Interdisciplinary Mathematics
=
Modeling + Analysis + Simulation

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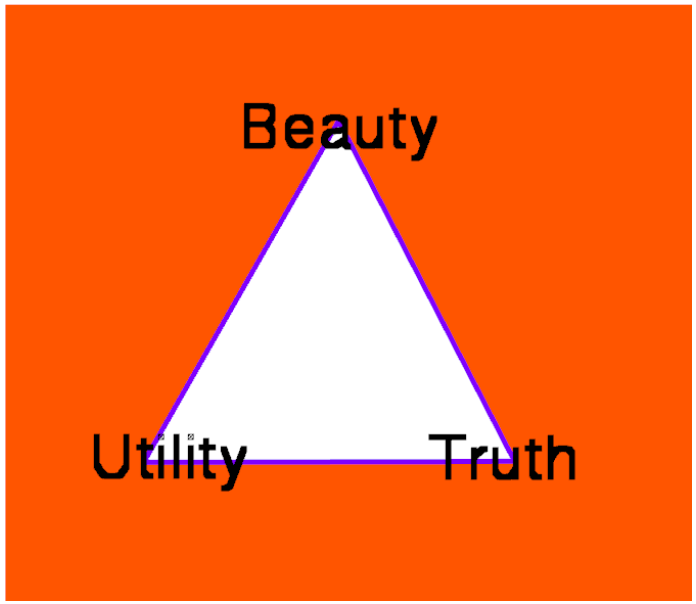
[*http://www.math.oregonstate.edu/people/view/mpesz*]

“Applied Mathematics is not ... a subject classification”

“It is an attitude”

- Projects contribute
  - to Mathematics itself
  - to other disciplines
  - across disciplines
- Modeling + Analysis + Simulation



Experiments vs Modeling vs Simulation

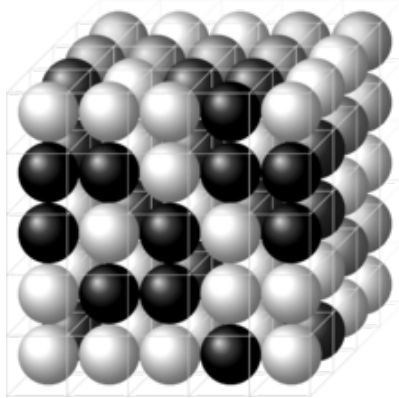
For continuum models at macroscale or mesoscale

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

. . . need data A and more . . .

