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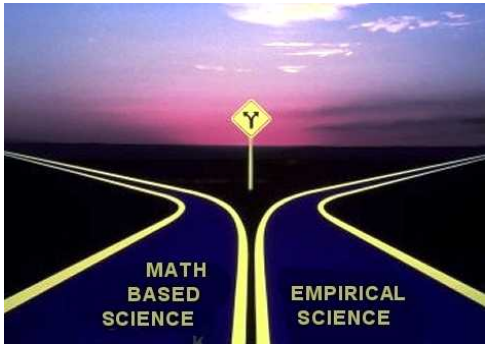

Model/Use Characteristics that Can Challenge Current VVUQ : Building Credible Models

June 22, 2016

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U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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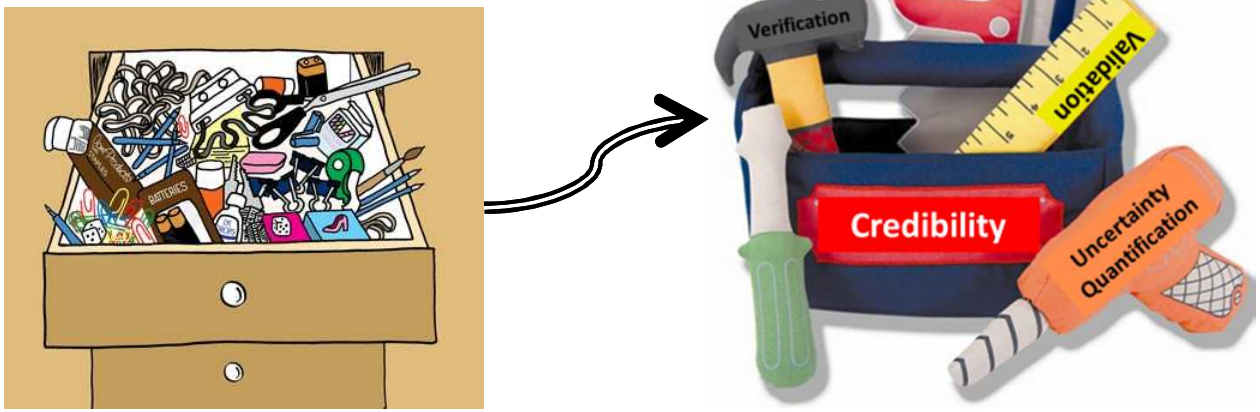
Outline

- Modeling process
- Characteristics of complex systems
- Purpose of VVUQ in modeling complex systems
- Model uses for complex systems
- When can modeling challenge current VVUQ?
- Opportunities for further research
- Summary



Modeling process

Model use as well as validation will likely lead to refinement or even new generation of problem questions

