

# Цифровой керн: модели диффузной границы и математическое моделирование микротечений многофазных сред в пористых средах

«Digital Core»: Diffuse interface models and simulation of multiphase flows in porous medium

V. Balashov, E. Savenkov

Keldysh Institute of Applied Mathematics RAS

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# Outline

- 1 «Digital core» technology
- 2 Pore scale simulation
- 3 Basic mathematical model
- 4 Multiphase model
- 5 Simulation results
- 6 Current research and future work



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# Reservoir simulation

## Purpose:

- Optimal reservoir treatment
- Optimization of type and parameters of IOR techniques
- Optimization and control of reservoir development
- Prediction reservoir performance and risks management

## Basic tool:

*Predictive* model of pore fluid displacement accounting for contemporary IOR techniques

## Difficulties:

- Complex (multi)physics (multi-phase/components flows, surface effects, temperature effects, bulk and surface chemistry, ...)
- Wide range of scales (micrometers  $\rightarrow$  kilometers)



## Basic requirement:

Necessity of *correct* integration of huge amount of heterogeneous data in reservoir model

## Solution:

- *Hierarchy* of models at different scales + multiscale solvers
- Physically-based re-scaling and transfer of reservoir properties (existing techniques → mainly deal with static properties)

## Examples:

- “macro” Simulation on «geologic» grids  
(multi-scale solvers for 1+ b. of cells)
- “meso” pores/vugs, Stokes-Brinkman, etc.
- “micro” **Direct simulation at pore-scale**  
(core micro sample,  $\sim 1\text{mm}$  → core sample,  $\sim 1\text{cm}$  → ...)

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# Flow and displacement processes at pore scale

## Pore-scale:

- Defines flow parameters at macro-scale (static and dynamic properties of macroscopic reservoir-scale models, e.g. «black oil»)
- Actual space scale of the physics which governs macroscopic displacement and IOR techniques

## Characteristic properties of pore-scale models:

- Detailed accounting for pore space geometry
- Multi-(phase,component) hydrodynamics at pore space with direct treatment of *primary* physical mechanisms (+ surface and bulk chemical reactions, etc.)

# Laboratory studies

## Difficulties:

- Need for high quality specimens
- High cost and practical impossibility of massive utilization of a number of laboratory experiments
- Principal impossibility of multiple experiments using single core sample
- Impossibility to implement a full spectrum of reservoir conditions
- Impossibility of full-featured parametric studies



# Numerical experiments: basic possibilities

## Possibilities:

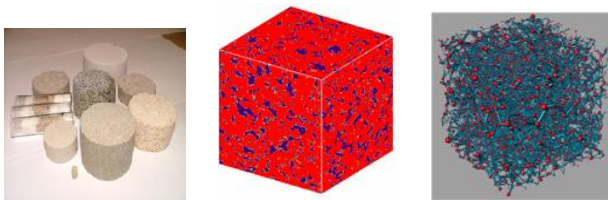
- Full quantitative information with manageable uncertainty quantification
- Account for wide range physical mechanisms
- Massive and (relatively) fast “virtual” experiments
- Full-featured parametric studies
- “Complex” specimens, un-consolidated samples, mud, *etc.*

Flexible tool which complements and  
extends laboratory measurements



# Basic components of the «digital core» model

- Geometric model of the specimen:
  - $\mu$ -CT + stochastic modelling
  - pore network
- Flow model:
  - multi-(phase,component) flow in pores
  - pore network models
- Model calibration tools
- Upscaling tools



Core sample and its models<sup>1</sup>

<sup>1</sup>Imperial College Consortium on Pore-scale Modelling



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# QHD equations

QHD = Quasi HydroDynamics

- QHD-equation = N.-S. equations + dissipative terms  $\sim \mathcal{O}(\tau)$ ,  
 $\tau$  — small parameter
- Can be derived as temporal averages of N.-S. equations  
(Elizarova T.G. 2011; Sheretov Yu.V., 2009)
- Can be derived phenomenologically (Sheretov Yu. V., 2009)
- Physically-based (parabolic) regularization of N.-S. equations
- Easy to implement stable centered approximations