Old way: laboratory experiments

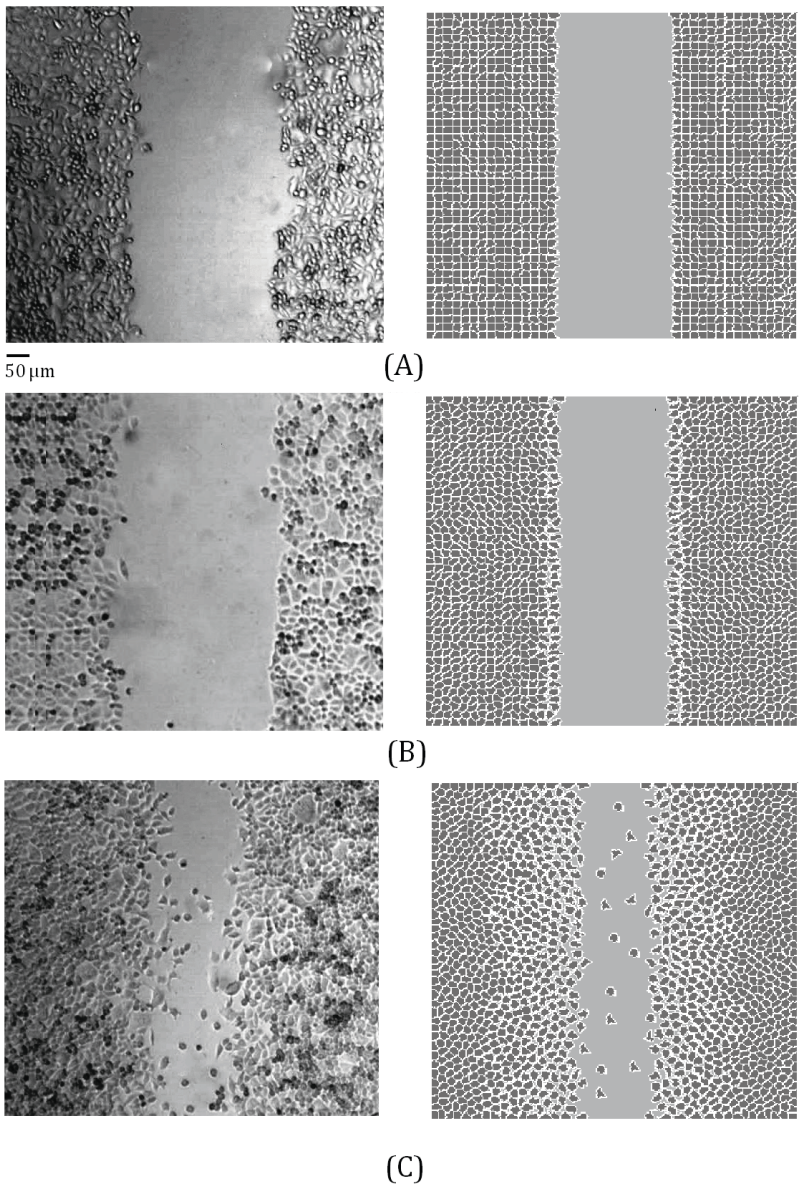
New way: *In silicio* experiments



In silicio modeling and experiments

Performed on computer or via computer simulation

Wound modeling



Capillary pressure in pores

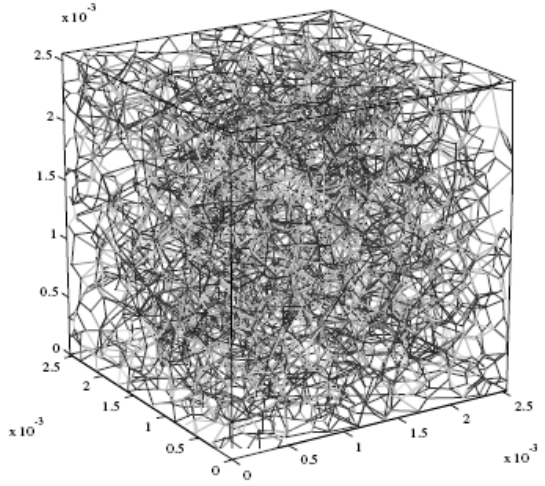


Fig. 5—3D network representation of a water-wet sandstone sample; the network description is courtesy of Statoil. The network dimensions are in meters.

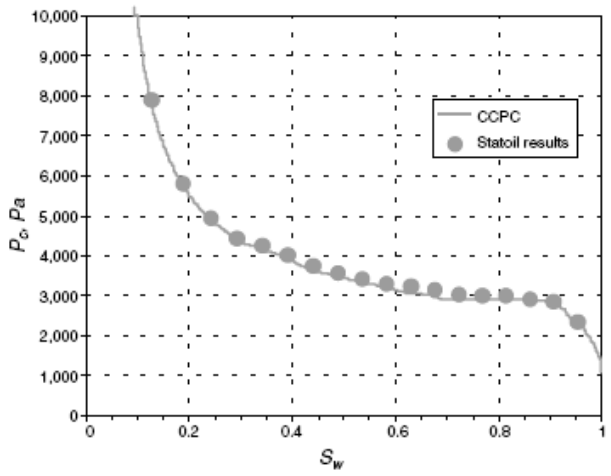


Fig. 18—The calculated capillary-pressure curve in primary drainage of the Bentheimer sandstone network vs. the Statoil results (circles) from P.-E. Øren, *et al.*

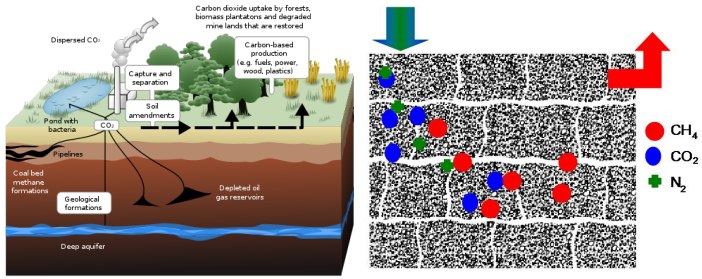
Computational modeling across scales

Example: energy recovery/carbon sequestration

[With M. Ossiander, L. Madsen (OSU Stat) + OSU CEAOS + OSU Chemistry + NETL scientists]

