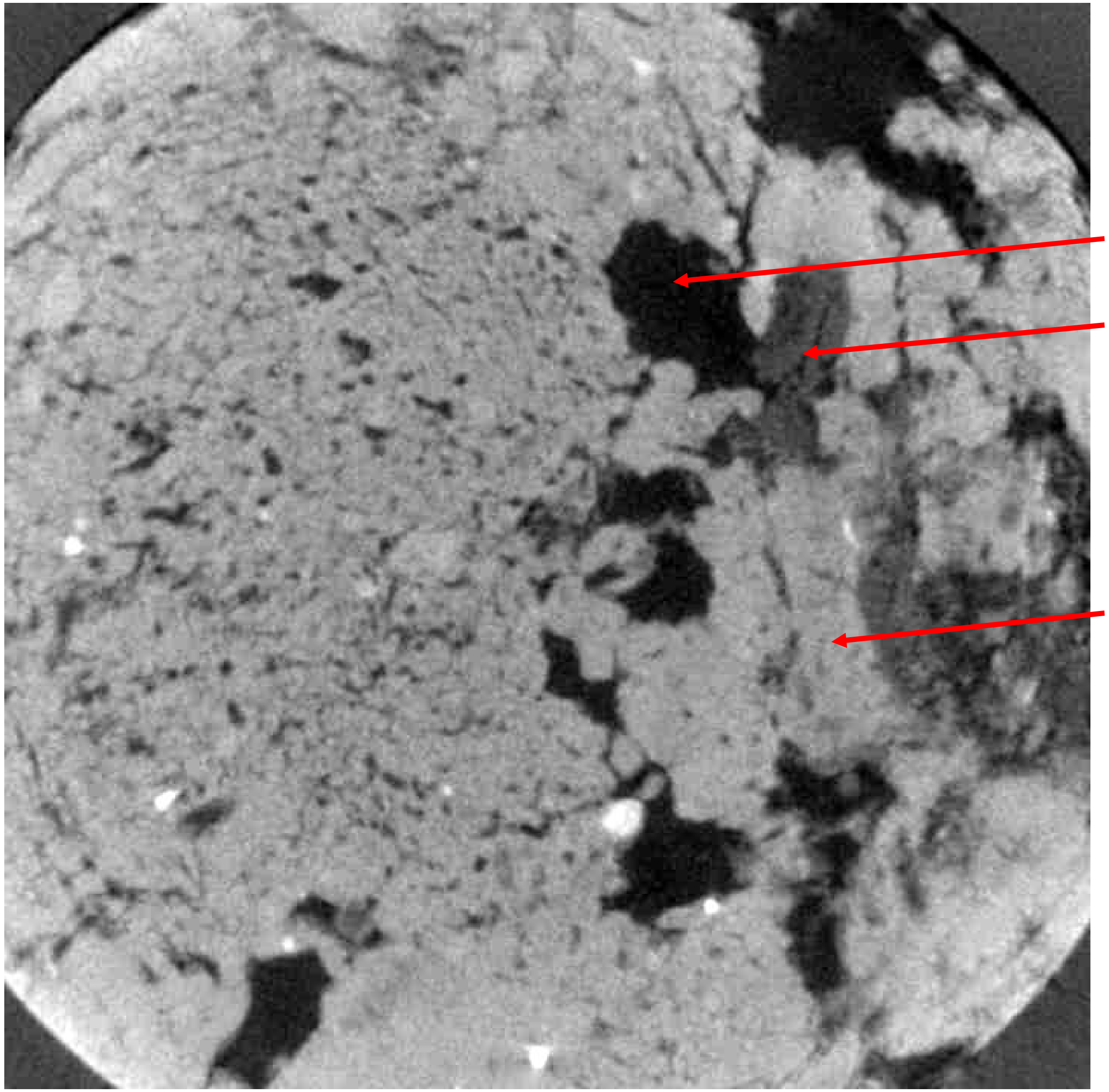
- *712x712x712 voxels*
- *resolution of 68 μm*