# QHD-equations I (1-phase, 1-component)

## QHD-equations

$$\frac{\partial \rho}{\partial t} + \operatorname{div} j_m = 0$$

$$\frac{\partial \rho u}{\partial t} + \operatorname{div} (j_m \otimes u) + \nabla p = \operatorname{div} \Pi$$

$$\frac{\partial}{\partial t} \left[ \rho \left( e + \frac{1}{2} u^2 \right) \right] + \operatorname{div} \left[ j_m \left( e + \frac{1}{2} u^2 + \frac{p}{\rho} \right) \right] + \operatorname{div} q = \operatorname{div} (\Pi \cdot u)$$



# QHD-system I (1-phase, 1-component)

- Mass flux:

$$\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w}), \quad \mathbf{w} = \frac{\tau}{\rho}(\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla p),$$

- Stress tensor:

$$\Pi = \Pi_{NS} + \rho \mathbf{u} \otimes \mathbf{w}$$

- Parameter  $\tau \sim h$  is small



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# Intro

QHD approach was extended to multiphase multicomponent flows with surface effects (surface tension, coalescence, ...)

The developed model belongs to *diffuse interface models*.

Model development is based on:

- QHD-approach
- “microforce” concept [Morton Gurtin, 1996]



# QHD approach (reminder)

- Basic idea of QHD-approach “in large”:

$$\mathbf{j}_m \neq \rho \mathbf{u} \quad \Rightarrow \quad \mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w})$$

- Derivation of constitutive relation for  $\mathbf{w}$  is based on the 2-nd law thermodynamics
- Physically based regularization of Navier-Stokes equations, which allows using *simply implementable* explicit finite difference schemes



# Diffuse interface method

- Idea: Van-der-Waals; development: Kortweg, Ginsburg, Landau, Cahn, Hilliard;  $\Rightarrow$  “weakly non-local” or “gradient” theories  $\Rightarrow$  Navier-Stokes-Cahn-Hilliard-Ginsburg-Landau equations
- Phases are separated by thin layer of finite thickness, where interphase forces take place
- Interface finite thickness is physical rather than numerical effect

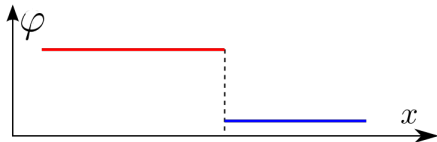


Рис.: “sharp interface”

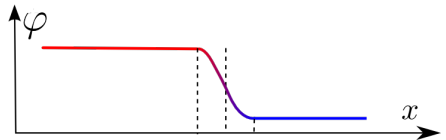


Рис.: “diffuse interface”



# “Microforce” concept

There are different ways to derive model equation.

In the present work is used

Approach suggested in [M.E. Gurtin, Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance, 1996, Physica D]:

Fundamental physical laws involving energy should account for the working (expenditure of power) associated with each operative kinematical process (order parameter evolution). So it seems plausible that there should be “microforces” whose working accompanies order parameter changes.



# Fluid composition model

- Fluid is composed of  $N$  components
- In arbitrary physically infinitesimal volume all of them could be presented

$$dm = \sum_{\alpha=1}^N dm_{\alpha}, \quad \rho = \frac{dm}{dV}, \quad \hat{\rho}_{\alpha} = \frac{dm_{\alpha}}{dV_{\alpha}}, \quad \rho_{\alpha} = \frac{dm_{\alpha}}{dV}$$

$$\rho = \sum_{\alpha=1}^N \rho_{\alpha}, \quad C_{\alpha} = \frac{\rho_{\alpha}}{\rho}, \quad \Rightarrow \quad \sum_{\alpha=1}^N C_{\alpha} = 1$$





