Modeling and Simulation (Breakout #2, Thursday am)

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participants (6):

Artie Kressner (ConEd/Columbia)

Steve Phillips (AT&T Research): CS in conservation biology, statistical modeling

Maria Ilic (CMU): modeling/control electric power grid, center for smart grid research CMU, systems level integration

Youssef Marzouk [moderator/scribe] (MIT): energy conversion, inverse problems in the environment, uncertainty quantification and decision-making under uncertainty

Pierre Deymier (Univ Arizona): former life = atomistic modeling of materials, multiscale approaches, cellular systems; directs "school of sustainable engineered systems" (SSES)

Neo Martinez: directs Pacific Eco-informatics And Computational Ecology Lab (PEACE lab); ecologist, simulates ecological networks

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Briefing points

1) Answer what-ifs via simulation. ConEd example (Artie Kressner). Ecological networks. Put results in games (WoW, SimCity).

2) data-driven/identified models (prob graph model) versus first-principles modeling (Schrodinger? Navier-Stokes? Newton's laws)

   Common goal = *Predictive modeling*: correlations to mechanisms to predictions?
   And to *actions*!

   How well do mechanisms need to be understood? Interpolatory versus extrapolatory? Outside the realm of historical data. Predictive = ability to extrapolate (accurately?)

  how to integrate data-driven/identified models with first-principles

modeling;
advantages of each, of putting them together.

3) Simulation ==> action and decision.

Need answer that is "better than a guess." How good/reliable of an answer do you need? How much uncertainty is okay. Quantify uncertainty im model predictions to drive methods for decision-making and planning.

Visualization and
communicating the results of simulation.

- Need to put researchers (simulation scientists) in the same room as the people with the problems. Need the right people in the room. Need time.

4) SCALE and BOUNDARIES

- Issues of scale: diverse language here:

- Phase changes and emergent behavior: blackouts in electric power grid; phase change in materials; small-scale rules lead to large-scale changes. From eating rule of an organism to the overall behavior of an ecosystem.

- Multiscale: correlation in space *and* in time

- Multiphysics (where do different contexts meet?). "Mixed excitation." Interactions between different media/networks.

- Boundaries: do you consider economic factors? Things from outside?

features to describe structure: cross-scale coupling, consistent embedding (spatial/temporal), {"multiphysics" / "multi-domain" / "multi-context" / "multi-platform"}, upscaling and downscaling

- Tools: Can one identify structure of the problem (e.g., time scale separation) and map it to the *right* simulation tools?

5) COMPUTING INFRASTRUCTURE, BROADER INFRASTRUCTURE---

- do needs of simulation for sustainability drive computing infrastructure in a particular direction?

--> need sensors and sensor networks

--> "computational sensing" = solve an inverse problem. How much information do you want from inversion? What do you actually need to measure? Minimal sensing networks.

--> Design the sensors that will help us solve that problem. Let science drive *what* we measure. Avoid making a bad problem (drowning in data) bigger!

--> usability (big machines are not enough)

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Actual notes from discussion:

- exchange between very different fields has led to transformative fields and new processes: "disease" of an electric network; statistical tools; control group

- ConEd: created "vertical slices" based on historical data: *what if* you had replaced this or that at some point in the past, or performed a stress test, would that have led to better outcomes in the present? Did not actually do the experiment, but created a slice through historical data to mimic having done it.

- Look at patterns from data

- More "what ifs" via simulation: As simulations become more accurate and comprehensive, incorporate them into games (SimCity, WoW, etc): so people can understand the results and make decisions, play out interdependence.

- Research area that needs to be tackled: integrate data-driven/identified models versus first-principles modeling; advantages of each, of putting them together.
  --> Good for *integrating* models
  --> Weather correlated to

- Defining model versus simulation; Schrodinger/NS versus computational implementation/expression of it

- Model could be PDEs; could also be probabilistic (Bayesian network)

---> CS issues: how to incorporate dynamics into probabilistic models; frequencies that the model can capture?

- *Predictive modeling*: correlations to mechanisms to predictions?
   And to *actions*!
   How well do mechanisms need to be understood? Interpolatory versus extrapolatory? Predictive = ability to extrapolate (accurately?)
   -- species distributions: everyone wants to extrapolate (new climate conditions, etc)

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BETTER-THAN-A-GUESS
(UNCERTAINTY, FIDELITY)

- Answer that is "better than a guess"
- Simulation leads to a decision.

Correlation to mechanism to prediction to action

Visualization!!!

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MATCHING TOOLS TO PROBLEMS

- General
- Identify structure of the problem (e.g., time scale separation) and map it to the *right* simulation tools.

features to describe structure: cross-scale coupling, consistent embedding (spatial/temporal), {"multiphysics" / "multi-domain" / "multi-context" / "multi-platform"}, upscaling and downscaling

How to design man-made system (e.g., grid, water system) so that you can sustainably manage an ecological resource. Need to have the right knobs, intelligence, switching capacity. Different switches for different resources and users.

Elena Rostrum?

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SCALE

- Issues of scale (coarse-graining)

- Phase changes and emergent behavior: blackouts in electric power grid; phase change in materials; small-scale rules lead to large-scale changes...

- Multiscale: correlation in space *and* in time

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- Multiphysics (where do different contexts meet?). "Mixed excitation." Interactions between different media/networks.

- Defining *boundaries* of the system: do you consider economic factors? Things from outside?

- Climate: multi-network systems

- Are these *complex systems*

- Model comparison: multipe models for same purposes

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TECHNOLOGIES AND INFRASTRUCTURE

- do needs of simulation for sustainability drive computing infrastructure in a particular direction?

--> need sensors and sensor networks

--> "computational sensing" = solve an inverse problem. How much information do you want from inversion? What do you actually need to measure? Minimal sensing networks. A

    --> Design the sensors that will help us solve that problem. Let science drive *what* we measure. Avoid making a bad problem bigger!

--> usability (big machines are not enough)

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EXERCISES:

- Need to put researchers in the same room as the people with the problems. Need the right people in the room. Need time.

SRC = semiconductor research corporation

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ADDITIONAL INPUT FROM ANOTHER PARTICIPANT OF THE GROUP:

Sustainability is, to a large extent, about designing and implementing better human-environment interactions.

Simulations are very useful to the understanding, decision making and education needed to achieve this aspect of sustainability

There is a general need for simulations to integrate and generate multi-scale understanding.   We have better and better models that discover and describe mechanisms key to the behavior of systems at different scales. However, this understanding at restricted scales (and from restricted perspectives) has yet to be integrated to the point of simulating, for example, the effects of a farmers operations choice (organic or conventional?) to the income and employment of people in the fishing industry. To do that, on needs to connect knowledge of agriculture with that of watersheds, with that of oceans with that of resource economics of fishing.

While pursuing this, simulations have to accommodate disciplines that are at various locations on the scientific spectrum from correlation to mechanism to prediction to action. These latter areas of prediction and especially action requires significant advances in the visualization and communication of simulations and their results. Gaming can provide a major contribution to this.

Communication brings up a final point addressing the interdisciplinary aspects of multi-scale understanding.   The same words have very strong and very different definitions in different disciplines.   Different disciplines also have very importantly different world views, goals, and senses of priorities. Focused analysis and understanding is needed to address this critical challenges of communication among disciplines needed to generate larger integrated multi-scale understanding of the interconnected systems that determine human sustainability.

ps.. science usually reacts to developments in sensor technologies but rarely gets a chance to direct such developments towards that which is more scientifically productive. therefore, major advances in sensor technologies would emerge from asking scientists what data they need and then going out and designing those sensors.