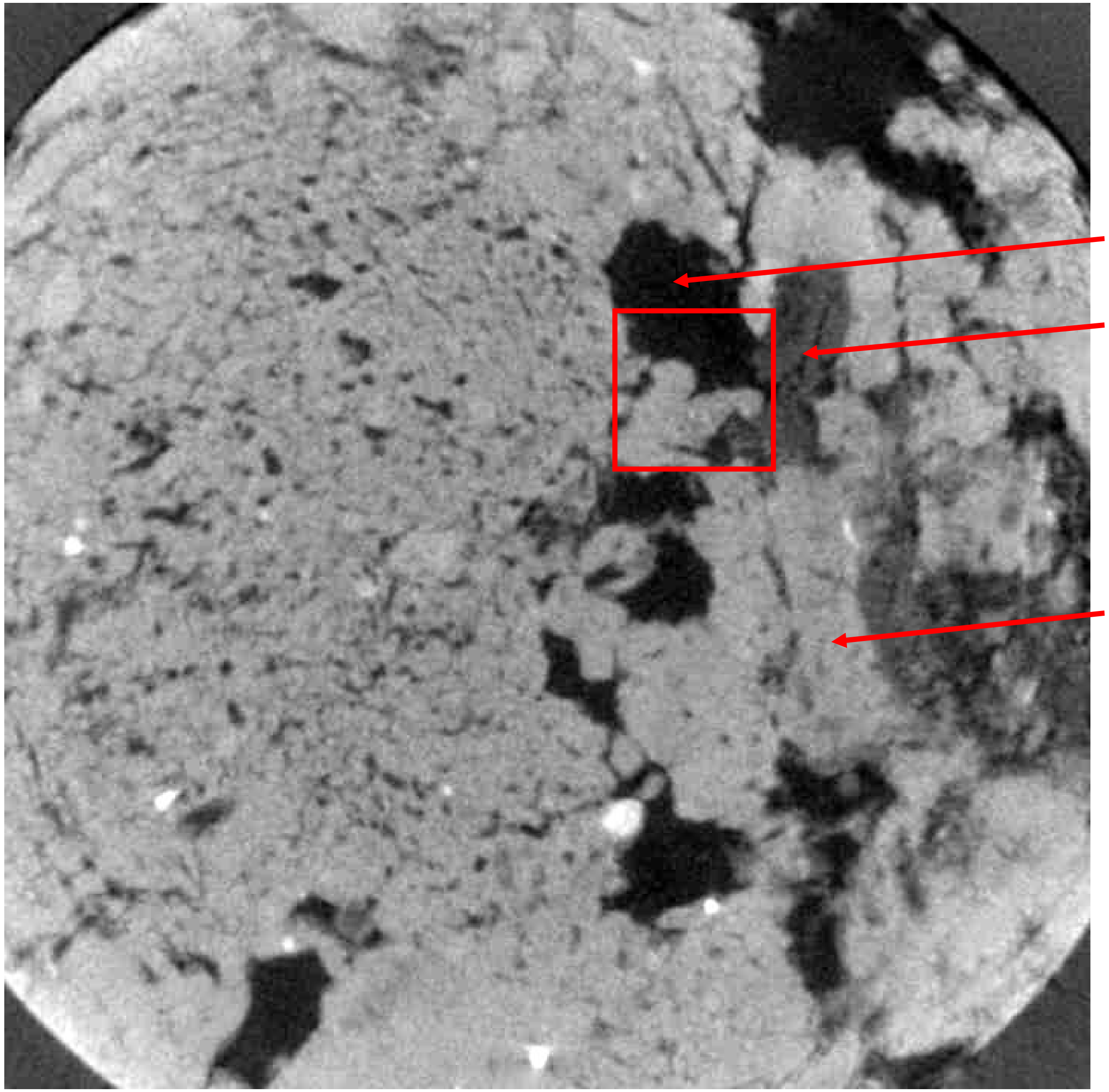
5 cm^3 soil image

EGC

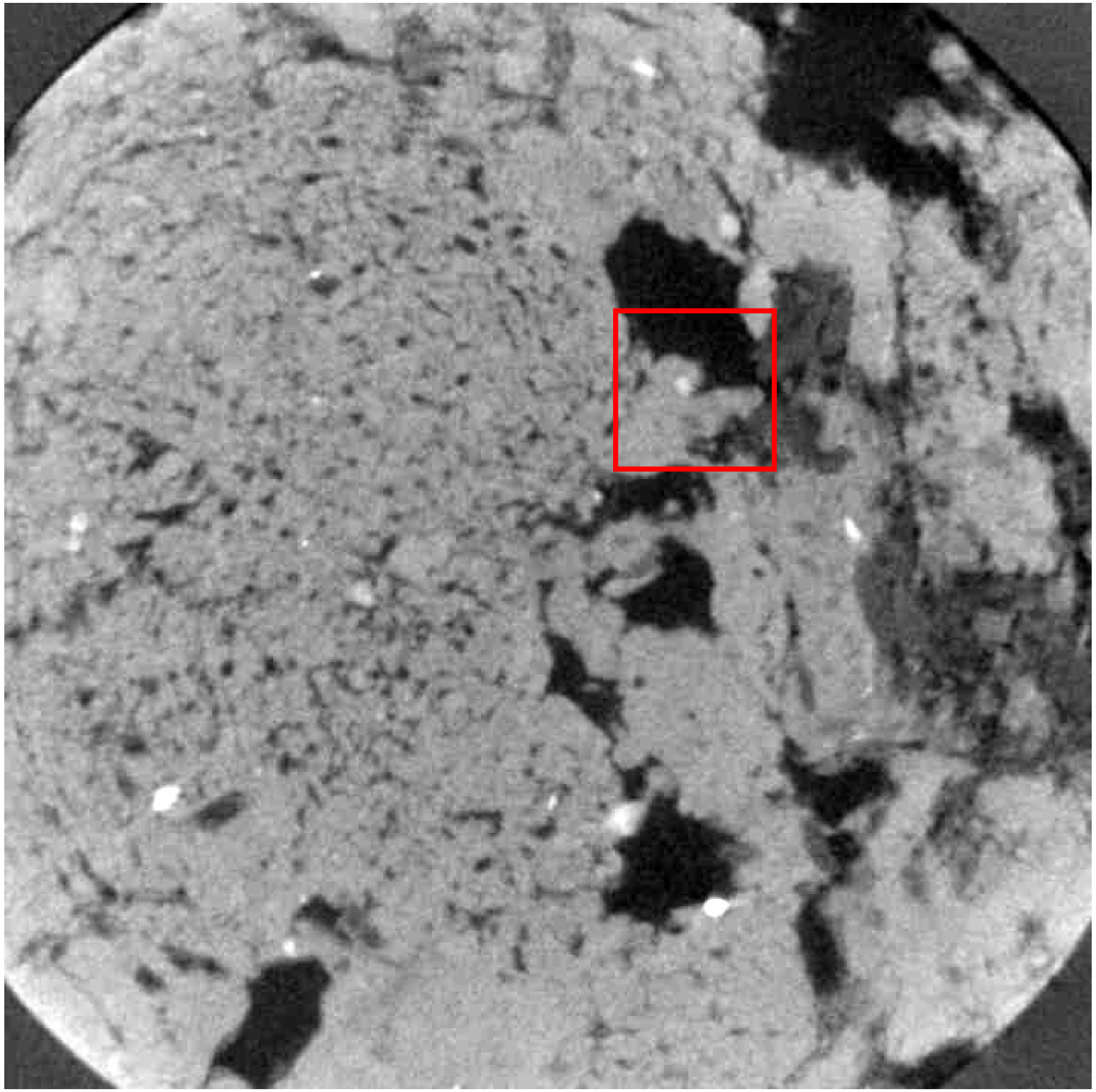
3D CT images of soil sample (2/4)



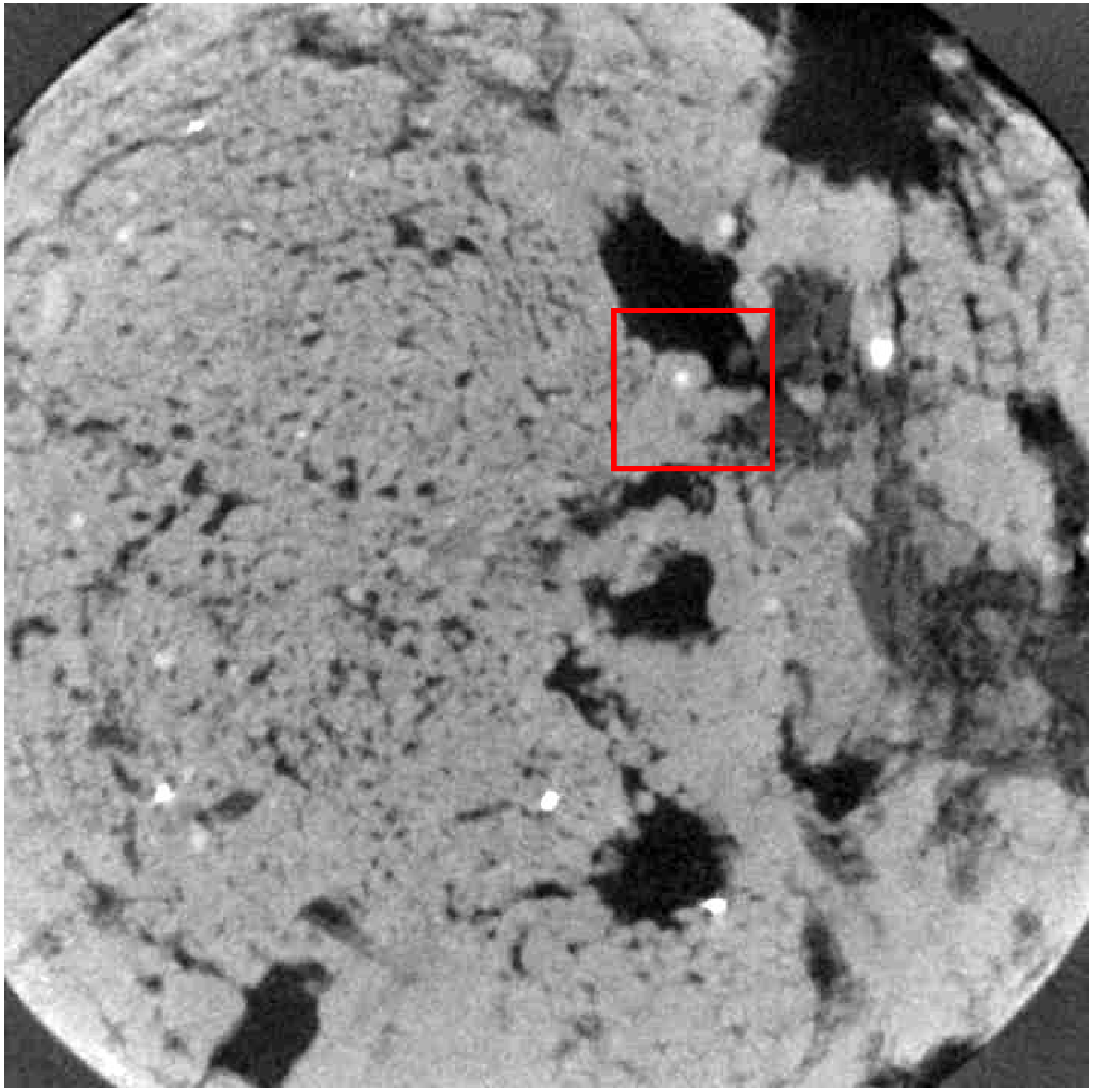
3D CT images of soil sample (2/4)



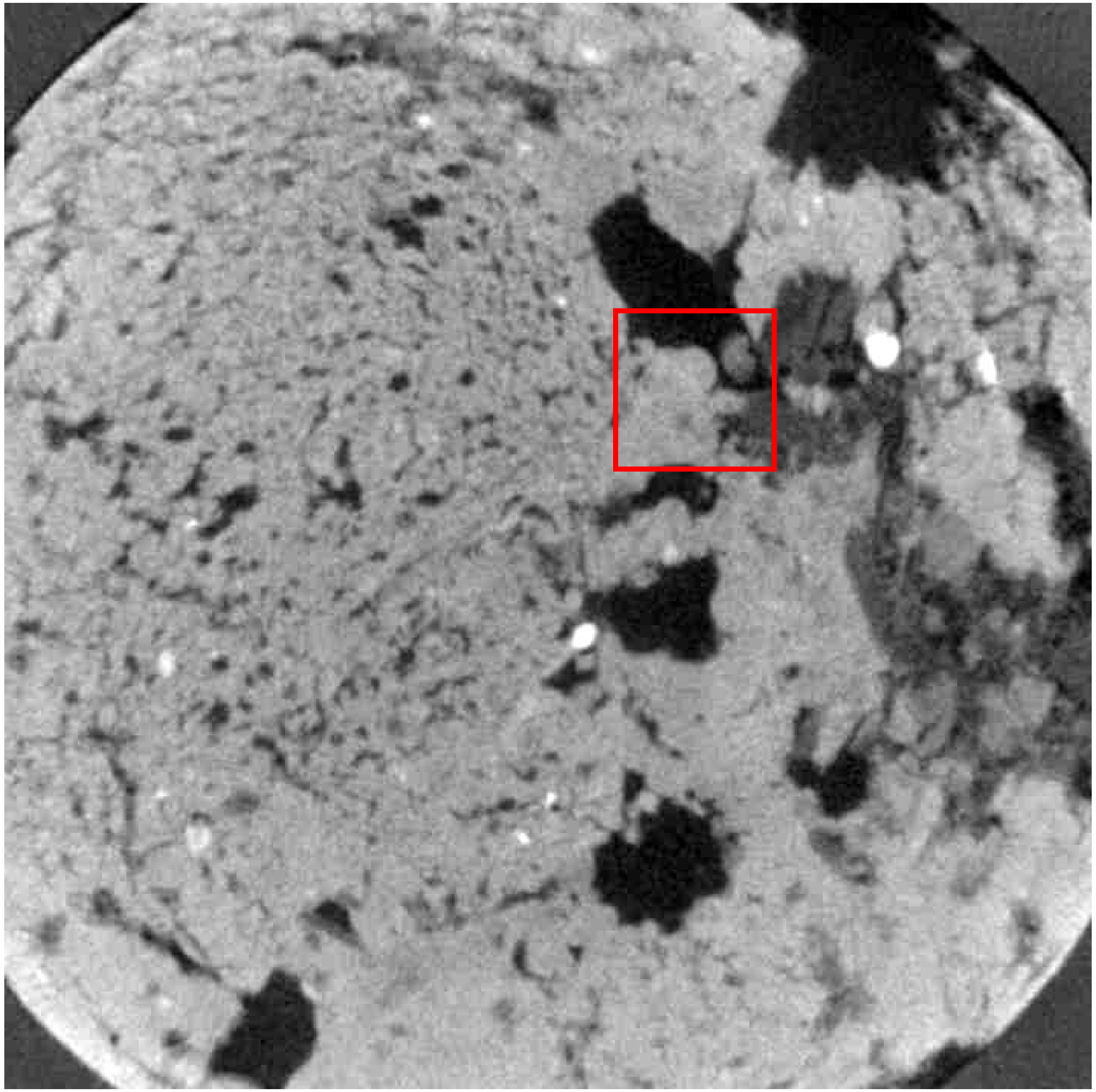
3D CT images of soil sample (2/4)