# Derivation of constitutive relations

## Two basic ideas

- derivation of constitutive relation for microforces and QHD-terms are based on 2-nd law of thermodynamics (Coleman-Noll procedure [B.D. Coleman, W. Noll, 1963])
- phase constitution (microstructure) of fluid in space is defined by order parameter field (fluid density and/or components concentration)

$$\frac{\partial \rho s}{\partial t} + \operatorname{div} \left( \mathbf{j}_m s + \frac{\mathbf{q}}{T} \right) - \frac{\rho r}{T} \geq 0.$$



# Special case

Isothermal two-component flow with surface effects

## Basic equations

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{j}_m &= 0 \\ \frac{\partial (\rho C_\alpha)}{\partial t} + \operatorname{div} (\mathbf{j}_m C) &= \operatorname{div} (M \nabla \mu) \\ \frac{\partial (\rho \mathbf{u})}{\partial t} + \operatorname{div} (\mathbf{j}_m \otimes \mathbf{u} - \mathbf{P}) &= 0\end{aligned}$$

## Helmholtz free energy

$$\Psi(\rho, C, \nabla C) = \Psi_0(\rho, C) + \frac{\lambda_1}{2} |\nabla C|^2$$

$$\Psi_0 = C\Psi_1 + (1 - C)\Psi_2 + \Psi_{sep}$$

$$\Psi_1 = \Psi_2 = c_s^2 \ln \rho, M = M_0 C(1 - C)$$

## Constitutive relations

$$\mathbf{w} = \frac{\tau}{\rho} [\rho(\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p + \operatorname{div} \mathbf{Q}]$$

$$\mathbf{Q} = -\rho \lambda_1 \nabla C \otimes \nabla C$$

$$\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w})$$

$$\mathbf{P} = \mathbf{P}_{NS} - p\mathbf{I} + \mathbf{Q} + \mathbf{P}_{QHD}$$

$$\mu = \frac{\partial \Psi_0}{\partial C} - \frac{\lambda_1}{\rho} \operatorname{div} (\rho \nabla C)$$

$$p = \rho^2 \frac{\partial \Psi_0}{\partial \rho}$$

# Special case: $\Psi_{sep}$ and $P$

“Separating” free energy

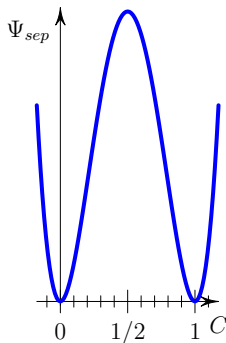
$\Psi_{sep}$  provides phase separation

$$\Psi_{sep} = A_\psi C_1^2 C_2^2 = A_\psi C^2 (1 - C)^2$$

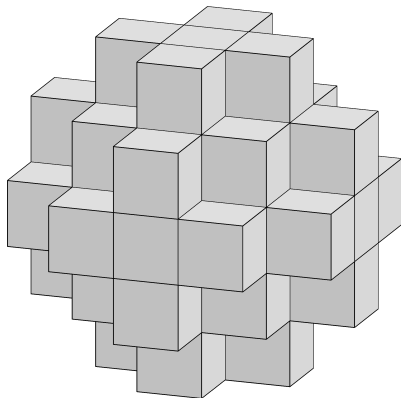
Stress tensor

$$\mathbf{P} = \mathbf{P}_{NS} - p\mathbf{I} + \mathbf{P}_{QHD} + \mathbf{Q}$$

- Capillary stress tensor  $\mathbf{Q} := -\rho\lambda_1 \nabla C \otimes \nabla C$   
Provides capillary forces on interface
- QHD-stress term  $\mathbf{P}_{QHD} := \rho \mathbf{u} \otimes \mathbf{w}$ .