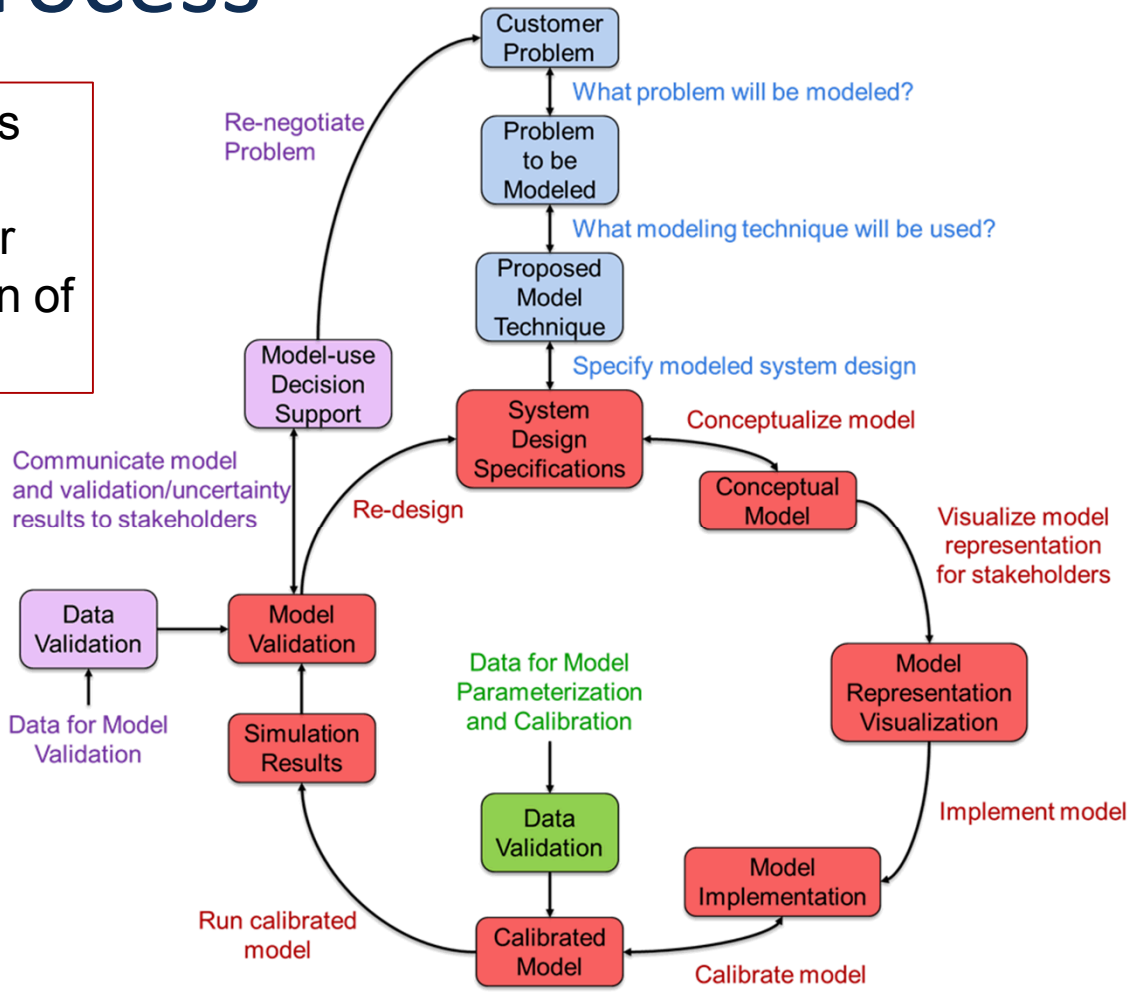


*Diagram is a modification of Balci modelling process diagram (Balci, 1998).

Modeling is an iterative process to build confidence and understanding.

Model uses

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According to Shannon (Shannon, 1975)

- Evaluation of system behavior
- Forecasting
- Comparison of different operating policies
- Optimization
- Sensitivity analysis
- Determination of functional relationships
- Training

Formal model validation

$$E = S - D$$
$$E = (T + \delta_S) - (T + \delta_D) = \delta_S - \delta_D$$
$$E = \delta_{\text{model}} + \delta_{\text{numerical}} + \delta_{\text{input}} - \delta_D$$
$$\delta_{\text{model}} = E - \left(\delta_{\text{numerical}} + \delta_{\text{input}} - \delta_D\right)$$
$$u_{\text{validation}} = \sqrt{\delta_{\text{numerical}}^2 + \delta_{\text{input}}^2 + \delta_D^2}$$
$$\text{if } |E| \leq u_{\text{validation}} \text{ then "valid"}$$

Formal validation: compare simulation results with experimental or observational data

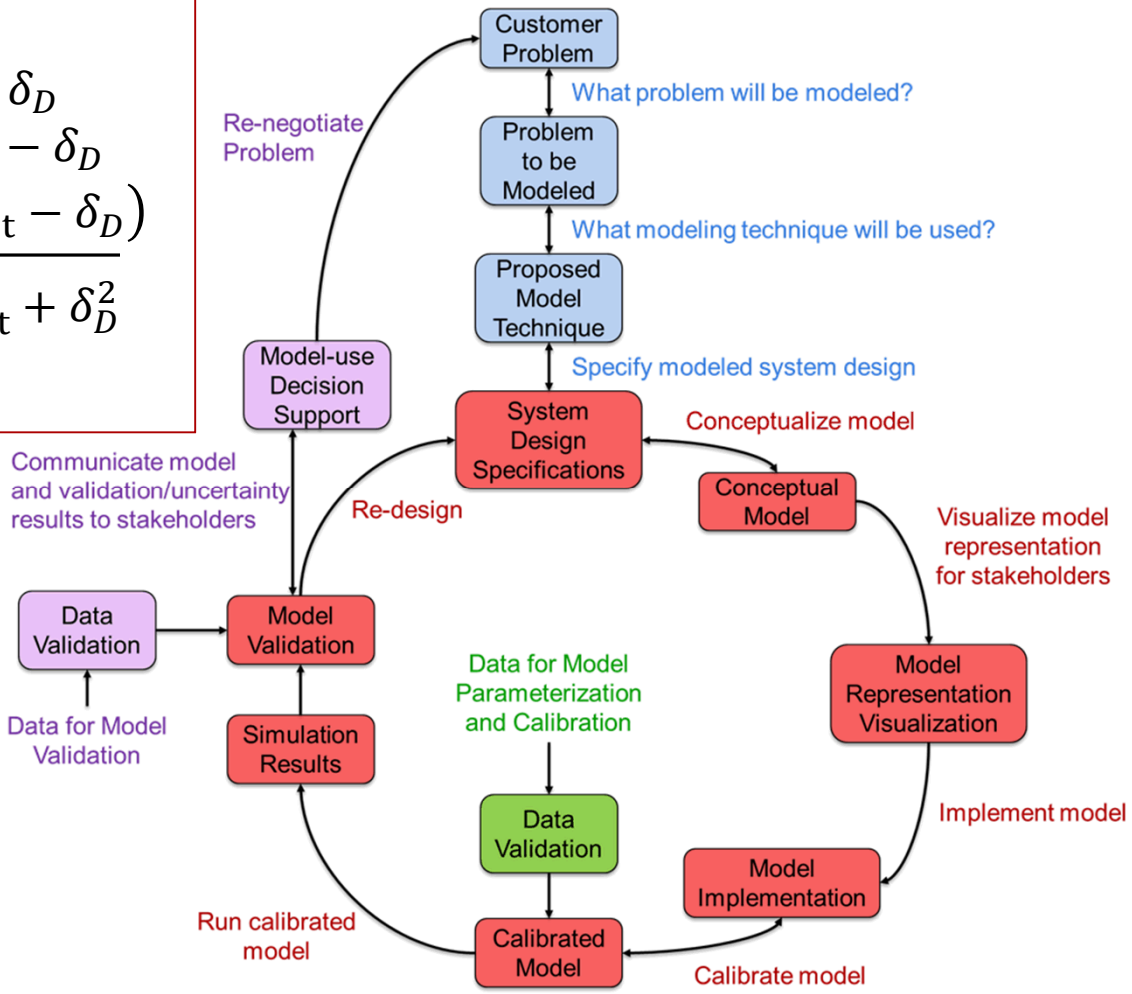

*Diagram is a modification of Balci modelling process diagram (Balci, 1998).