3D CT images of soil sample (2/4)

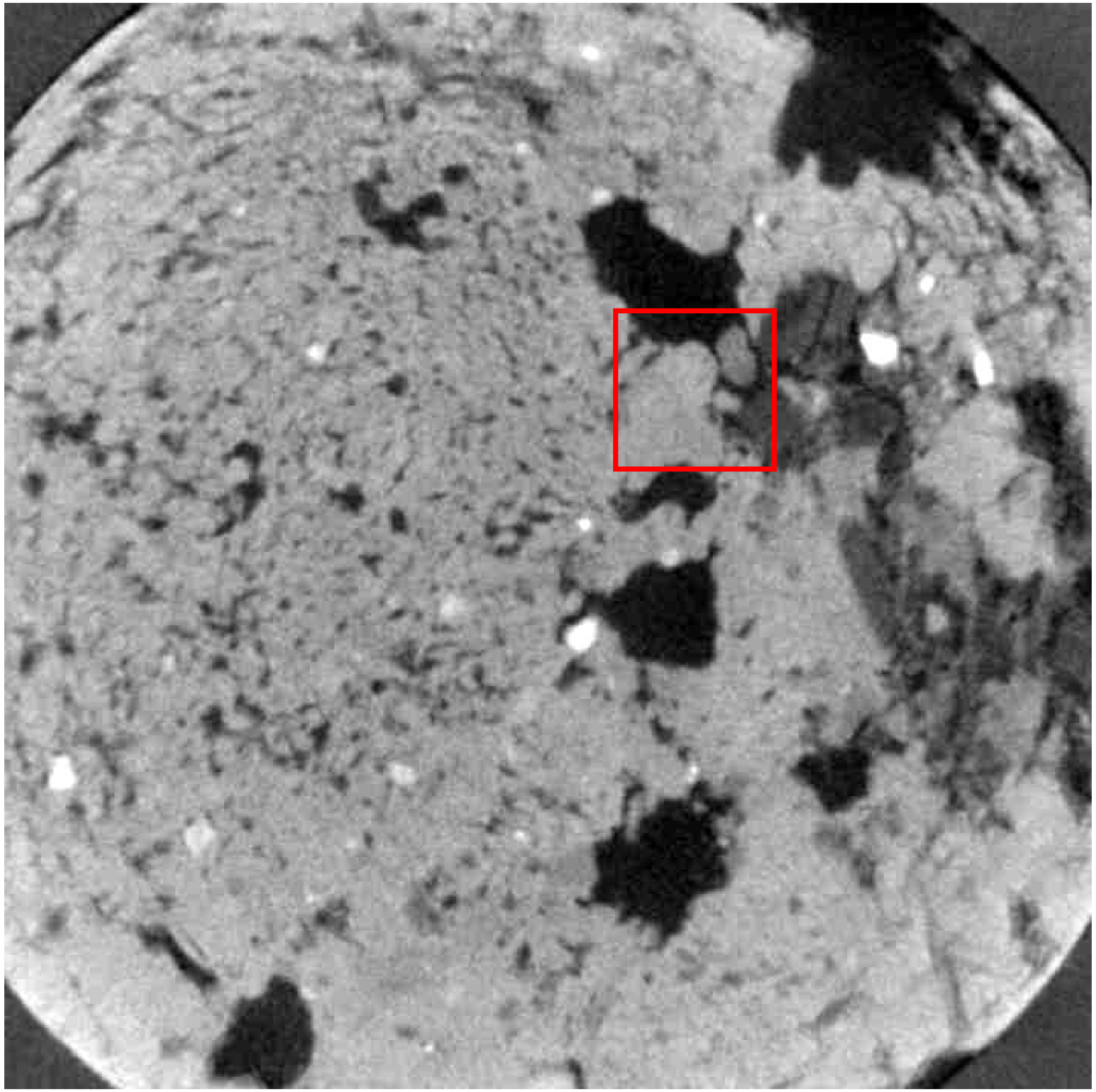


3D CT images of soil sample (2/4)

