Interdisciplinary Mathematics
= Modeling + Analysis + Simulation

Małgorzata Peszyńska

Department of Mathematics, Oregon State University

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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

![Diagram with points labeled Beauty, Utility, Truth]
Experiments vs Modeling vs Simulation

For continuum models at **macroscale** or **mesoscale**

\[ U_t + A(u) = 0 \]

\[ \text{... need data } A \text{ and more ...} \]

**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. Oren, 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)**
  \[ U_t + A(U) = 0 \]

- **lab=core (meso)**
  \[ u_t + a(u) = 0 \]

- **pore (micro)**
  \[ \frac{d}{dt} \sum_i u_i + a_i \sum_j u_i u_j = 0 \]
Example: adsorption models \cite{Peszynska11}

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

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]

\[ u_t + v_t + u_x = 0; \quad v \in g(u, u_t) \]

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

experiments ... or continuum models [PShowalter'97]... or discrete models [P'11-12]
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. Augustston’06, PTrykozko’2010-, 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 $\psi$)
- 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

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

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 . . .

\[
B_t + \nabla \cdot (Bv) - \nabla \cdot (D_B \nabla B) + \Lambda = F(B, N)
\]

\[
N_t + \nabla \cdot (Nv) - \nabla \cdot (D_N \nabla N) = G(B, N)
\]

\[
F(B, N) = k_B B \frac{N}{N + N_0}, \quad G(B, N) = -k_N B \frac{N}{N + N_0}
\]

Challenges:

degenerate/singular \(D_B, D_N\), variational inequality associated with \(\Lambda\)
Example: networks and multiscale networks

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

Many applications and models . . .

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 $\in \{\text{Modeling, Analysis, Simulation}\}$

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(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 ~ 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]