# Finite difference scheme



- Additional dissipative terms provide numerical stability of central difference approximations
- Cartesian orthogonal grid
$$h_x = h_y = h_z$$
- $\tau \rightarrow \tau_h = \alpha^* \frac{h}{c_s}$
- 51-point stencil in 3D



# Details

Other details about the model (including derivation) can be found in the following work:

V.A. Balashov, E.B. Savenkov, Quasihydrodynamic equations for diffuse interface type multiphase flow model with surface effects // Preprints Keldysh IAM. 2015. № 75. 37 p. [in russian] URL: <http://library.keldysh.ru/preprint.asp?id=2015-75>

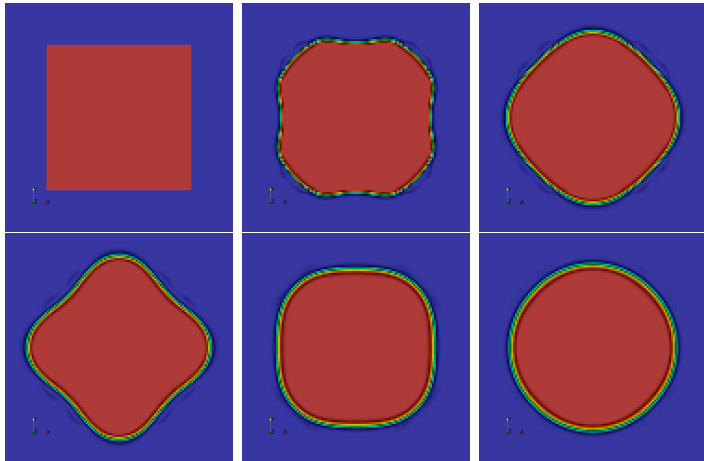


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# Evolution of «square» droplet: (one of the) 1st simulation



red —  $C_0 = 0.85$ , blue —  $C_0 = 0.15$



# Fluid focusing device I

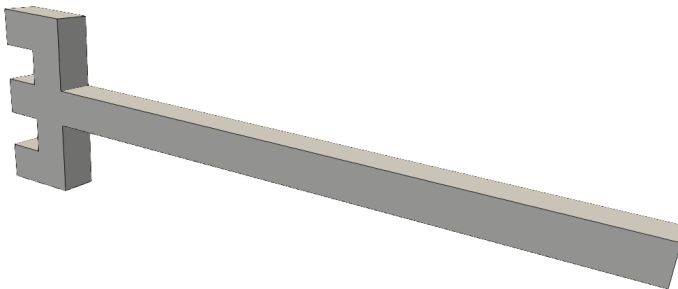


Рис.: Fluid focusing device

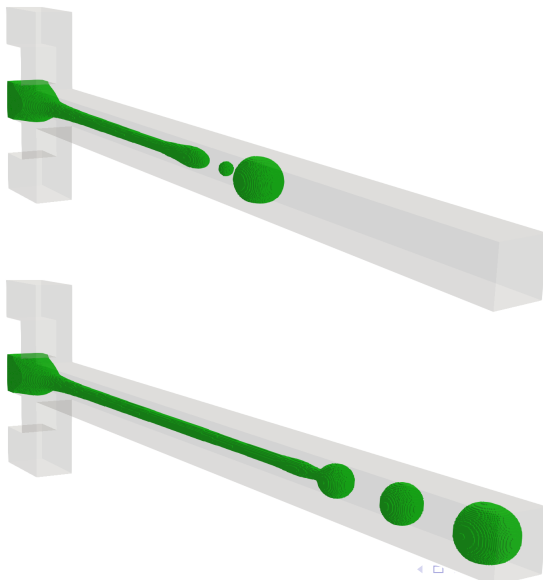
Rich structure of flow depending on flow parameters:

- threading, jetting, dripping, tubing, displacement

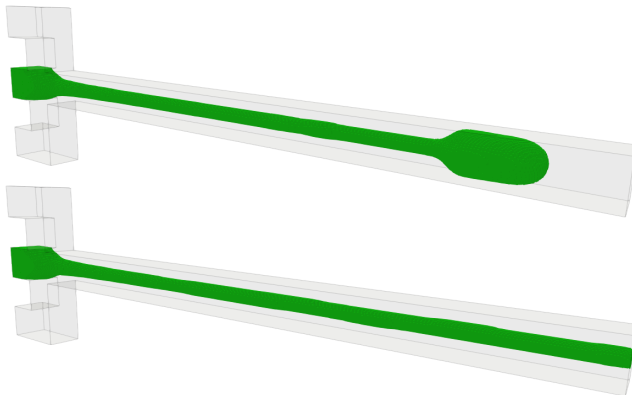




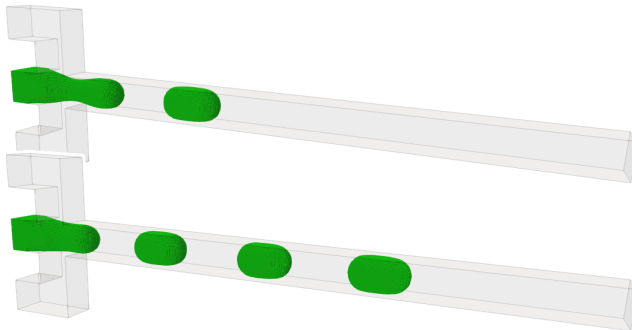
# Fluid focusing device (jetting, струйный режим)



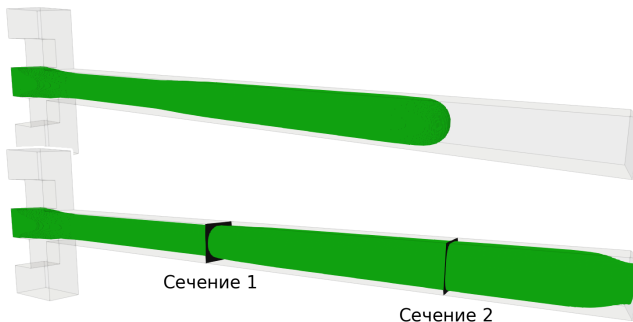
# Fluid focusing device (threading, нитеобразный режим)



# Fluid focusing device (dripping, капельный режим)



# Fluid focusing device (tubing, пленочный режим)



# Fluid focusing device: a map

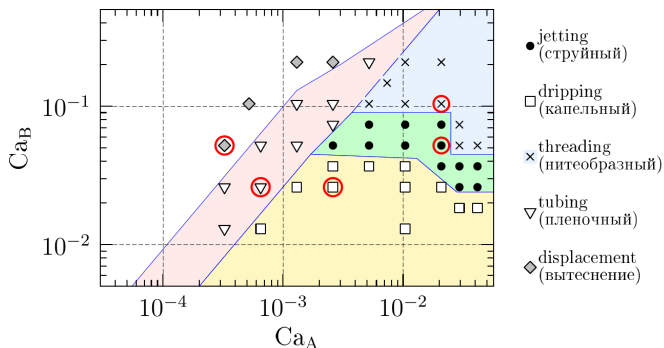
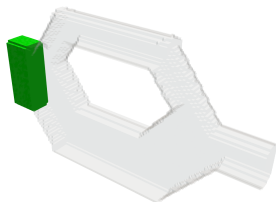


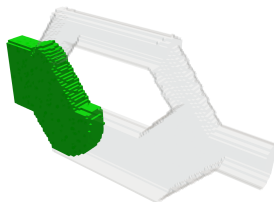
Рис.: Flow regimes map,  $Ca_A$  vs.  $Ca_B$ .



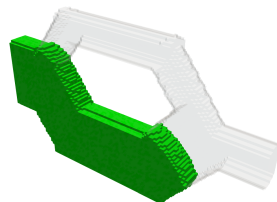
# Pore doublet (drainage)



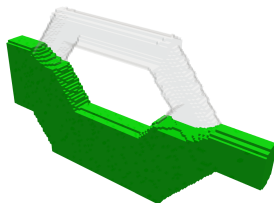
(a)  $t = 0$



(b)  $t = 5 \cdot 10^5 \Delta t$



(c)  $t = 10 \cdot 10^5 \Delta t$

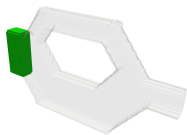


(d)  $t = 29 \cdot 10^5 \Delta t$

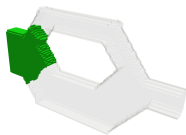


Рис.: Вытеснение при дренаже в поровом дублете.