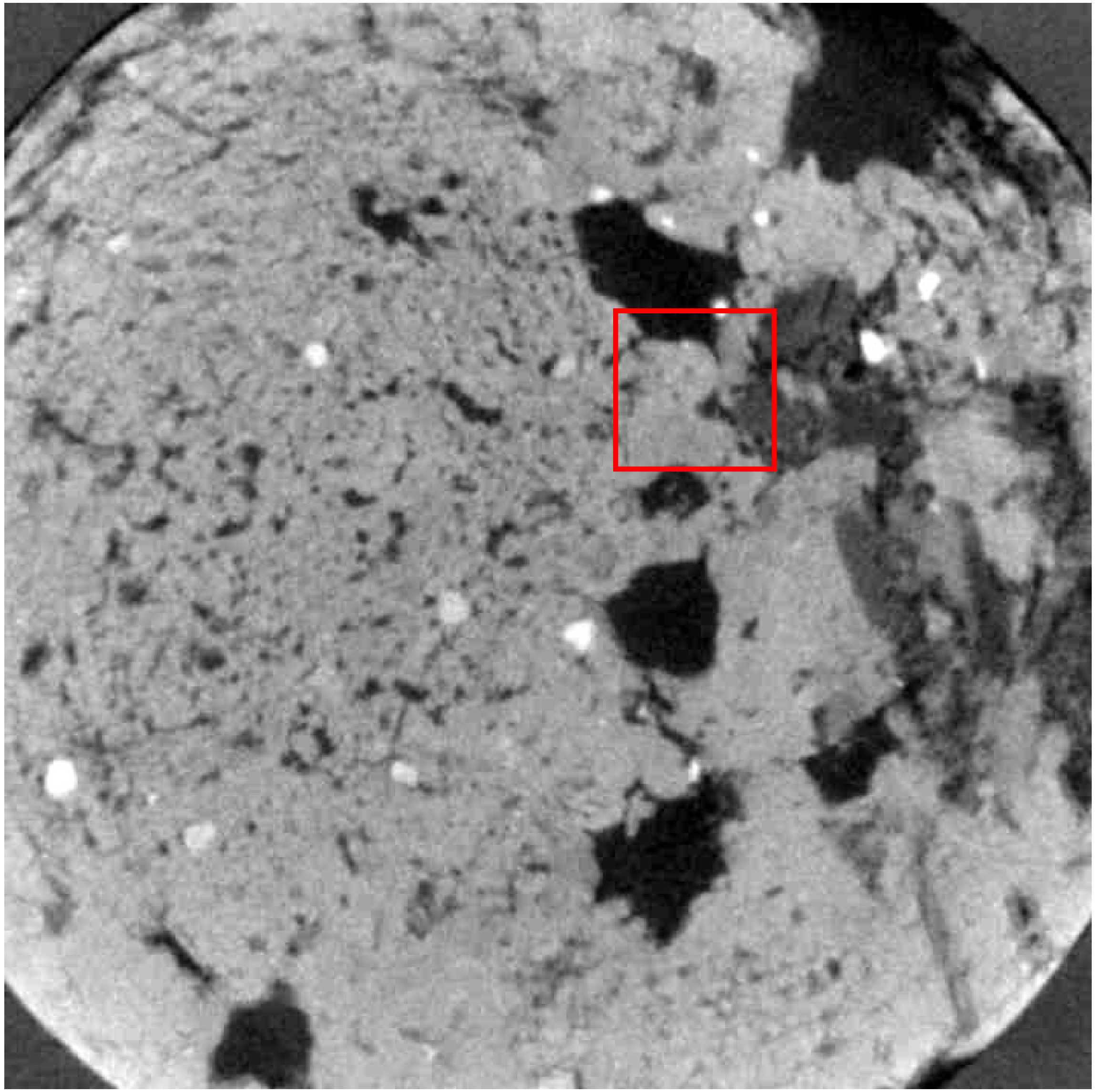


EGC

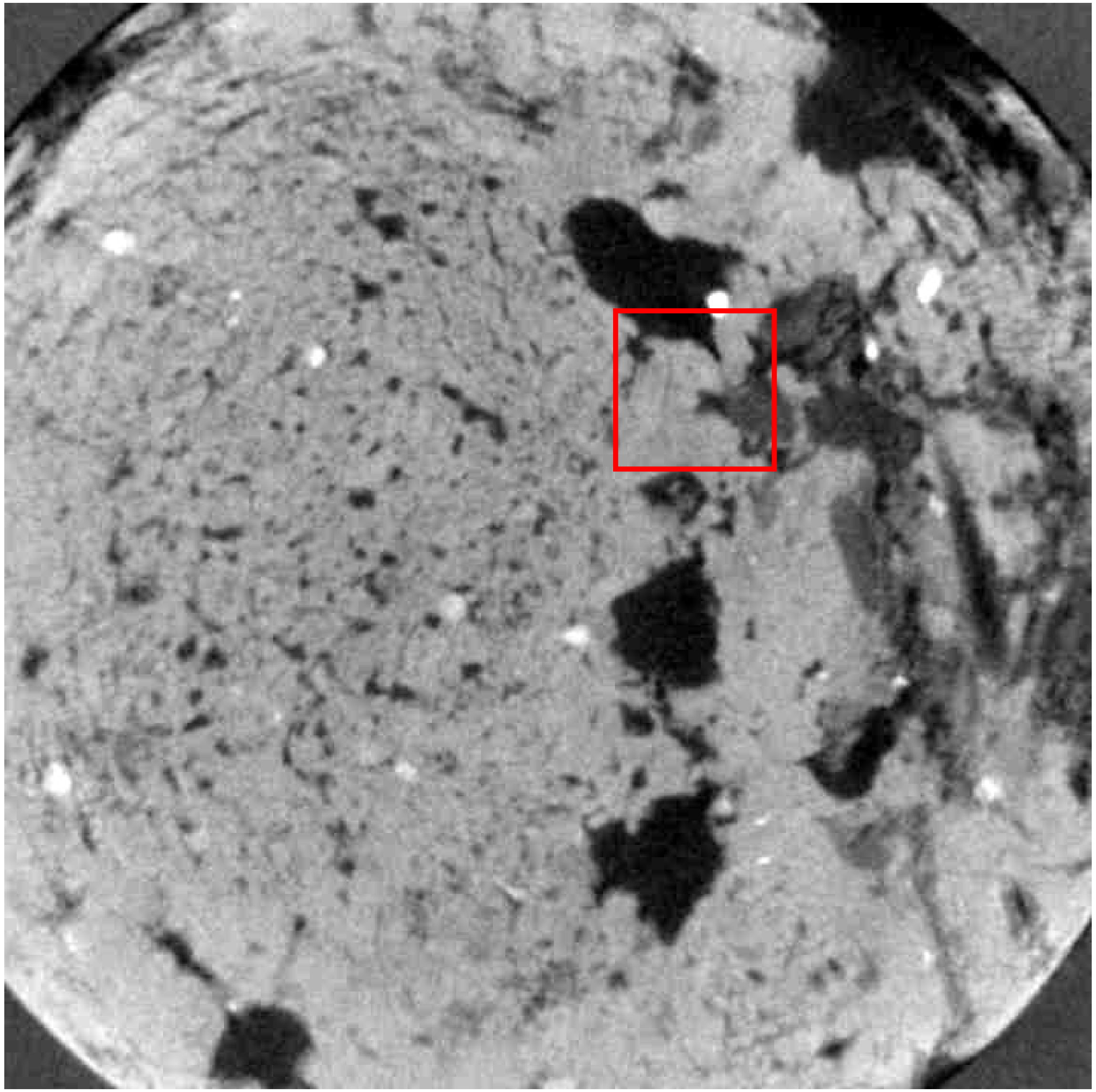
3D CT images of soil sample (2/4)



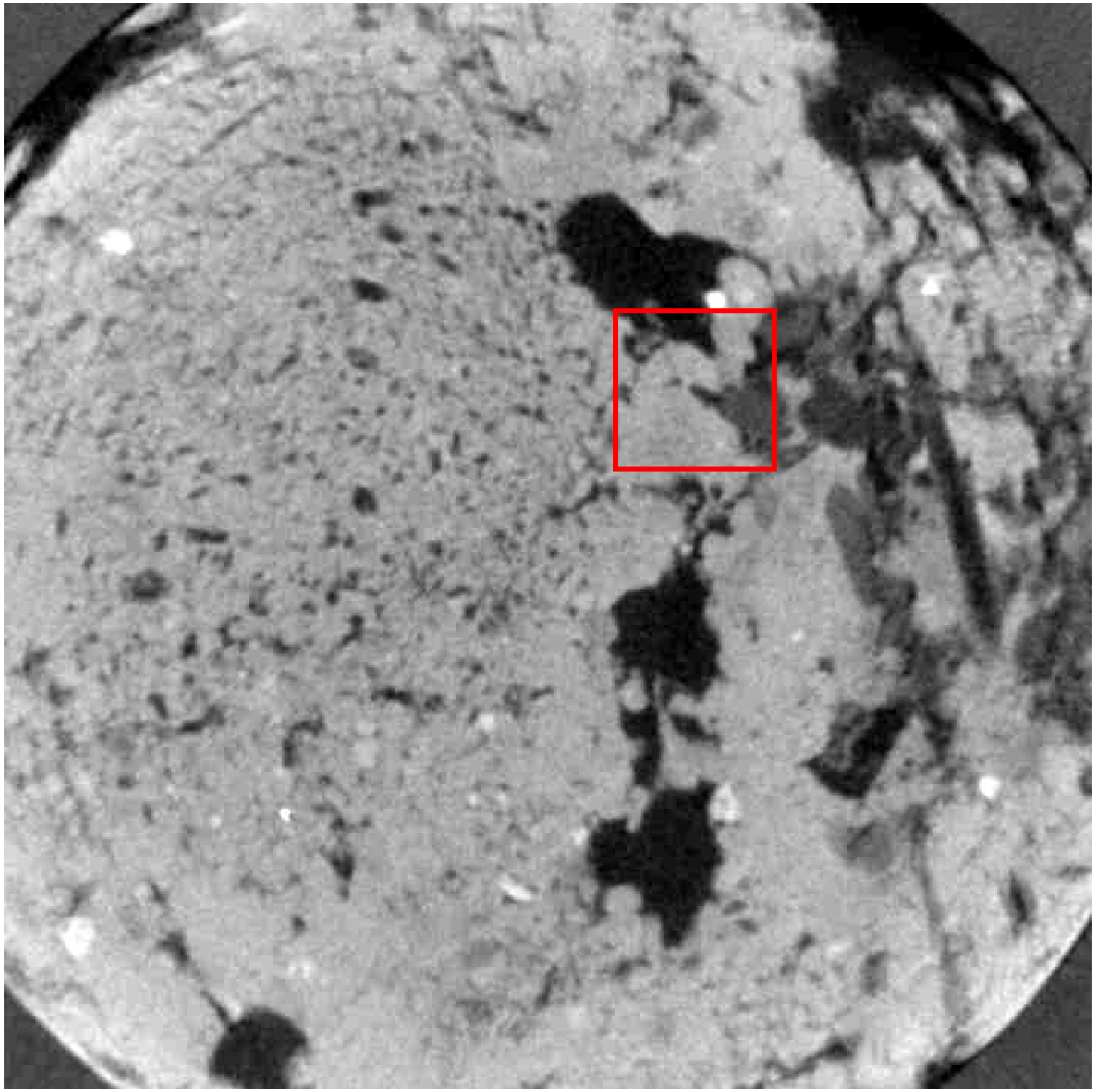
3D CT images of soil sample (2/4)



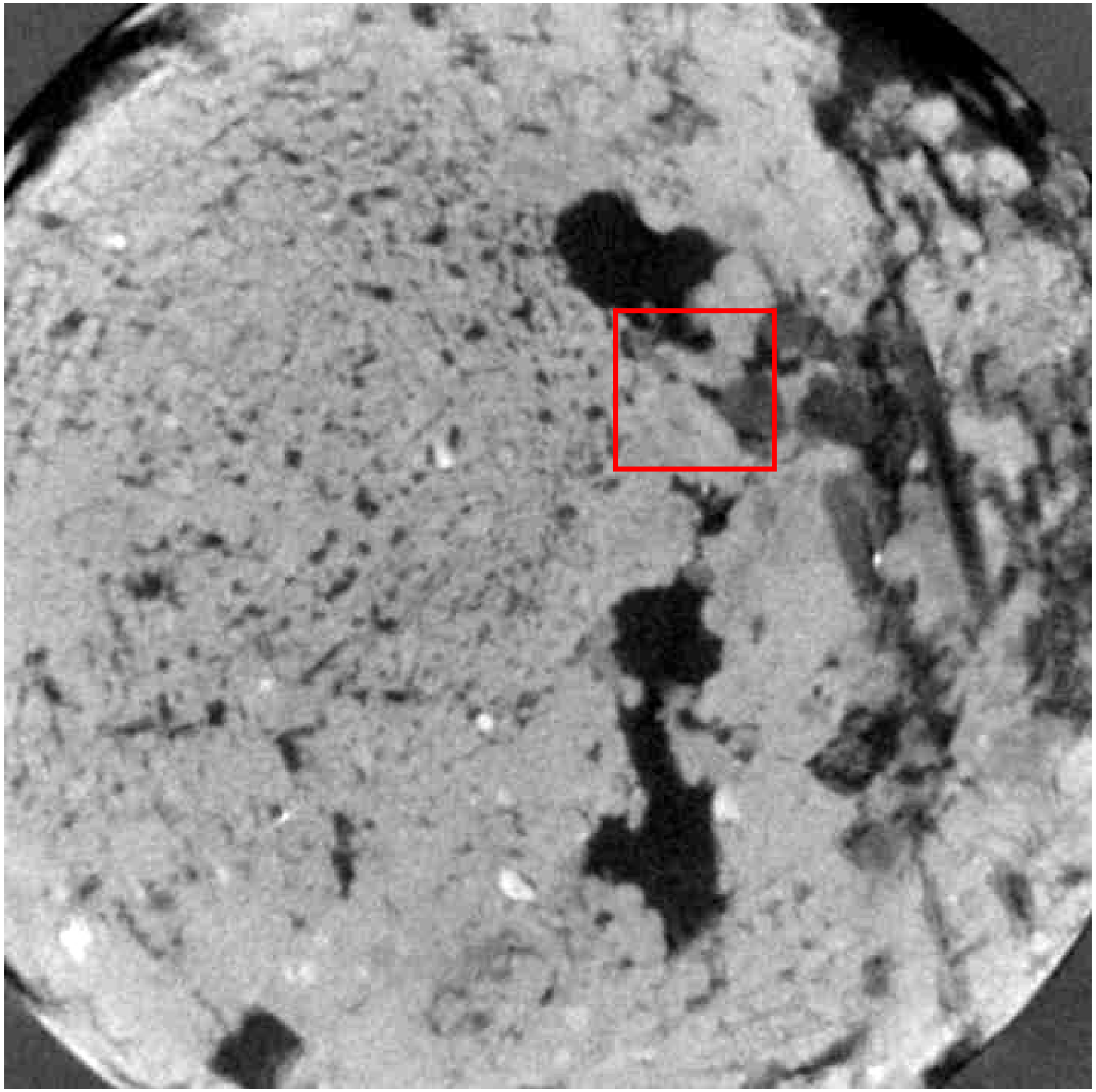
3D CT images of soil sample (2/4)