- field (macro)
  $U_t + A(U) = 0$

continuum models

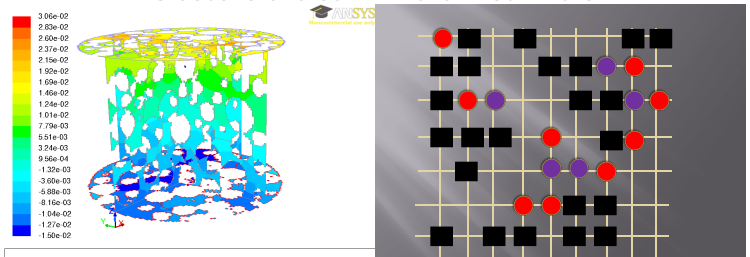


- lab=core (meso)
  $u_t + a(u) = 0$

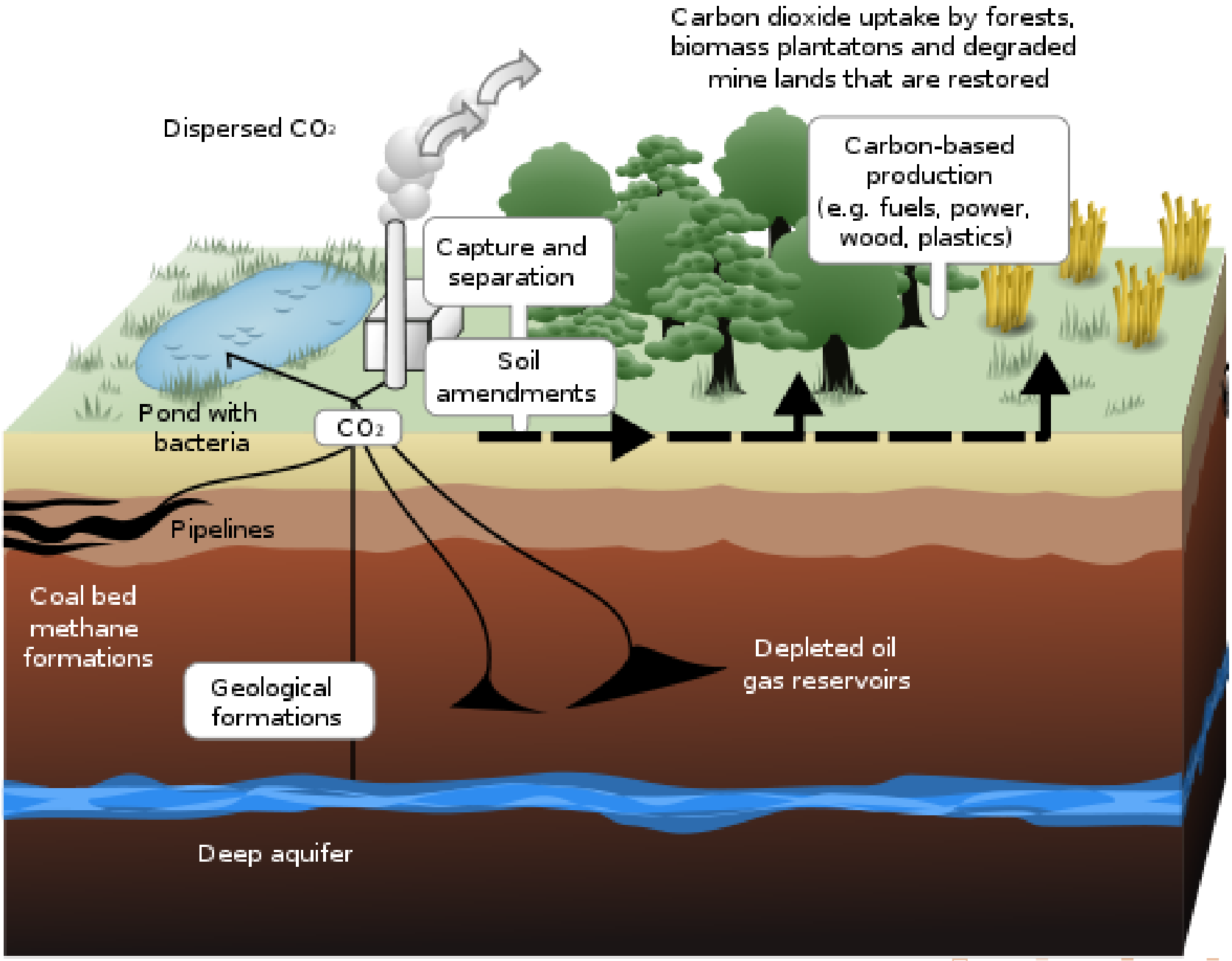
continuum or discrete models

- pore (micro)
  $\frac{d}{dt}\sum_i u_i + a_i \sum_j u_i u_j = 0$

statistical mechanics



Reservoir reality and modeling

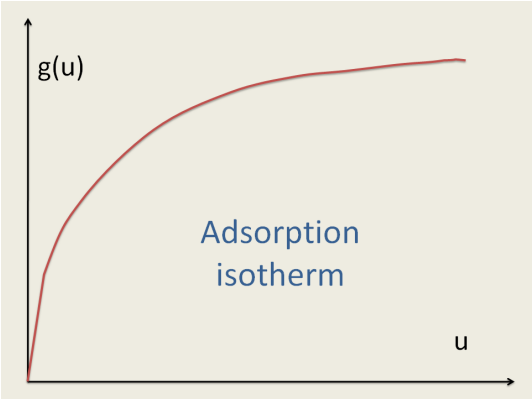


Example: adsorption models *[Peszynska'11-]*

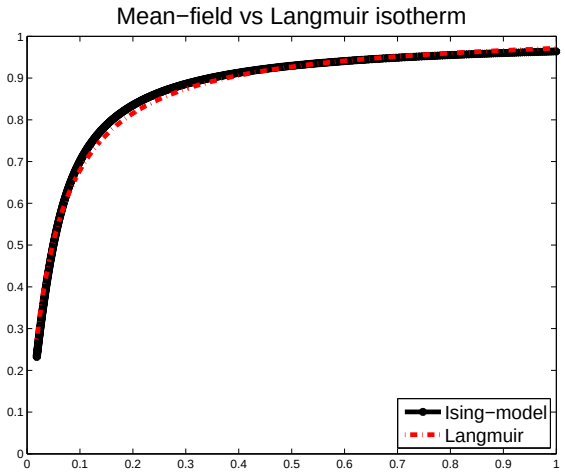
$$u_t + v_t + u_x = 0;\ v = g(u)$$

Traditional experiment-based model
(Langmuir isotherm)