Model error within noise level imposed by numerical, parameter input and experimental data uncertainties → "valid".

Characteristics of complex systems

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- adaptive or self-organized behavior
- high throughput
- heterogeneity of subcomponents
- multi-scale interaction
- bifurcations and phase change
- cascading and/or emergent behavior
- synergistic components
- feedback loops
- non-linearity
- humans in the loop
- lack of established theory and/or unknown basic physical laws
- feedback from model to system
- inability to conduct experiments, lack of data and/or low signal-to-noise
- reliance upon soft quantity data
- out of equilibrium
- results and assessment focus on dynamics or dynamical behavior
- reductionist approach is inappropriate (irreducible)
- open system
- imbalanced information exchange
- exhibits power laws
- multi-objective behavior
- non-locality
- complementary quantities of interest
  - Heisenberg uncertainty principle
- inability to specify closed-form description but can be simulated
- potentially unpredictable
- social dynamics

List is incomplete, non-orthogonal and not definitive or universally agreed upon.

Purpose of VVUQ in modeling complex system

- Continue to use formal validation where possible
- Build confidence in modeling process where formal validation cannot be applied

Includes stakeholders and potential stakeholders

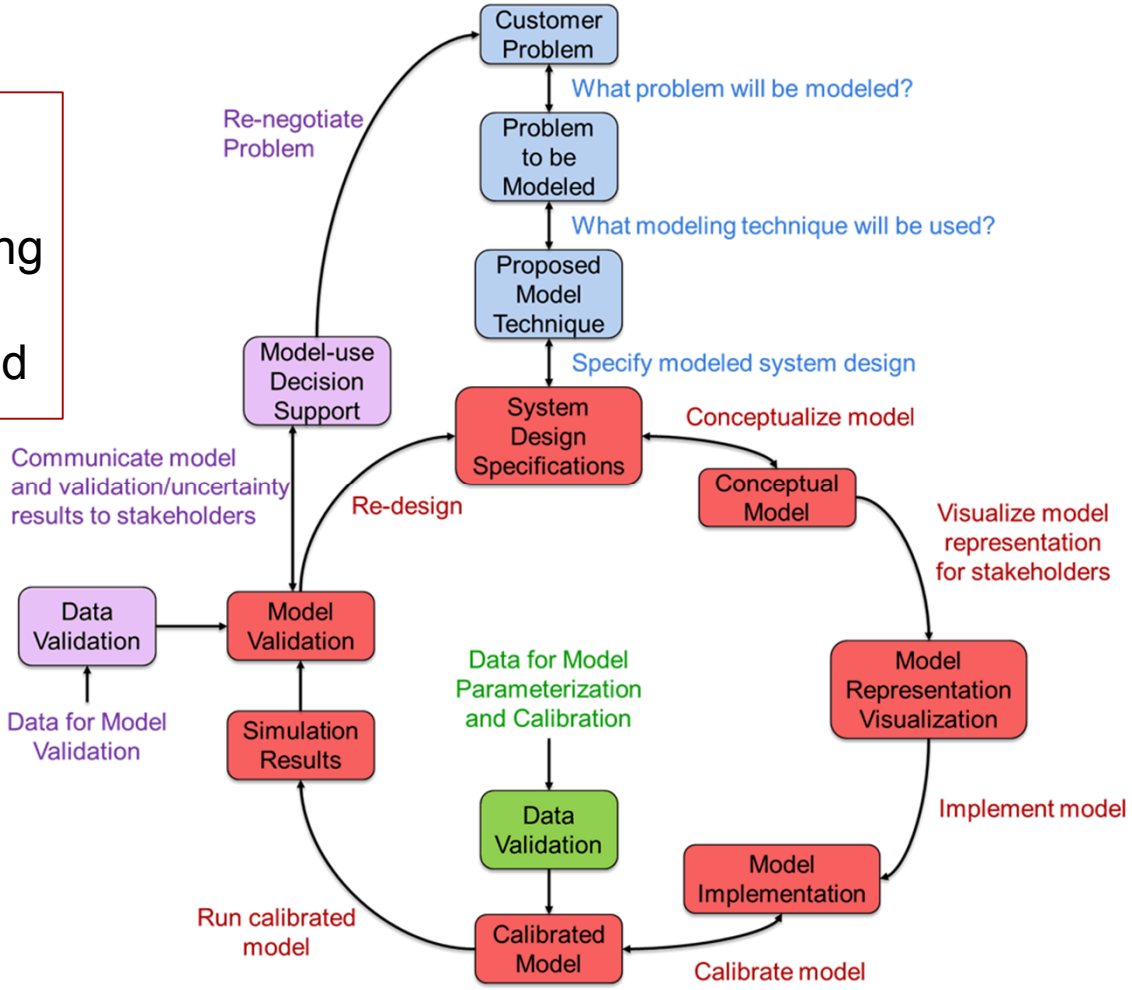

*Diagram is a modification of Balci modelling process diagram (Balci, 1998).

