Hybrid modeling

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[*http://www.math.oregonstate.edu/people/view/mpesz*]

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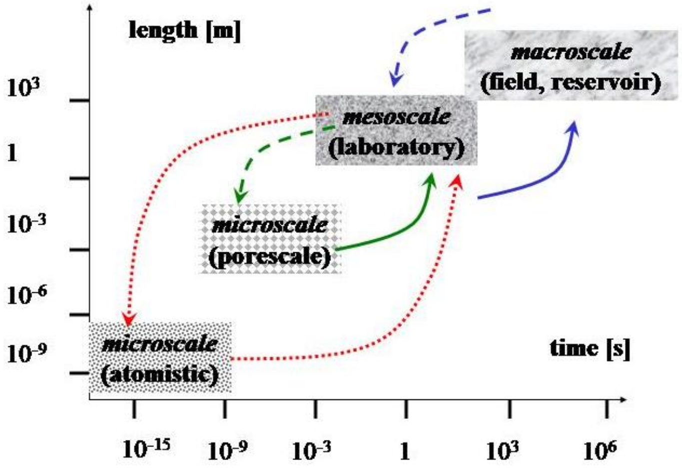
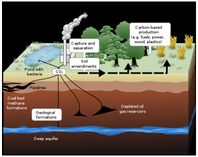
Multiple scales

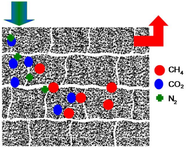


Computational modeling across scales

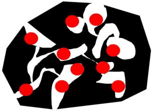
Example: energy recovery/carbon sequestration

- field (macro)

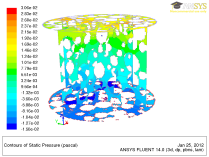


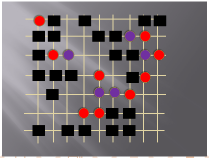


- lab=core (meso)



- pore (micro)



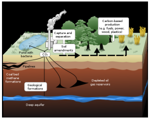


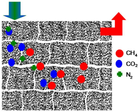
Computational modeling across scales

Example: energy recovery/carbon sequestration

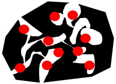
- field (macro)
  $U_t + A(U) = 0$
- lab=core (meso)
  $u_t + a(u) = 0$
- pore (micro)
  $\frac{d}{dt} \sum_i u_i + a_i \sum_j u_i u_j = 0$

continuum models

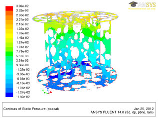


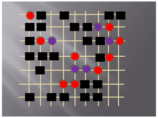


continuum or discrete models



statistical mechanics





Data for modeling

For continuum models at macroscale or mesoscale

$$U_t + A(u) = 0$$

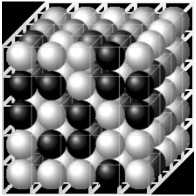
or

$$u_t + a(u) = 0$$

. . . need coefficients A, a and more . . .

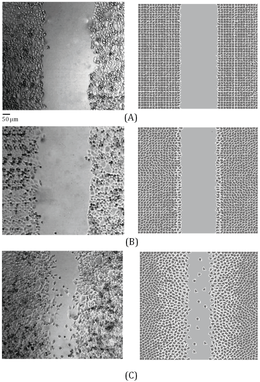
Old way: laboratory experiments

New way: *In silicio* experiments



In silicio modeling and experiments

Performed on computer or via computer simulation



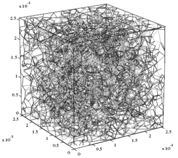


Fig. 5—3D network representation of a water-wet sandstone sample; the network description is courtesy of Statoil. The network dimensions are in meters.