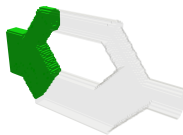
# Pore doublet (imbibition)



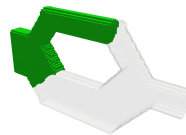
(a)  $t = 0$



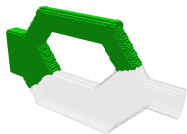
(b)  $t = 2 \cdot 10^5 \Delta t$



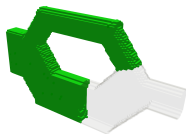
(c)  $t = 4 \cdot 10^5 \Delta t$



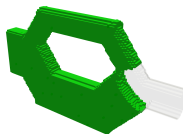
(d)  $t = 5 \cdot 10^5 \Delta t$



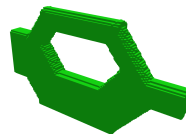
(e)  $t = 6 \cdot 10^5 \Delta t$



(f)  $t = 10 \cdot 10^5 \Delta t$



(g)  $t = 14 \cdot 10^5 \Delta t$



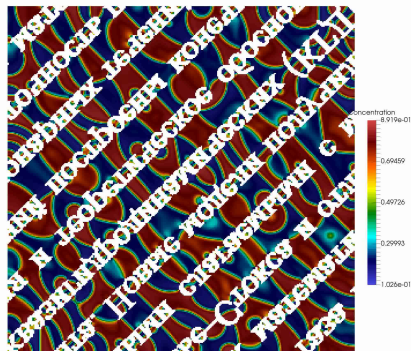
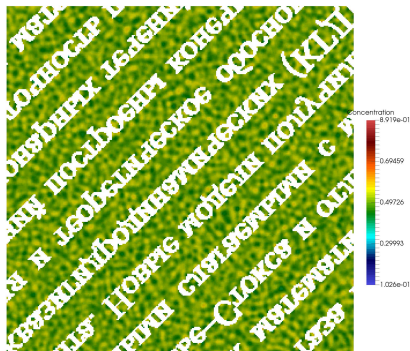
(h)  $t = 16 \cdot 10^5 \Delta t$

Рис.: Вытеснение при пропитке в поровом дублете.



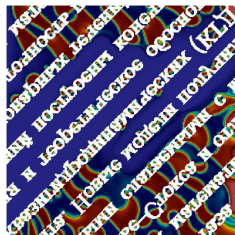
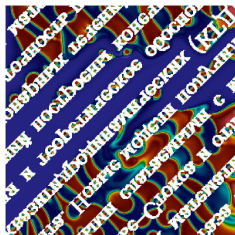
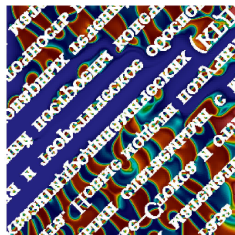
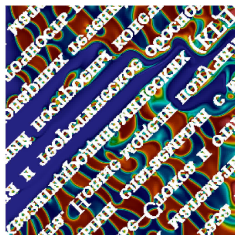
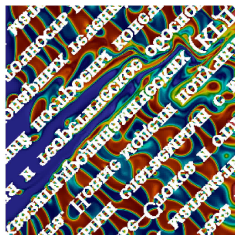
# Displacement in 2D: initial state computation