Understand and quantify credibility in the use of complex systems modeling approaches with respect to a particular use.

Model uses for complex systems

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Key model/use factors to be addressed

- What is the question of interest (knowledge of interest)?
- Which model is appropriate for answering this question?

Potential model uses

- Prediction
- Policy exploration
- Risk analysis
- Empirical demonstration of system theory
- Scientific exploration of alternate system theories
- Real-time operation (feedback & control)

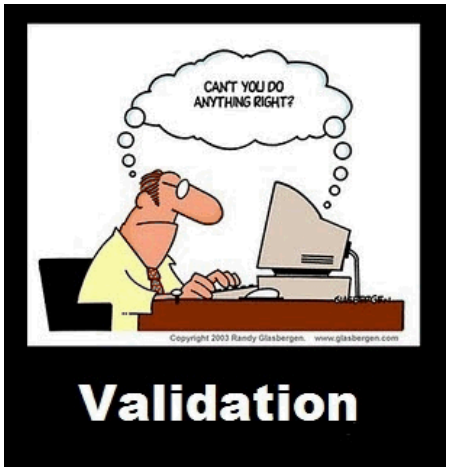
Model/use credibility

- Do we have the right model for our intended use?
  - Engineered systems – "Assurance that a product, service, or system meets the needs of customers and other identified stakeholders"
  - Software – "Process of evaluating software design and implementation to determine whether it satisfies specified requirements"

ISO/IEC 15288

IEEE SA 1012

- Are we asking the right question of our model?
  - Customers do not always know what they want
  - Customers need Y but ask for X
  - Have model Z that we want to apply
  - Want to research/build model W



Quote from Swiler, 2016.

"Perform due diligence and communicate frankly about assumptions, approximations, and limitations affecting simulation credibility."

Prediction is hard:

- *Limited* physical data (observational or experimental)
- *Limited* simulations (high computational demands…)
- *Imperfect* computational models (missing physics, etc.)
- *Under-resolved* approximations or numerics
- *Unknown* model parameters and boundary conditions
- *Imperfect* humans
- We want to *extrapolate* to conditions beyond validation regime…

Slide from Swiler, 2016.

When can modeling challenge current VVUQ?

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- Limited (observational or experimental) data
  - Modeled system is unpredictable
- Additional data challenges
- Imperfect models
  - Computation and/or physics
  - Complex behavior dynamics
- Limited model simulations (time & cost)

Current approaches to assess model credibility

- Limited data
- Additional data challenges
- Imperfect models
- Extrapolating beyond validated (validate-able) regime

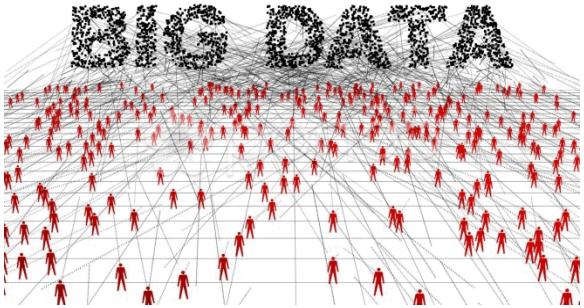
Limited data

- inability to conduct experiments
  - detonate “dirty bomb” in NYC
  - natural disaster
- imbalanced information
  - stealth
  - one-sided learning
- Modeled system is unpredictable

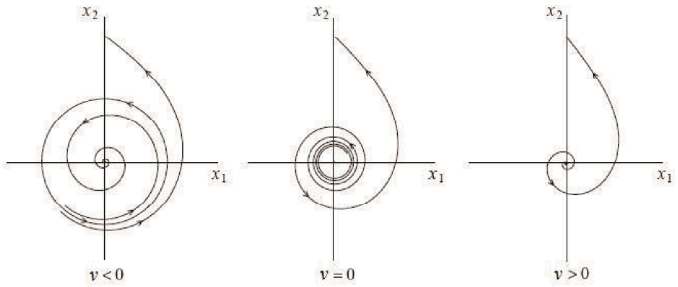
Need to understand potential effects we cannot create ourselves.

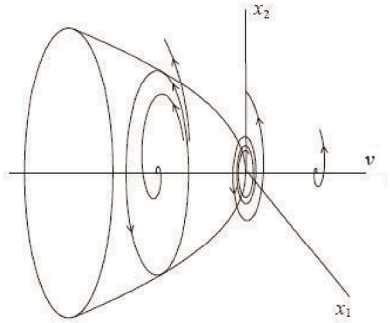
Additional data challenges

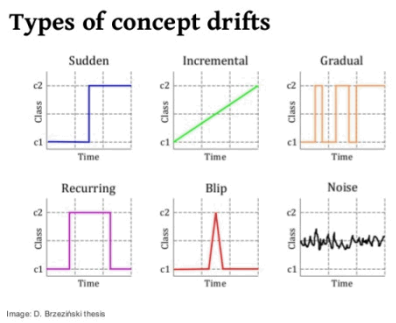
- Data quality
- Dimensionality
  - heterogeneity of subcomponents
- Too much data
  - multi-scale interactions
  - low signal-to-noise
- Continuous dynamic data
  - bifurcations and phase change
  - out of equilibrium