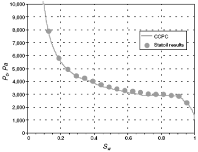
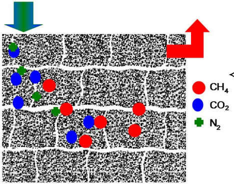


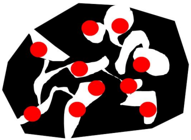
Fig. 18—The calculated capillary-pressure curve in primary drainage of the Bentheimer sandstone network vs. the Statoil results (circles) from P.-E. Øren, *et al.*

Hybrid modeling across scales

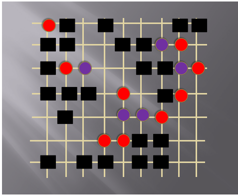
Combine dynamically the three scales



$\Longleftrightarrow$



$\Longleftrightarrow$

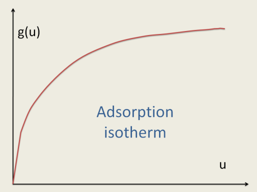


Example: adsorption models

$$u_t + v_t + u_x = 0,$$
$$v = g(u)$$

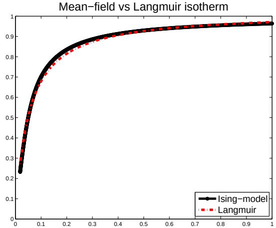
Traditional experiment-based model
(Langmuir isotherm)

$$v = g(u) = V_L \frac{bu}{1 + bu}$$

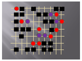


Need V_L, b from experiments

Computer simulation model
statistical mechanics,
equilibrium mean-field Ising-like model
[*Peszynska'11-12*]



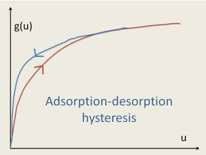
Uses a computer model



What is better? Why need extra models?

How to model adsorption hysteresis $v \in g(u, u_t)$?

$$u_t + v_t + u_x = 0$$



Get $v \in g(u, u_t)$ from

experiments . . . or continuum models [PShowalter'97]. . . or discrete models [P'11-12]

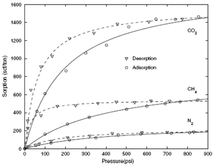
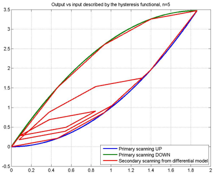
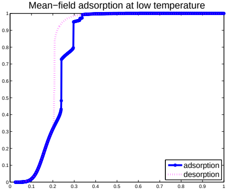


Fig. 2 Sorption characteristics of Power River Basin (Wyoming) coal. Measurements conducted at 295.15 K (71.6 F)



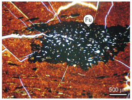


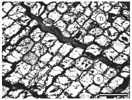
Example: how to get $g(\cdot)$ from porescale models

[with D. Wildenschild, A. Trykozko, others (OSU/UWarsaw)]

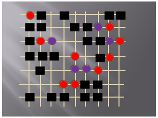
Tomography (x-ray) images $\Longrightarrow$ Porescale models $\Longrightarrow$ $v \in g(u)$

- Geometry from tomography

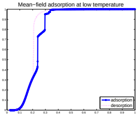





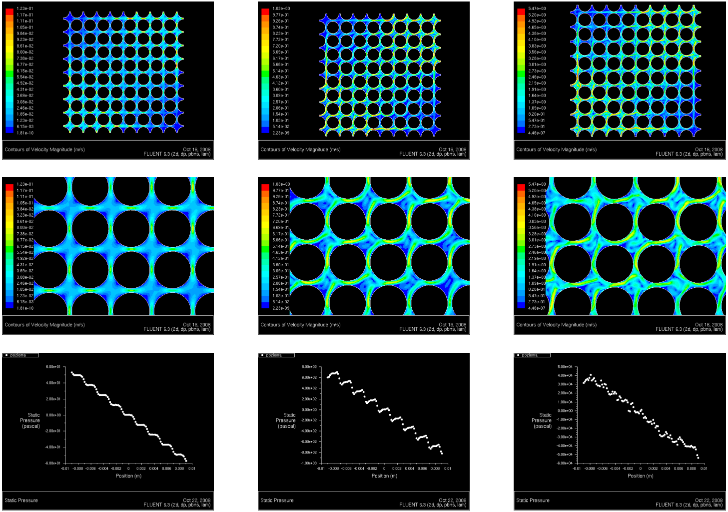
- Computational models (discrete: statistical mechanics)



- Result: $v \in g(u)$



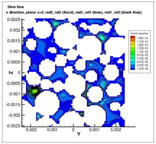
Example: slow, fast, very fast flow

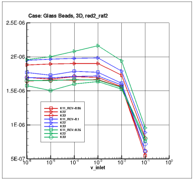


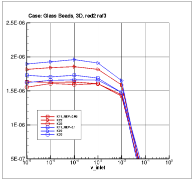
standard Darcy (new) non-Darcy ???