Spinodal decomposition to obtain initial state of the mixture

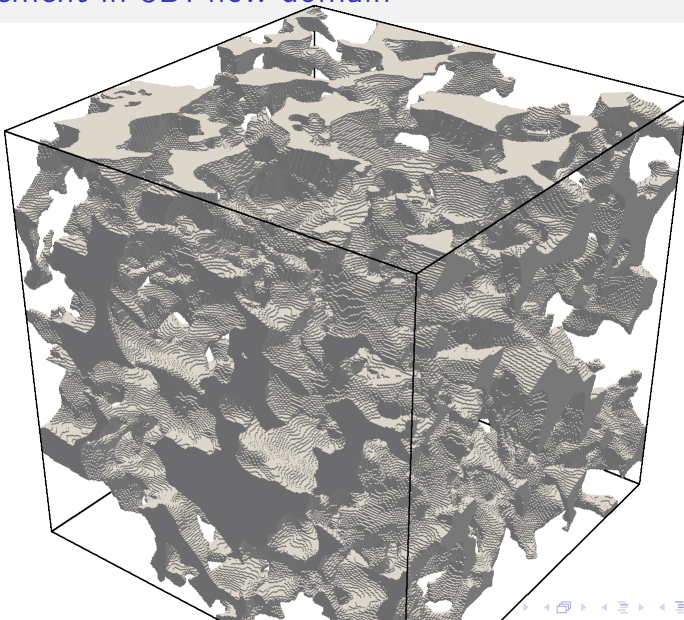




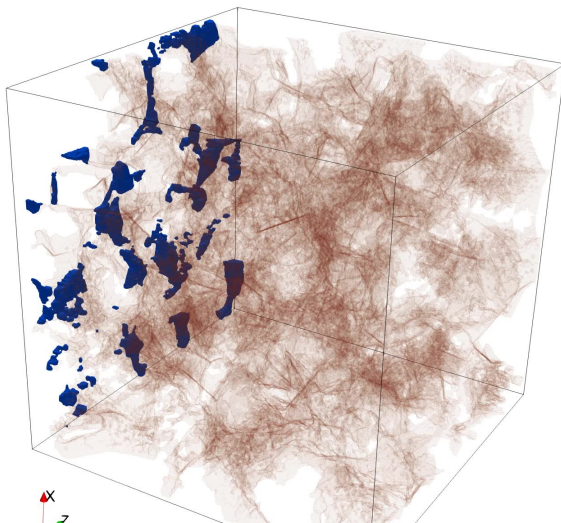
# Displacement in 2D



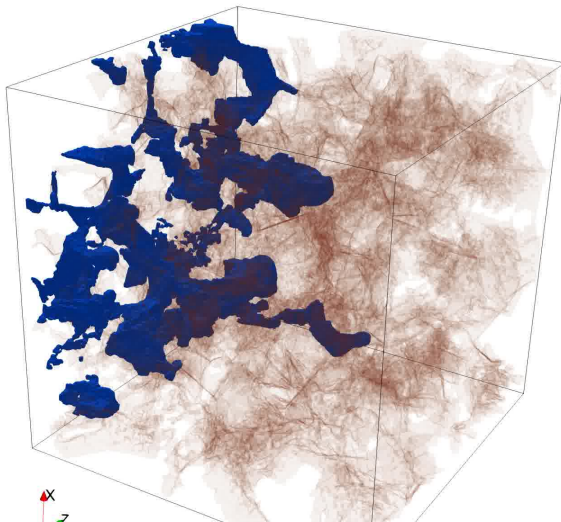
# Displacement in 3D: flow domain



# Displacement in 3D: $600^3$ sample: initial state



# Displacement in 3D: $600^3$ sample: developed state



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# Current research

## New models & numerics:

- “Solid-fluid interaction”: coupled HD in pore space coupled with elasticity in core, dynamics of suspension (elastic particles in the flow).
- New models for complex contact angle dynamics
- New algorithms for **3ph** flows —  $\times 10/100/1000$  jumps in viscosity/density/compressibility

## Validation and verification for industry-quality predictive simulations

- Laboratory experiments.

## HPC:

- Up to now we *practically* simulate 1ph flows for  $1600^3@10\%$  porosity — the goal is 3ph with  $2048^3$
- **GPGPU** in progress!

Thank you for your attention!