- Volume
- Velocity
- Variety
- Value
- Visibility







Imperfect models

Computation and/or physics

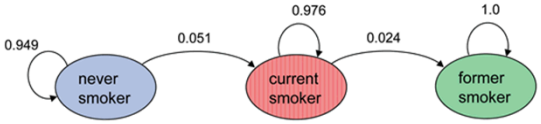
- non-linearity
- synergistic components
- open system
- reductionist approach is inappropriate (irreducible)
- lack of established theory and/or unknown basic physical laws

Exploratory modeling

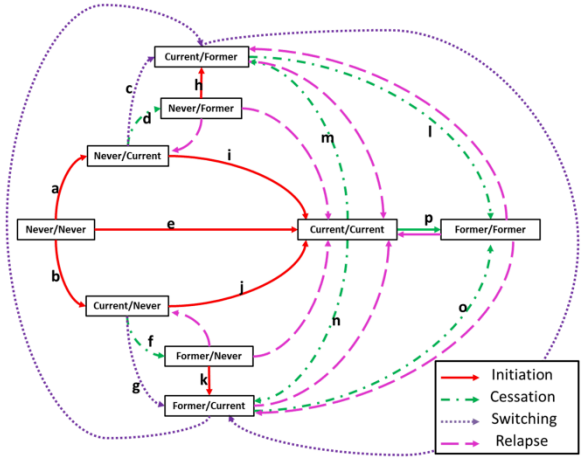
Complex behavior dynamics

- adaptive or self-organized behavior
- cascading and/or emergent behavior
- multi-objective behavior
- social dynamics
- humans in the loop

Re-negotiate problem



Verzi et al., 2012.



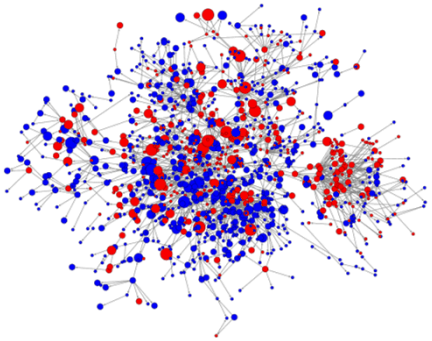
Vugrin et al., 2015.

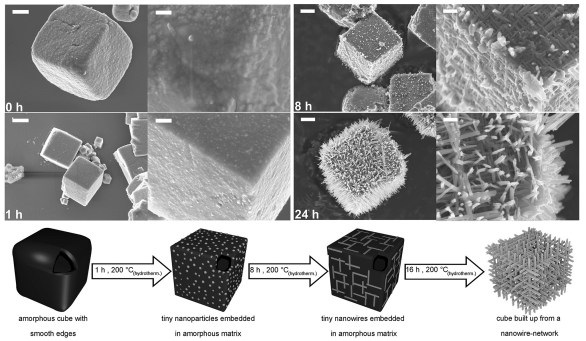
Limited model simulations

- high throughput
  - turbulent flow

- complex behavior dynamics

  {cascading, emergent, self-organized, multi-objective, adaptive}
  - self-organizing materials
  - social dynamics



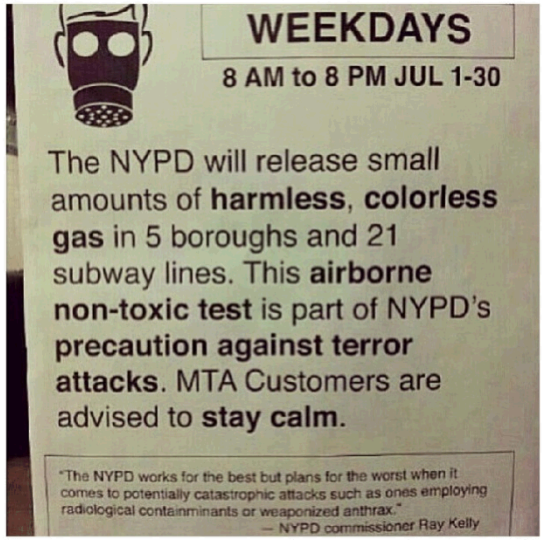


Need to understand potential effects that are too expensive to simulate completely (a large number of times).

Current approaches to assess model credibility

Limited data

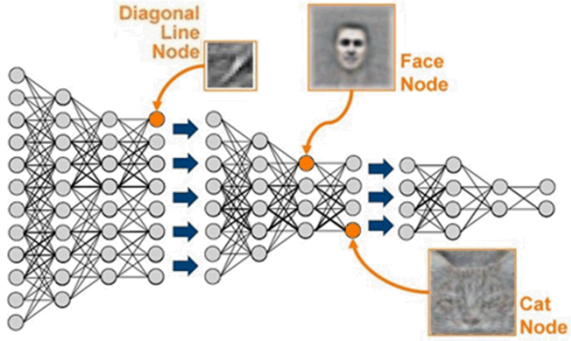
- Find surrogate source
- Simulate it
  - Use known data to design generative model
  - Use micro scale model to generate macro scale data
- Conduct our own experiment
  - Small sample size – biased?
- Survey subject matter experts (SMEs)
- Model without it
  - Use “best guess”