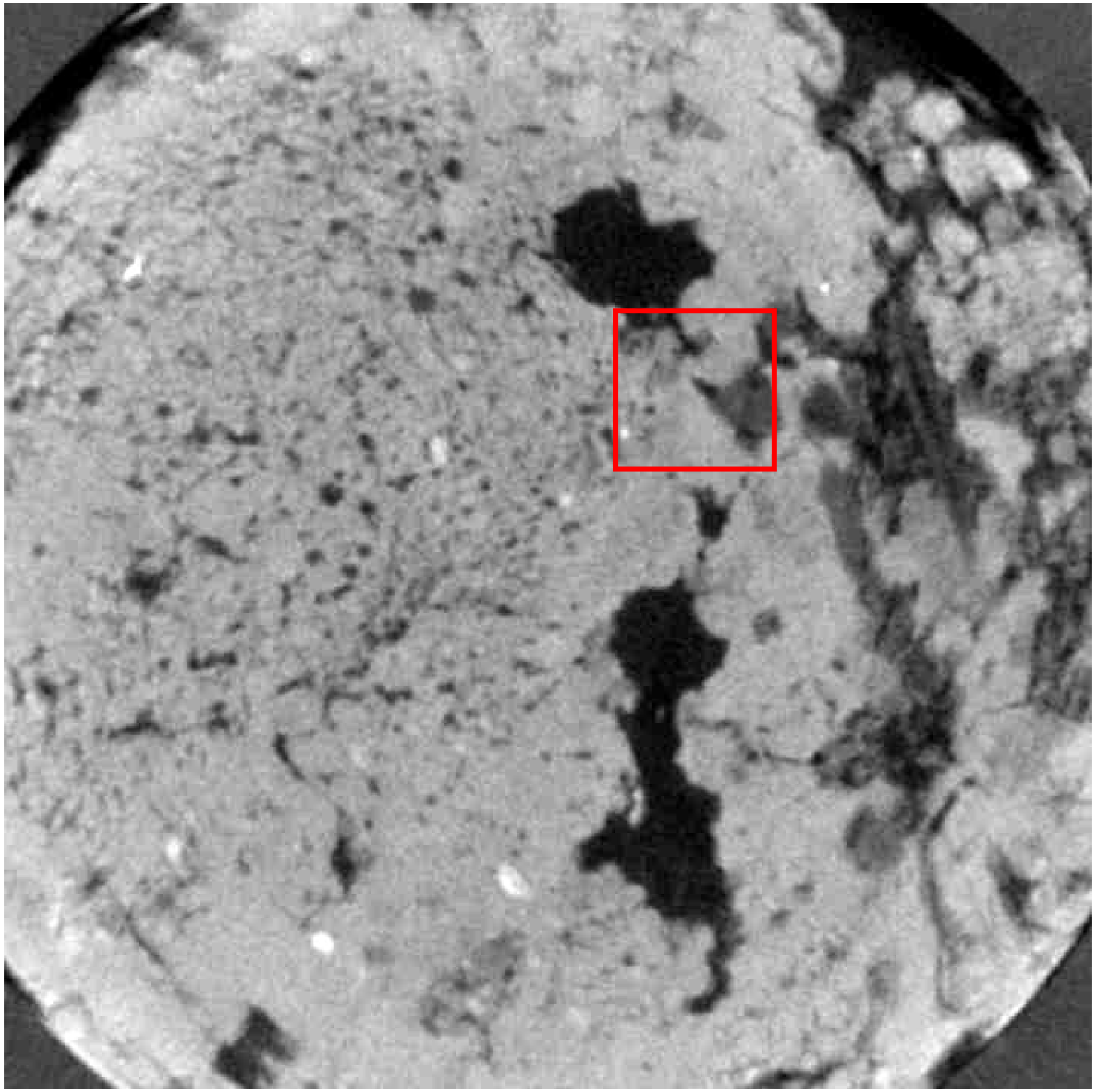
3D CT images of soil sample (2/4)



3D CT images of soil sample (2/4)



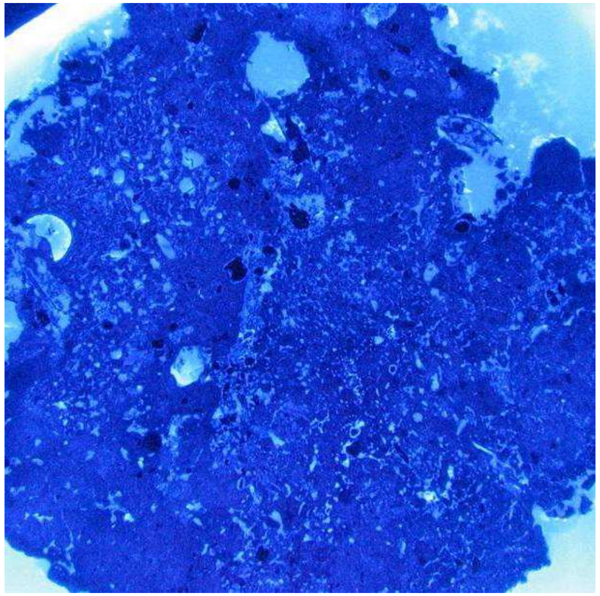
3D CT images of soil sample (2/4)



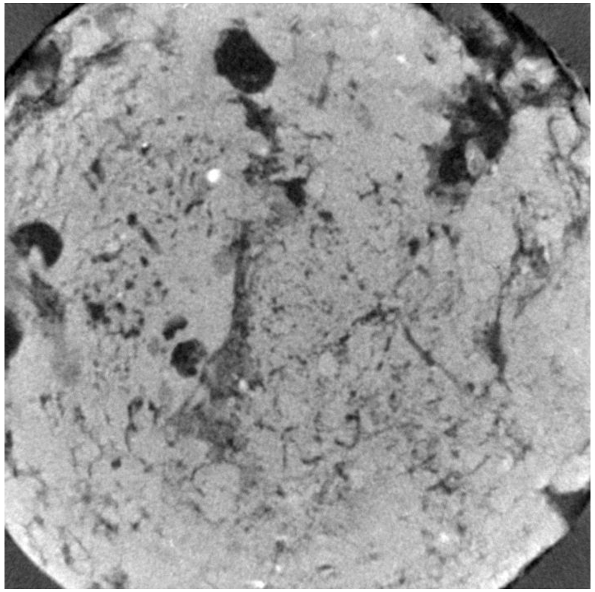
96x96x96 voxels
~ 1e6 LB sites

3D CT images of soil sample (3/4)

Comparison between 2D thin sections and CT section



Thin section

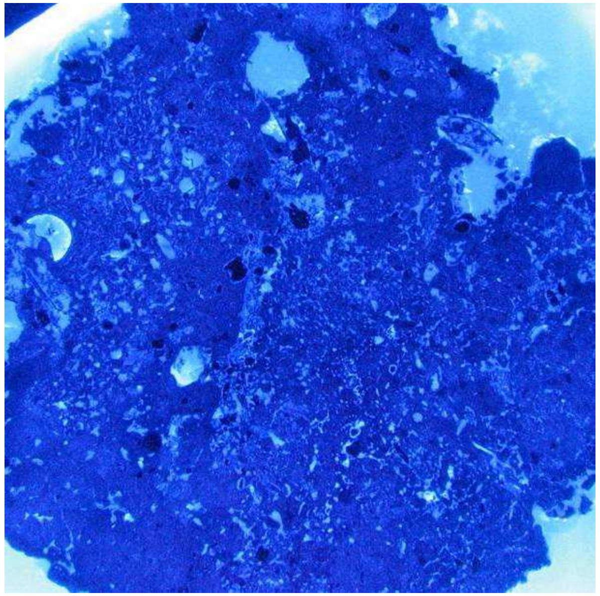


CT section

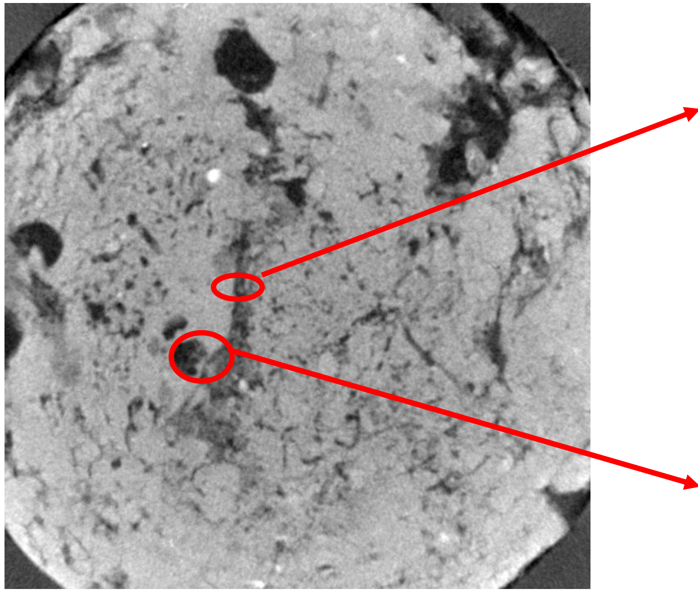
3D CT images of soil sample (3/4)