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

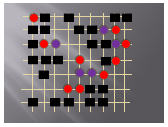


Computer simulation model
statistical mechanics



Needs V_L, b *from experiments*

Uses a computer model

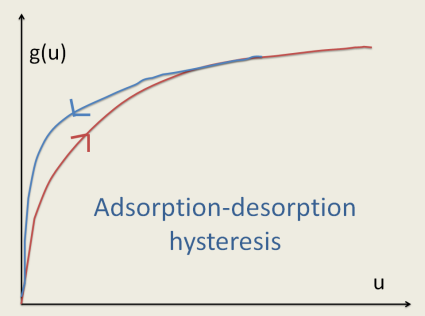


What is better? Why need extra models?

Example: adsorption hysteresis

[Work with R. Showalter, P. Medina, and others]

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



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

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

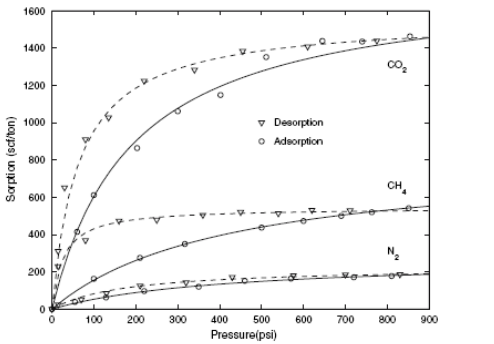
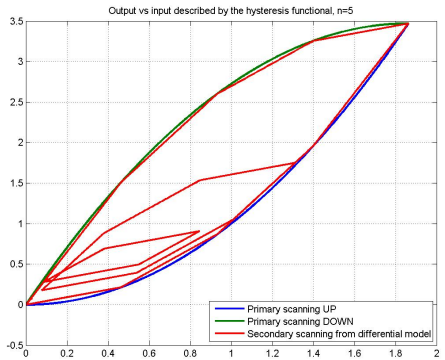
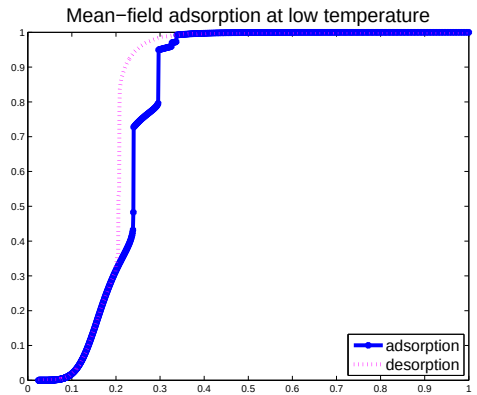


Fig. 2 Sorption characteristics of Power River Basin (Wyoming) coal. Measurements conducted at 295.15 K (71.6 F)

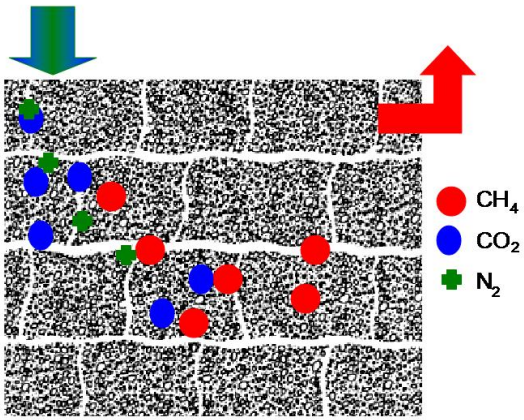


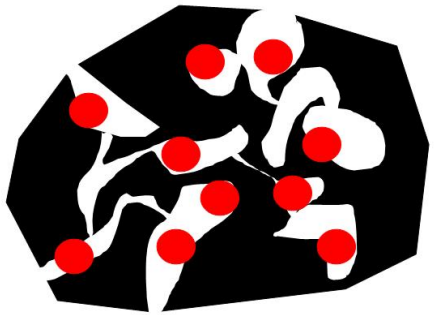


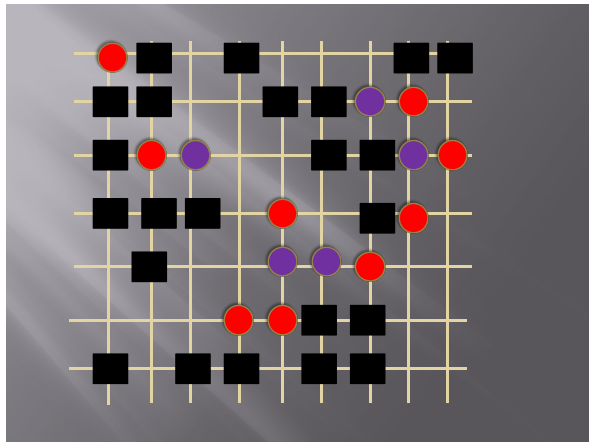
Current project: Hybrid modeling across scales