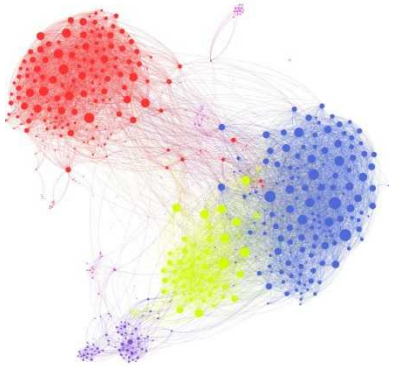


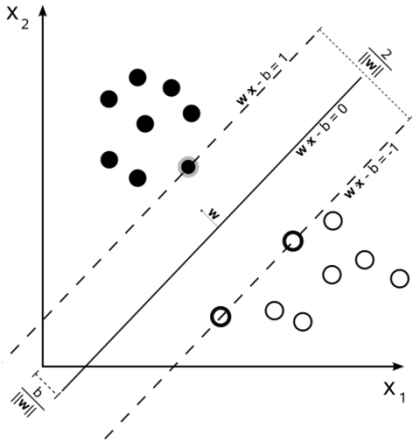
Current approaches to assess model credibility

Additional data issues

- Data quality V&V
- Dimension reduction
  - Feature extraction – deep learning
  - Principle components analysis
  - Compression
- Data clustering
- Machine learning







Current approaches to assess model credibility

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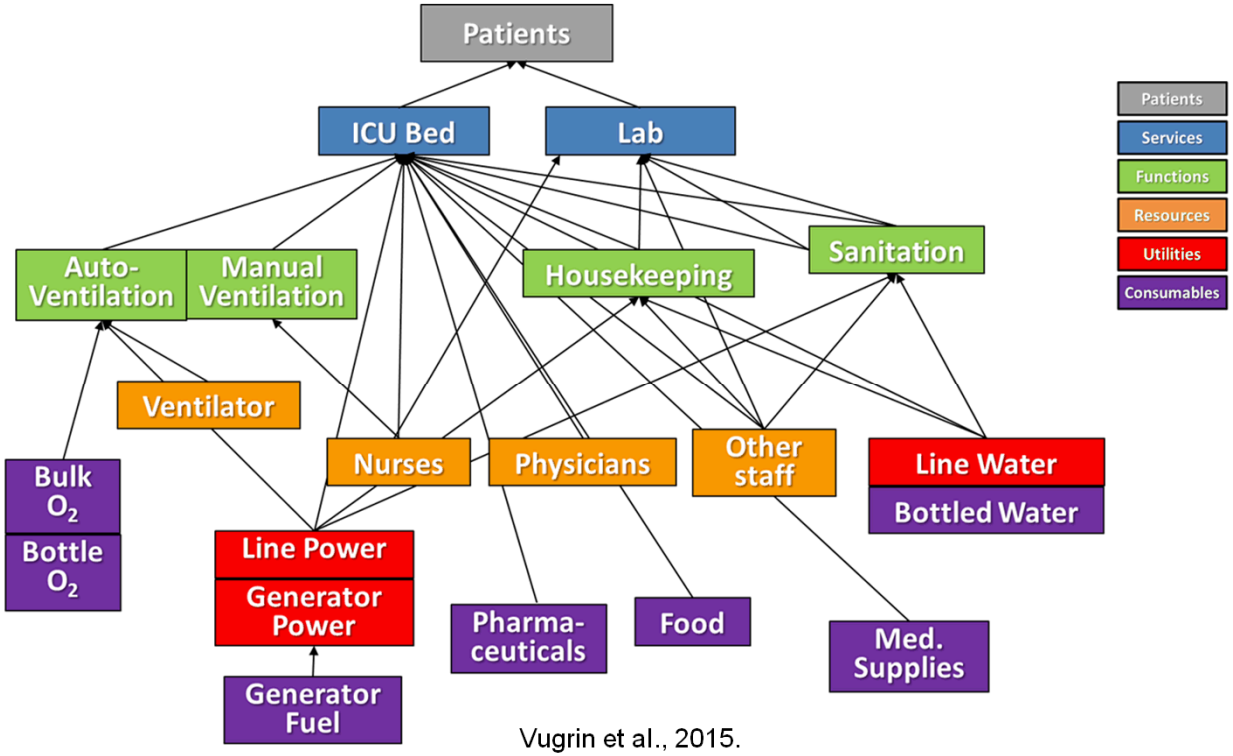
Model representation visualization

Imperfect models

- Adaptive resilience in hospital ICU



Vugrin et al., 2015.

Work with customers to derive insights from model for adaptive substitution and to build credibility by recreation of historical event.