Comparison between 2D thin sections and CT section

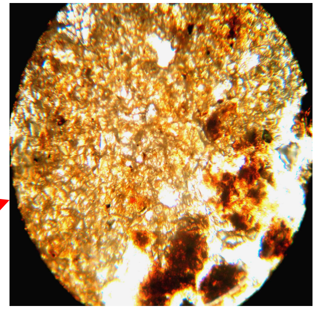
Issue: discretisation

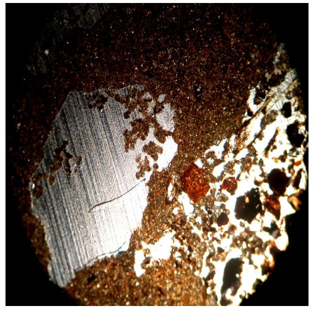


Thin section



CT section





Thin section
Optical microscopy

EGC

3D CT images of soil sample (4/4)

- Explicit description of:
  - physical heterogeneity (soil structure)
  - chemical heterogeneity (identification of organic matter and organo-mineral phases of soil)

The Lattice Boltzmann model (1/3)

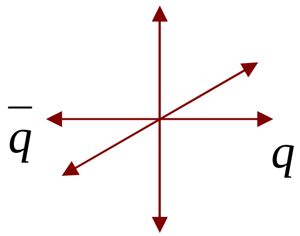
- ***Two-relaxation time LB model of Ginzburg (2005):***
  - more stable than the widely used One-relaxation time LB model (BGK)
  - intrinsic permeability does not depend on fluid viscosity for bounce-back collision on solid nodes

The Lattice Boltzmann model (2/3)

TRT LB model

Population density expressed by Boltzmann equation written with two relaxation times (λ_e,λ_d):

$$f_q(r+c_q,t+1) = f_q(r,t) + \lambda_e(f_q^+ - f_q^{eq+}) + \lambda_d(f_q^- - f_q^{eq-}) + Q_q(r,t)$$



$$f_q^+ = \tfrac{1}{2}\left(f_q + f_{\bar{q}}\right)$$
$$f_q^- = \tfrac{1}{2}\left(f_q - f_{\bar{q}}\right)$$
$$f_q^{eq+} = \tfrac{1}{2}\left(f_q^{eq} + f_{\bar{q}}^{eq}\right)$$
$$f_q^{eq-} = \tfrac{1}{2}\left(f_q^{eq} - f_{\bar{q}}^{eq}\right)$$

Equilibrium populations:
$$\begin{cases} f_q^{eq+} = t_q^* c_s^2 \sum_{q=0}^{Q-1} f_q \\ f_q^{eq-} = t_q^* \sum_{\alpha=\{1,2\}} \sum_{q=0}^{Q-1} f_q c_{q\alpha} \end{cases}$$

Source term (body force): $Q_q^m(r,t) = t_q^* c_q F_q$

Stability conditions: $-2 < \lambda < 0$

Stokes flow (D3Q19): $\lambda_e = -\dfrac{1}{3\nu - \frac{1}{2}}$ $\quad \lambda_d$ *is free*

Advection diffusion (D3Q7): $\lambda_d = -\dfrac{2c_s^2}{2D + c_s^2}$ $\quad \lambda_e$ *is free*

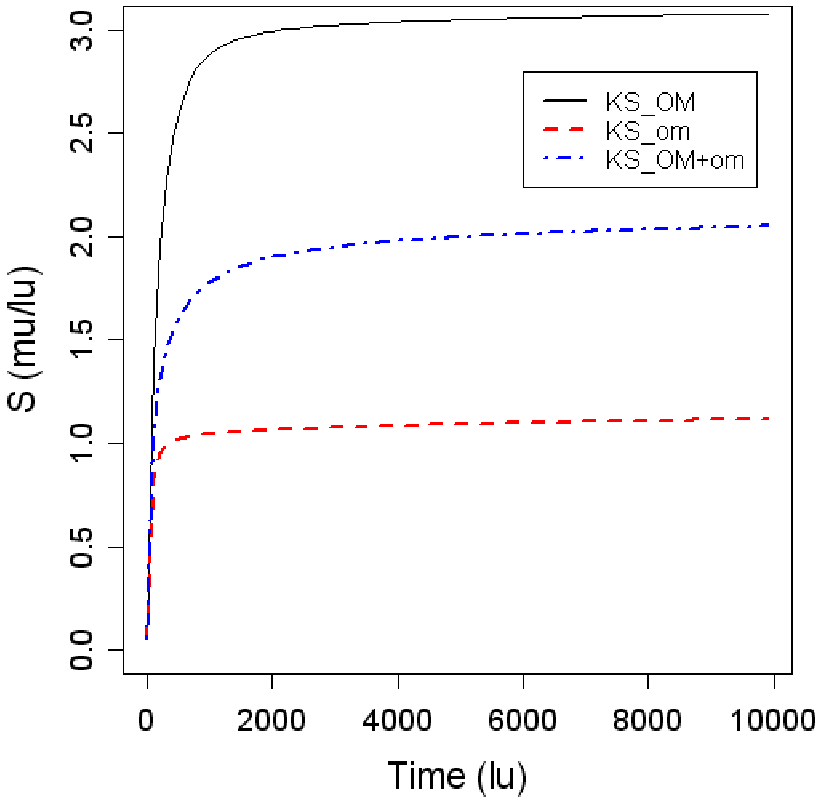
The Lattice Boltzmann model (3/3)

TRT LB model

Sorption Kinetics on solid sites:

$$f_{\bar{q}}(r_b, t+1) = f_q(r_b, t) - K_c f_q(r_b, t) + K_s s(r_b, t)$$
$$s(r_b, t+1) = s(r_b, t) + K_c f_q(r_b, t) - K_s s(r_b, t)$$

Sorption kinetics for high ($Kc=10^{-1}$, $Ks=10^{-3}$) and low ($Kc=10^{-1}$, $Ks=10^{-2}$) reactivity



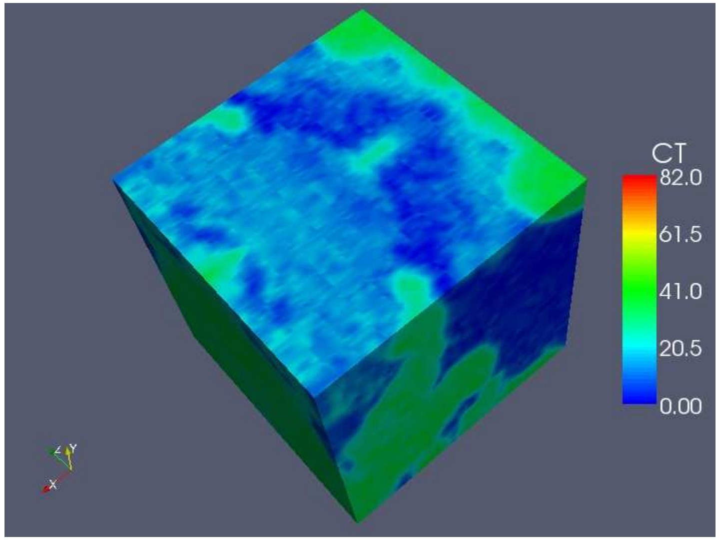
Linear adsorption isotherms

★ Homogeneous repartition of low reactive sites:
Kd = 1.55

★ Homogeneous repartition of high reactive sites:
Kd = 13.21

★ True repartition of high (OM) and low (om) sites:
Kd = 4.19

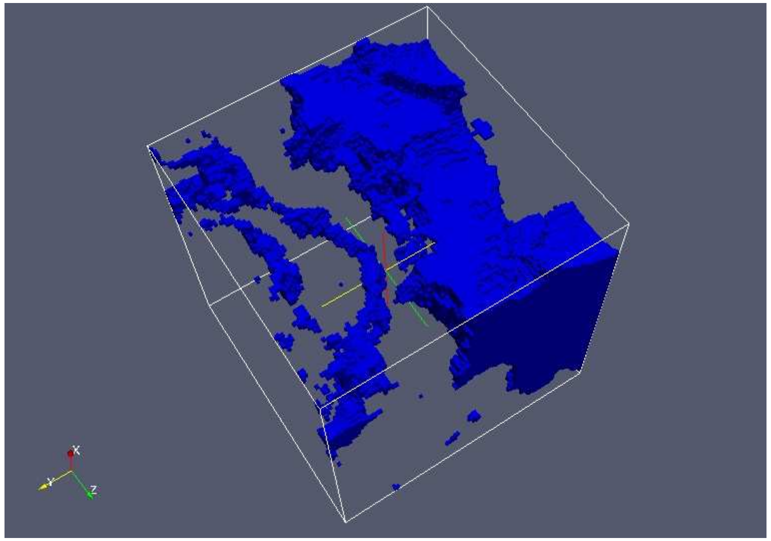
Numerical Results (1/5)