Combine dynamically the three scales in porous media

[With T. Costa, A. Trykozko]

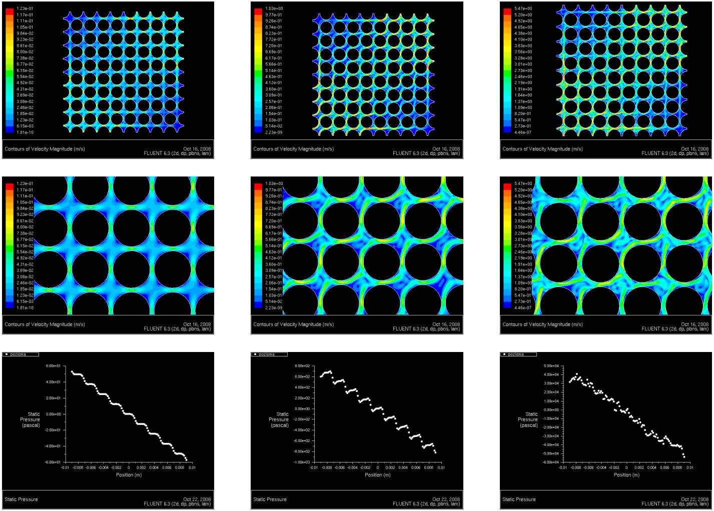






Example: multiscale flow

slow | fast | very fast flow



Standard Darcy model

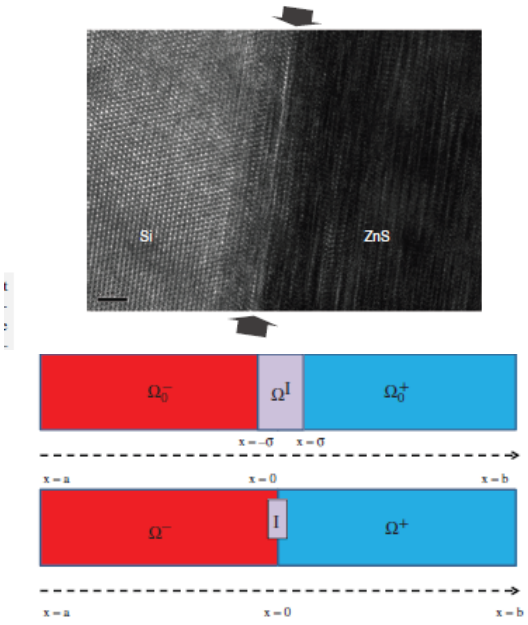
We found a new model (non-Darcy)

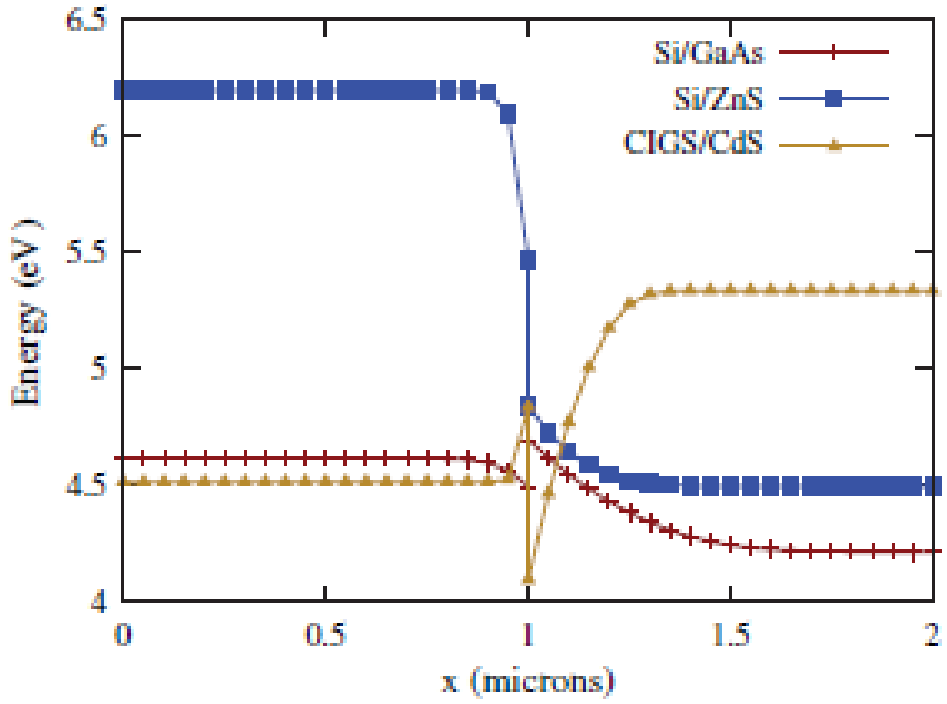
[K. Auguststonʼ06, PTrykozkoʼ2010-, D. Wildenschild (CBE)]

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)
- Delicate physics on interfaces *Heterogeneity Assisted Impact Ionization*
- MAIN ISSUE: how to couple them ?