Current approaches to assess model credibility

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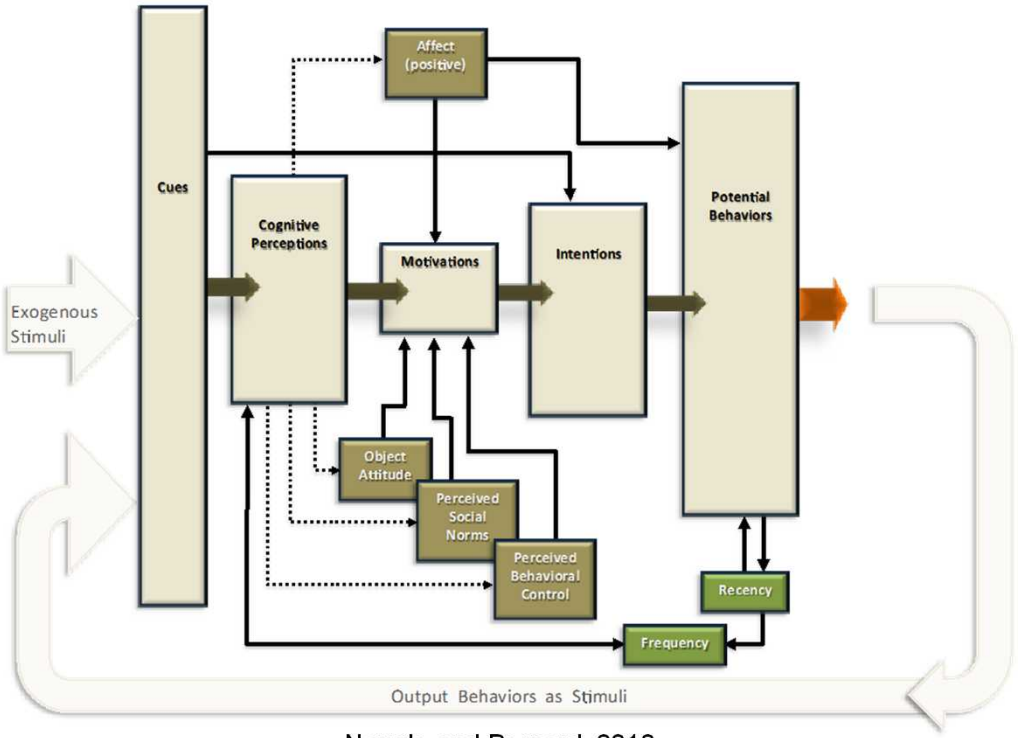
Model representation visualization

Imperfect models

- Complex socio-cognitive behavior



Naugle and Bernard, 2010.

Work with customers/stakeholders to derive insights from modeling process and to understand modeled behavior equations.

Current approaches to assess model credibility

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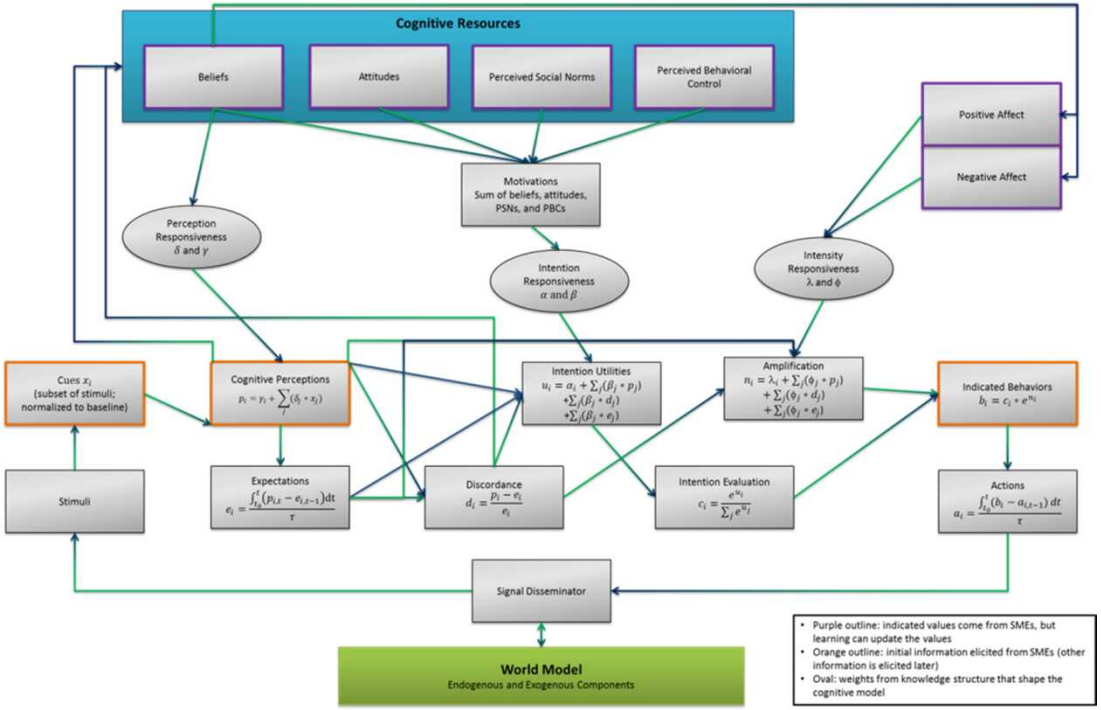
Model representation visualization