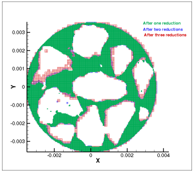
Porescale: computational math aspects

- Convergence of results models

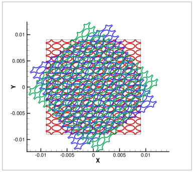
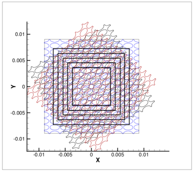
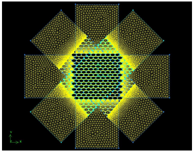








- Invariance with respect to rotation

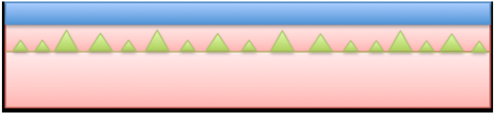
- New model at corescale found (non-Darcy, $\alpha \approx 2.5$ in 2D, $\alpha \approx 1.2$ in 3D)

[*PTrykozko'Comp.Geosci.2013,*]

Example: semiconductor modeling (solar cells)

[with G. Schneider, D. Foster, T. Costa, and others (OSU, UfO Physics, Chemistry)]

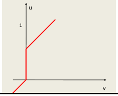
- Nonlinear coupled PDEs (electron/hole concentrations n, p, potential ψ)
- Discrete model to describe *Heterogeneity Assisted Impact Ionization* (on interfaces)
- MAIN ISSUE: how to couple them ?



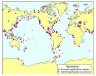
Schematic of a three-component HAII structure formed by self assembly of quantum dot harvesters (green) by Stranski-Krastanov growth on a narrower band gap host (red), followed by an additional layer of the host and a wide band gap capping layer (blue).

Example: methane hydrates modeling and phase transitions

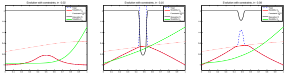
$$u_t - v_{xx} = 0, \quad u \in \alpha(v)$$



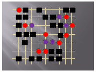
- At world scale



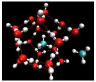
- At macroscale *[GMPS'12]*



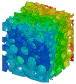
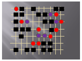
- At mesoscale



- At molecular scale



Models at pore2core

	core continuum	pore continuum	pore discrete
			
VARIABLE	V=average over ϕ	v=local value	$\langle V\rangle_{P[\mathbf{t},\mathbf{n}]}, \bar{V}, \sum_i V_i$
FLOW	DARCY	NAVIER-STOKES	LB
TRANSPORT			
porosity	ϕ	1	$\frac{\sum_i n_i}{L^3}$
mass (molar) fractions	pC	x_{pC}	ρ_a, ρ_b
flux	$J = -DS_p \nabla_{pC}$	$j = -d\nabla x_C$	
diffusivity	$D = \phi \frac{d}{\theta^2} \propto d\phi^m$	d	
ADSORPTION			
amount	$a_i = V_{L,i} \frac{b_i p_i}{1+\sum_j b_j p_j}$	b.cond. ?	mean-field approx.
PHASE BEHAVIOR			
saturation	S	s ?	
flow	k_{rl}, k_{rg}, P_c	multiphase N-S	LB
constraints	P_{sat} or $(_{IM}, S_l) \in F$	p_{sat} or $(x_{IM}, s_l) \in f$?	STAT.MECH.
ENERGY			
temperature T			
enthalpy	$cT + H_\phi(T)$	$cT + LH(T)$	STAT. MECH.

Interested in hybrid models ?

Modeling + Analysis + Simulation

- Modeling: existing and new models

  applications: geosciences, physics, engineering, biology

  - Continuum (empirical) models: ODEs, PDEs:
  - Discrete models (deterministic and stochastic)
    equilibrium and non-equilibrium (dynamic)
  - (Coupling) between continuum and discrete models

- Analysis

  understanding properties, analyzing well-posedness

- Computation and simulation

  - use/analyze/develop existing/new methods for new applications
  - implement/develop known/new algorithms
  - NEW technologies

Classes: *[PDEs + Analysis + Numerical Analysis/Computing + Probability]*

`Interested ?  Email me to meet.`