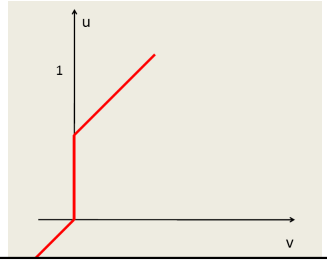
[FCPS'13 [Journal Coupled Systems Multiscale Dyn.] CFP'14,CFP'15 [JCSMD.]]

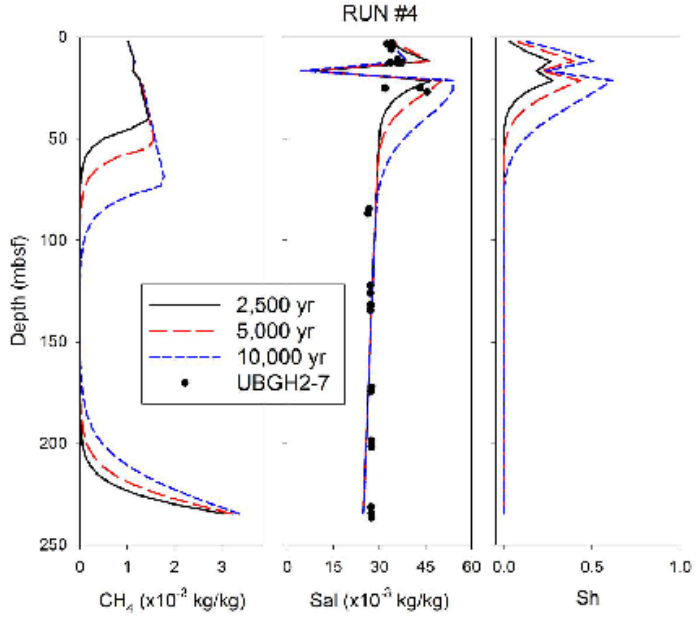
Example: Methane Hydrates

[with P. Medina, R. Showalter, J. Webster, M. Torres, WeLi Hong and others]

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

Recent analysis in *[GMPS'14, PSW'15]*





Current work *[PHT'*]* on $u \in \alpha(S, v); S_t - S_{xx} = 0$

Example: biofilm modeling *[with A. Trykozko, D. Wildenschild et al)]*

Data. . .

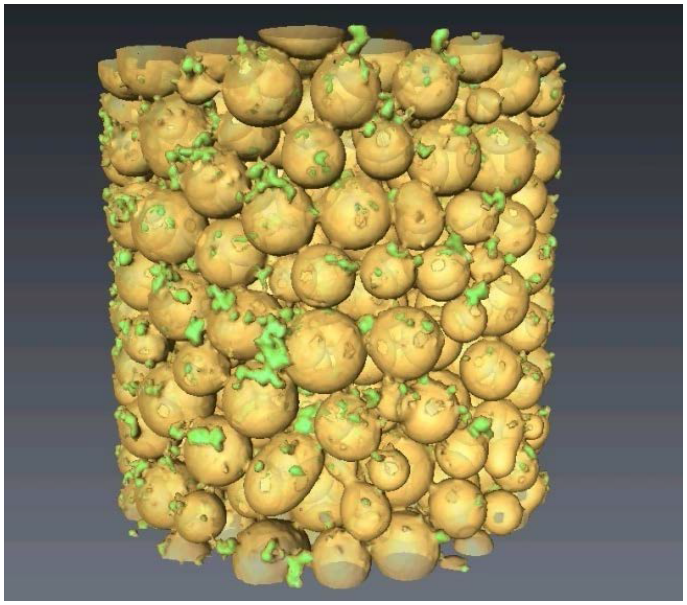
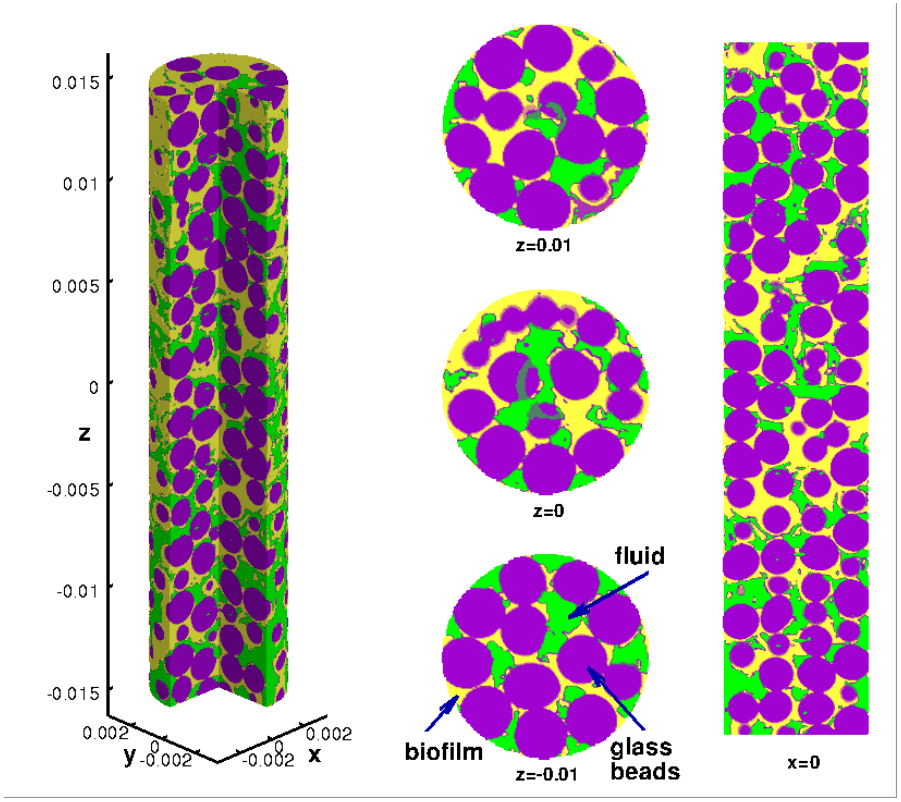