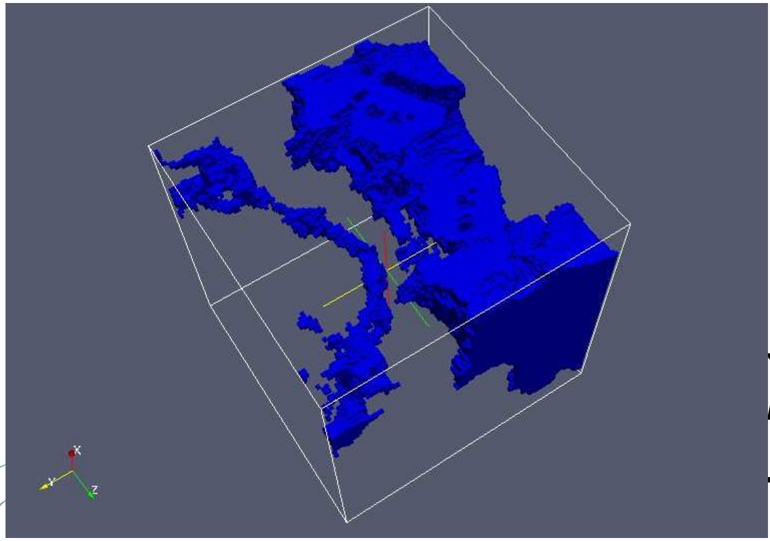


CT Soil Image: 884736 voxels

Issue: thresholding

Soil Porosity after thresholding:
178908 LB sites - $\theta = 0.20$



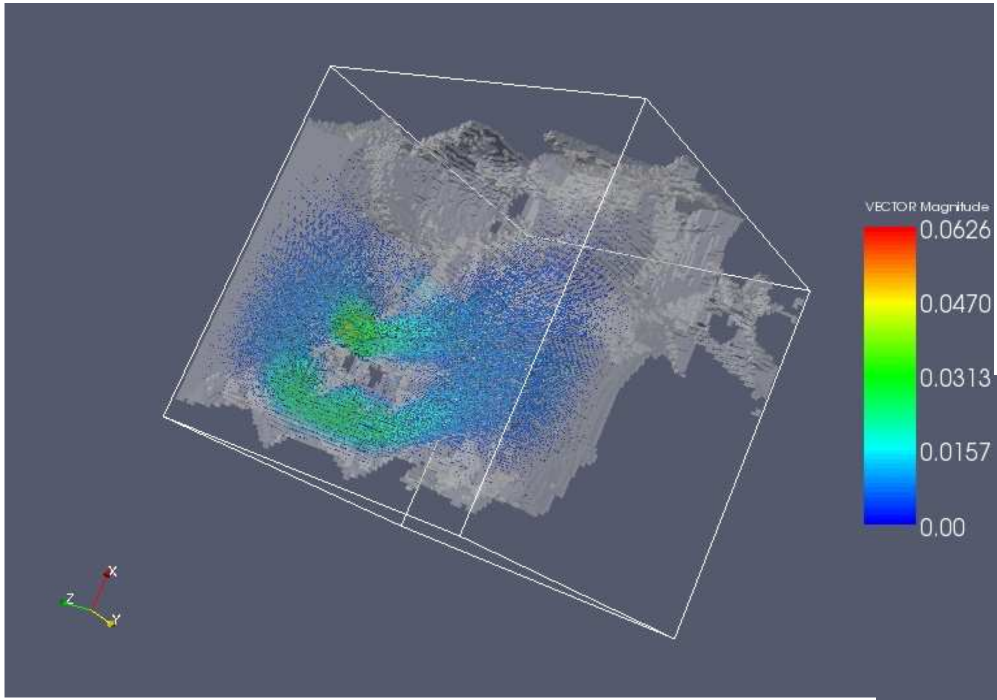


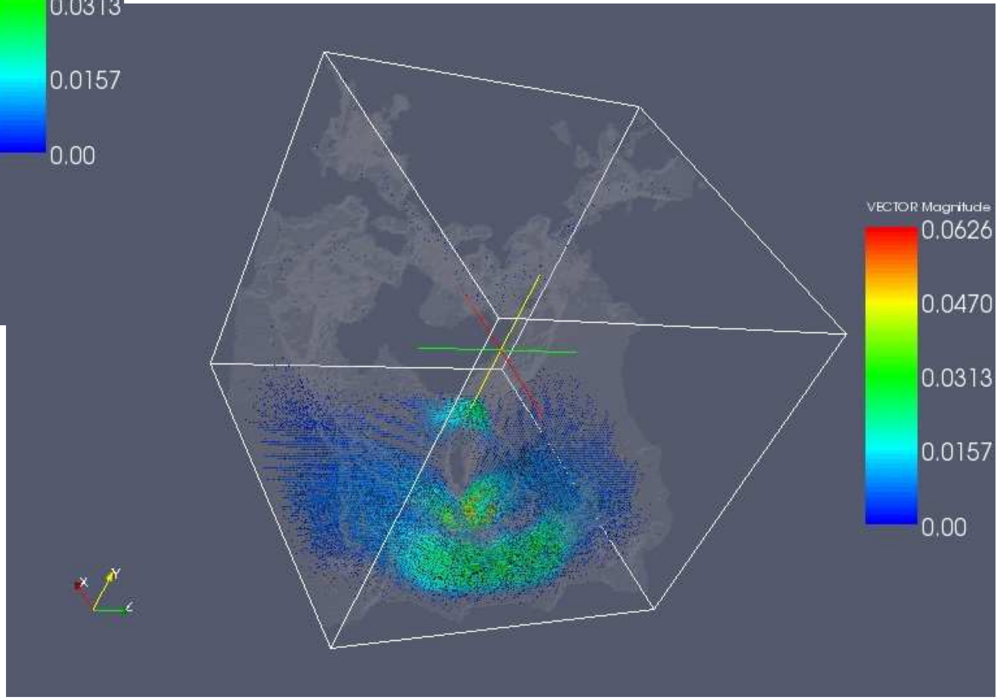
Soil Porosity after removal of non-connected porosity:
159252 LB sites - $\theta = 0.18$

Numerical Results (2/5)

Stokes Flow Field:

T = 50 000 tu



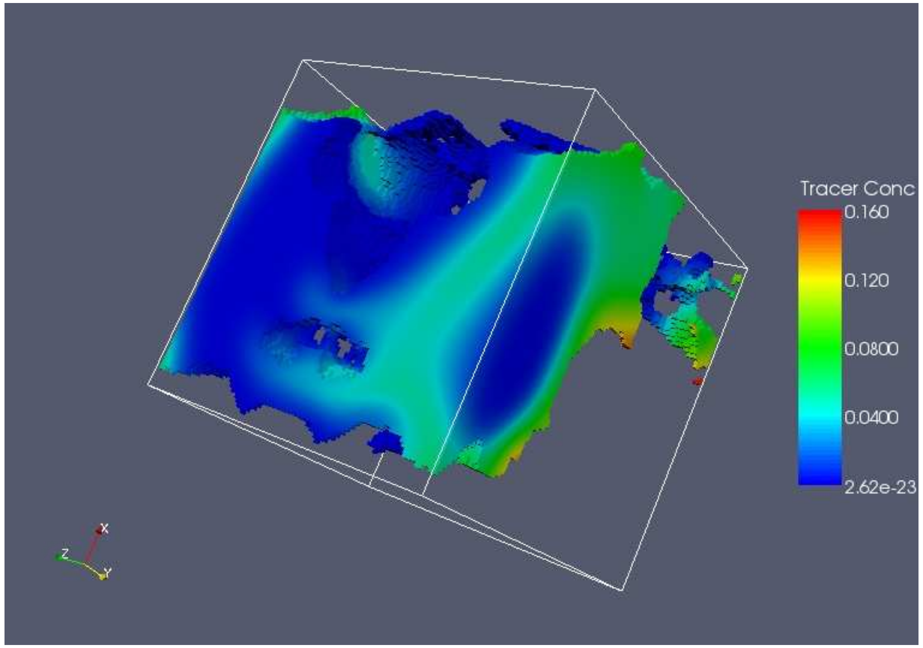


Body force: $F_z = 1\ e\text{-}3$

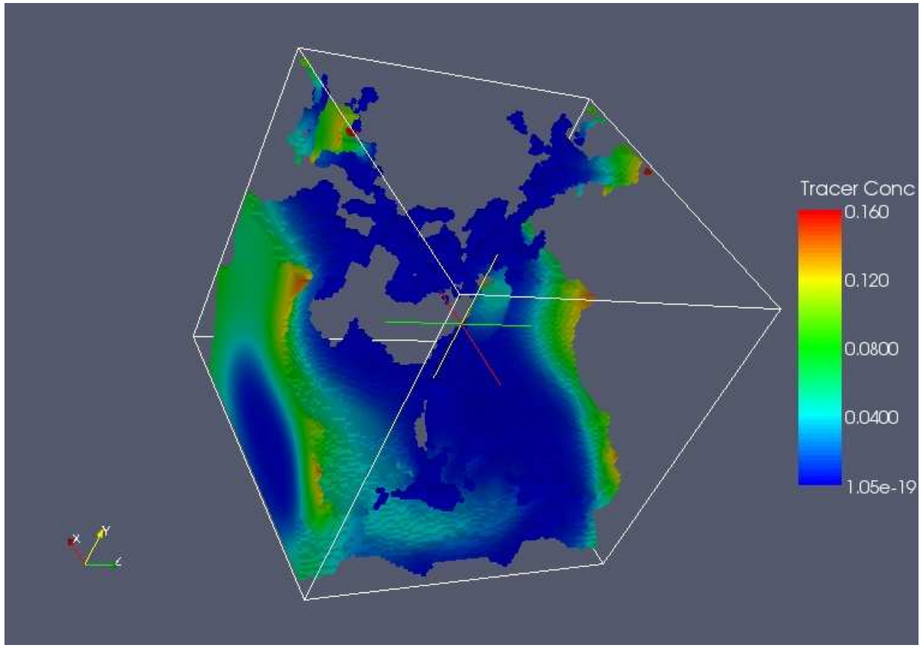
Numerical Results (3/5)

Concentration Field: Transport of a Dirac solute tracer plume

T=5000 tu



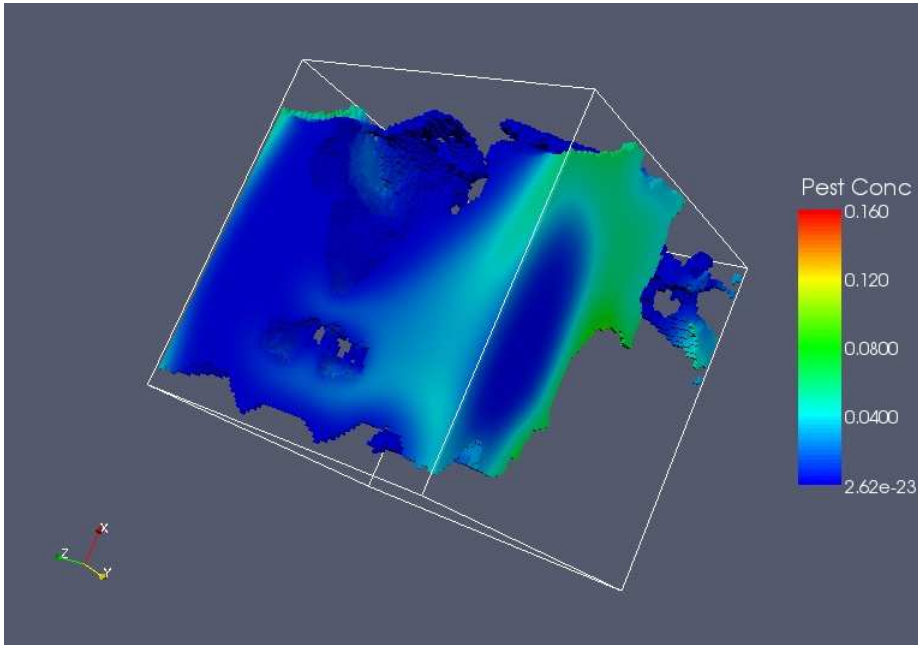
T=5000 tu



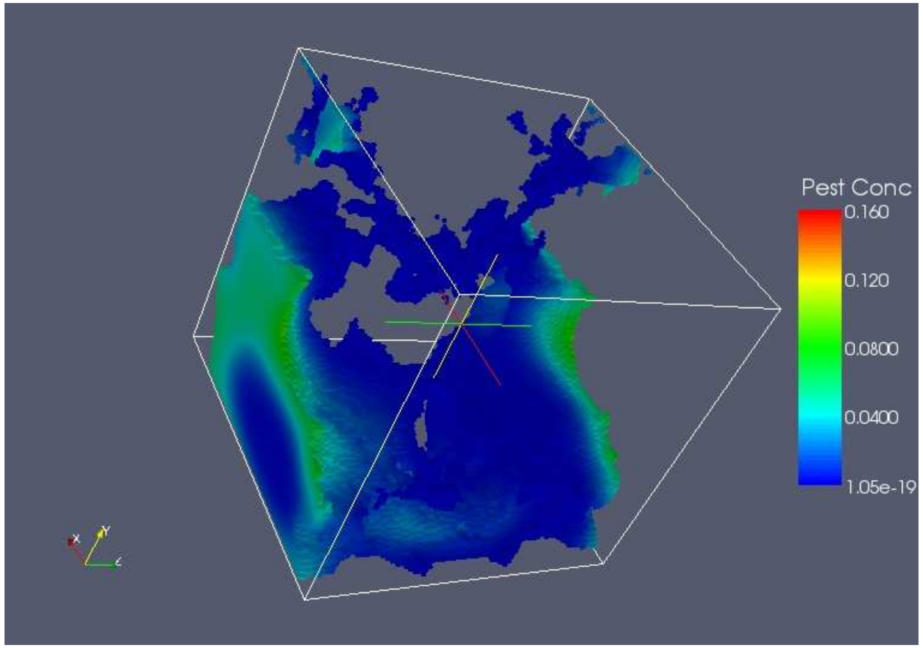
Numerical Results (4/5)

Concentration Field: Transport of a Dirac pesticide plume

T=5000 tu

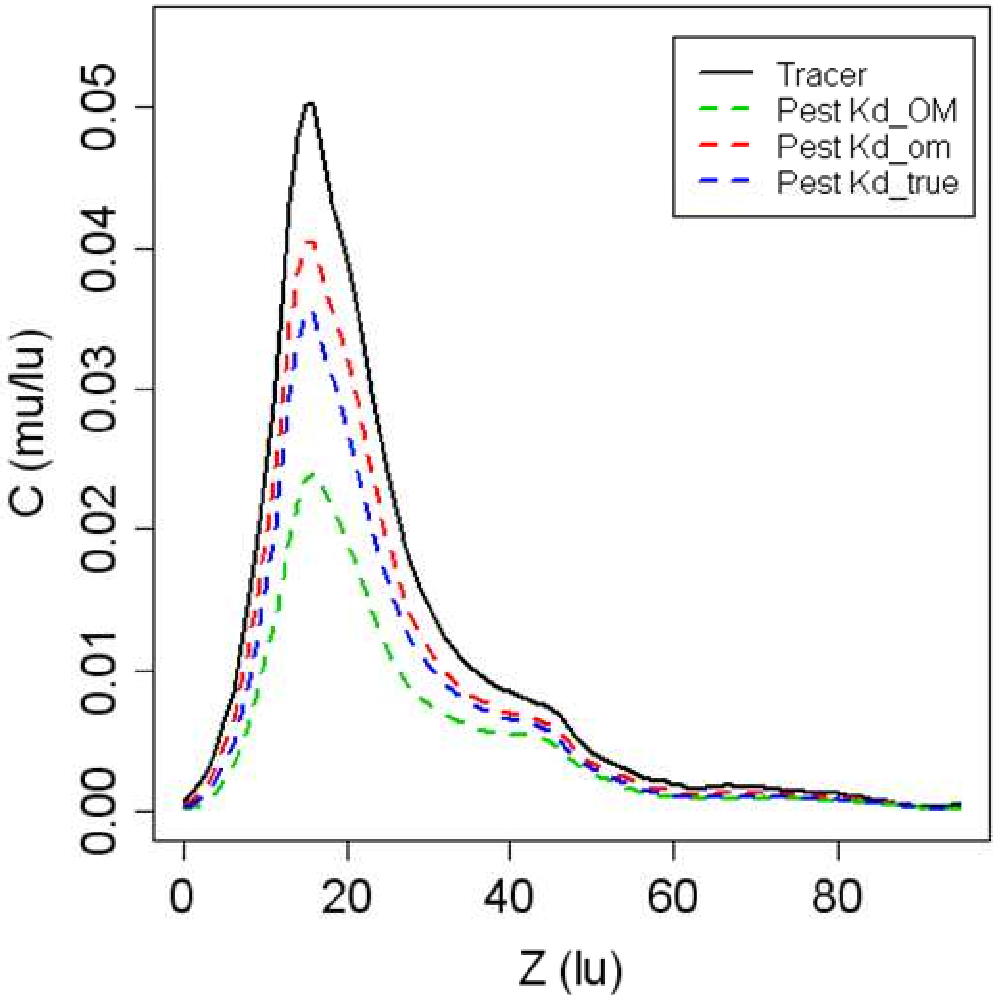


T=5000 tu



Numerical Results (5/5)

Mean Resident Concentration Profiles at 5000 tu



Conclusions – Future work

- ***Conclusions:***
  - *We successfully combined CT images and micromorphological observations of thin-sections on the same soil sample to identify and describe physical and chemical heterogeneities for pesticides*
  - *We developped sorption kinetics in the TRT LB model*
  - *We included the real physical and chemical heterogeneities in the TRT LB model*

- ***Future work:***
  - *Perform transport calculations on larger images (~ 1 cm^3)*
  - *Introduce biological reactivity of pesticides*

EGC