image from Iltis'13



data for computations

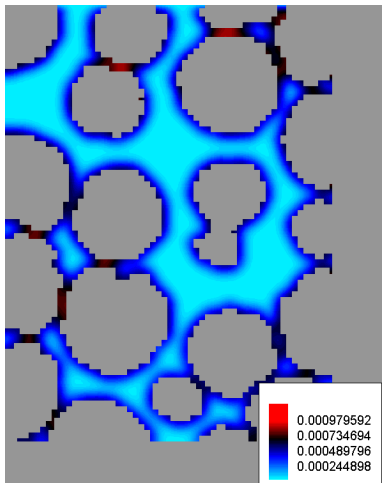
New biofilm model *[PTISW'to be submitted]*

Model and simulations . . .

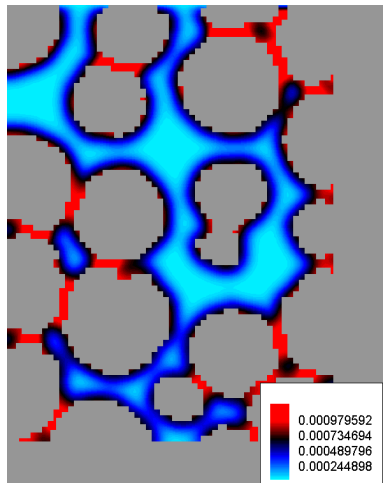
$$
\begin{aligned}
B_t + \nabla \cdot (Bv) - \nabla \cdot (D_B \nabla B) + \Lambda &= F(B,N) \\
N_t + \nabla \cdot (Nv) - \nabla \cdot (D_N \nabla N) &= G(B,N) \\
F(B,N) = k_B B \frac{N}{N+N_0} \quad , \quad & G(B,N) = -k_N B \frac{N}{N+N_0}
\end{aligned}
$$

Challenges:

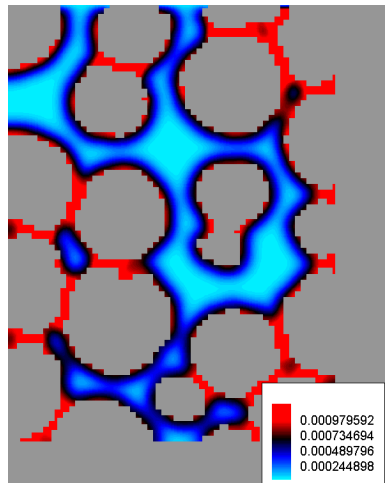
degenerate/singular D_B, D_N, variational inequality associated with Λ



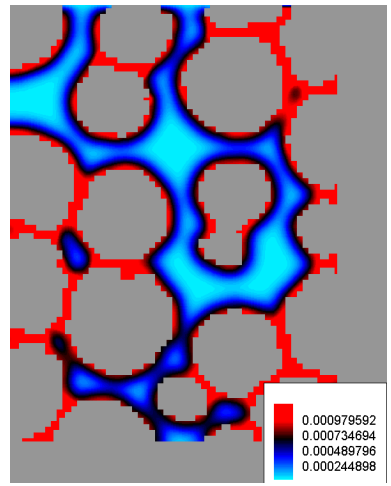
12h



18h



20h

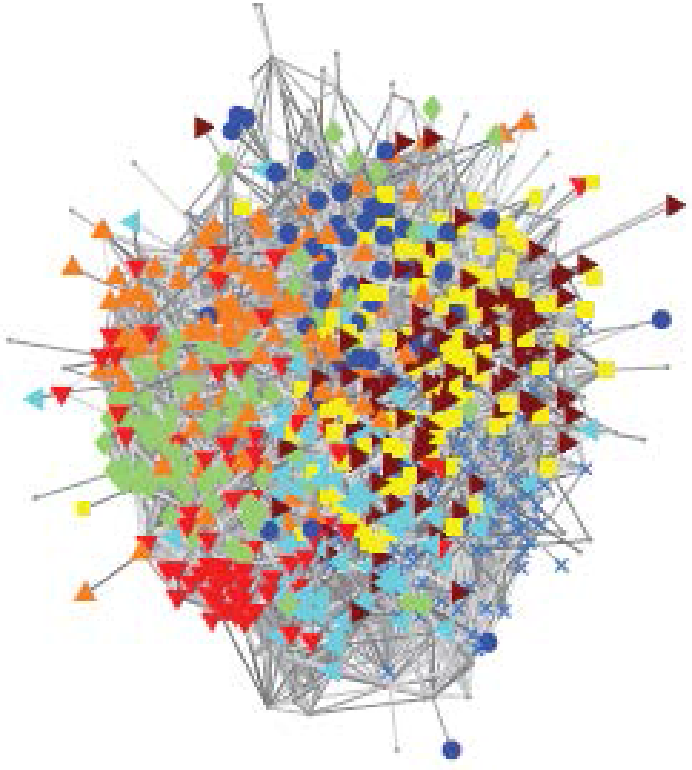


22h

Example: networks and multiscale networks

[Recent work with Masa Prodanovic, Ken Kennedy, Tim Costa]

Many applications and models . . .



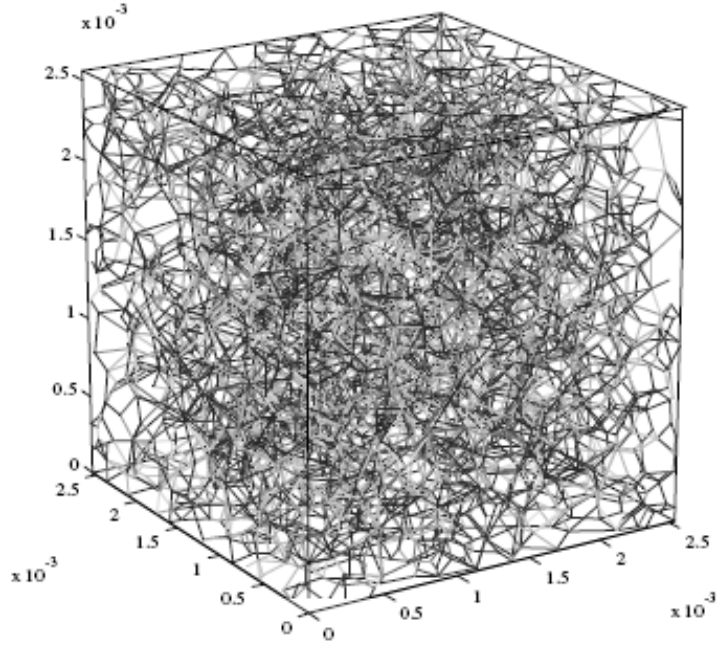
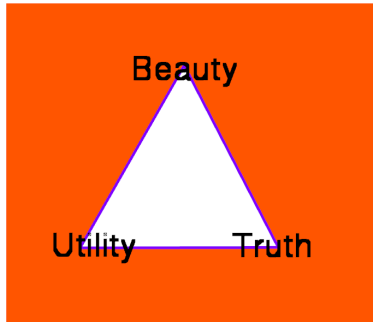


Fig. 5—3D network representation of a water-wet sandstone sample; the network description is courtesy of Statoil. The network dimensions are in meters.

`Social network (SIREV'13)` `pore network`

Funded research projects

Def. GRA := "Graduate Research Assistant". Also, internships.



- Projects contribute
  - to Mathematics itself
  - to other disciplines
  - across disciplines
- Projects aligned with (current) funding[(a)]
  - Porescale modeling
  - Biofilms
  - Hydrates and adsorption
  - Stochastic modeling
- Other projects: e.g., *snow and ice and microbes*
  - Any, as long as $\in \{$ *Modeling, Analysis, Simulation*$\}$

(a) NSF DMS "Hybrid modeling for porous media" and NSF DMS "SOLAR: Enhanced Photovoltaic Efficiency through Heterojunction Assisted Impact Ionization" and NETL projects

Interested ?

- 10,000 hours $\sim$ *Malcolm Gladwell "The Outliers"*
- Hugh Kearns `thinkwell.com` *The Seven Secrets of Highly Successful Research Students*

Modeling + Analysis + Simulation

- Modeling: existing and new models
  - applications: *geosciences, physics, engineering, biology*
  - continuum, discrete, and coupled
- Analysis
  - understanding properties, analyzing well-posedness
- Computation and simulation
  - use/analyze/develop . . . existing/new methods

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

`Interested ?  Email me to meet.`

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