Imperfect models

- Complex socio-cognitive behavior



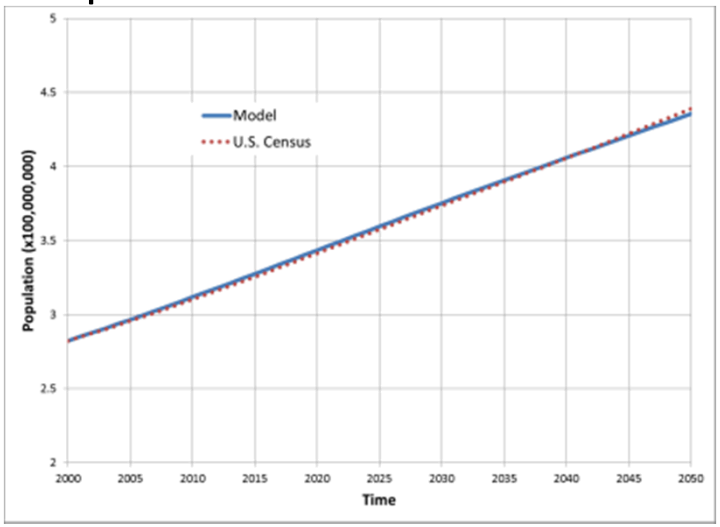
Naugle and Bernard, 2010.

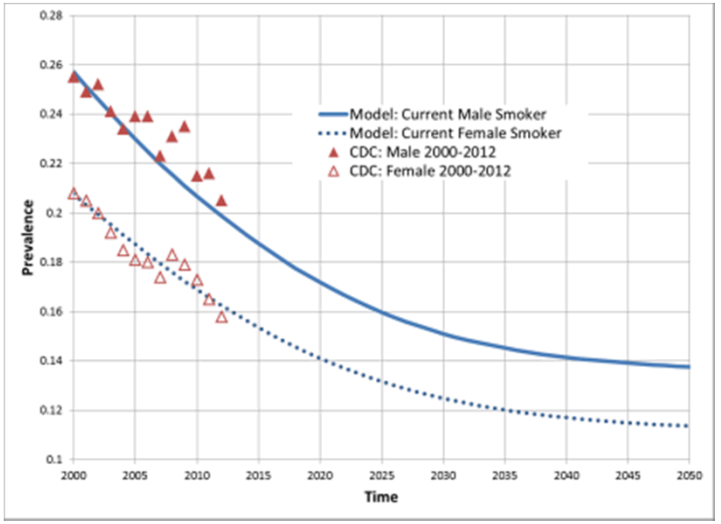
Work with customers/stakeholders to derive insights from modeling process and to understand modeled behavior equations.

Current approaches to assess model credibility

Extrapolating beyond validated (validate-able) regime)

- Model-to-model comparison
  - docking
  - co-validation (model verification)
- Independent review
  - subject matter experts
  - peers

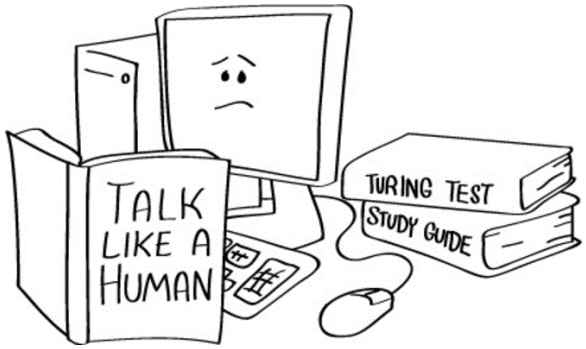




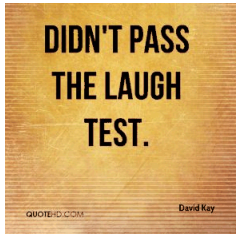
Vugrin et al., 2015.

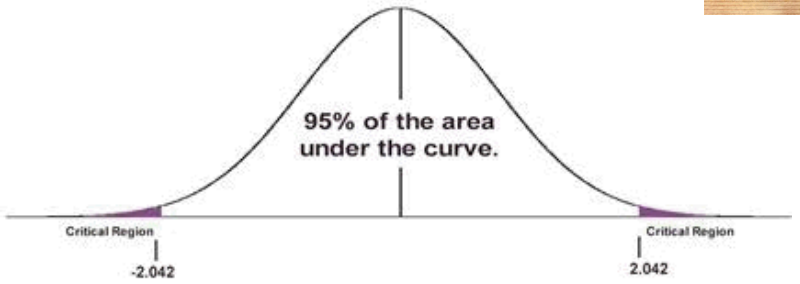
Opportunities for further research

- Lack of data
  - Use analogous, synthetic or expert-elicited data
  - Reproduction of
    - system theory
    - phenomena
    - behavior



- Extending model credibility
  - Face validation
  - Turing test
  - Extreme-value testing





Summary

- Modeling process
- Complex systems modeling characteristics
- Goal: understanding and quantifying model credibility
- VVUQ gaps
- Current approaches
- Opportunities

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Thank you

- Questions?

Backups

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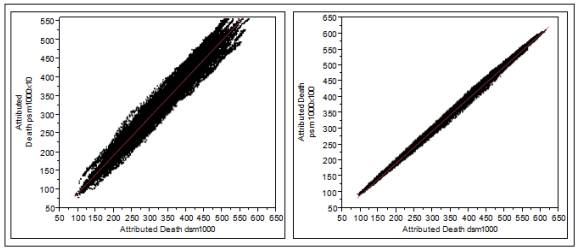
Dealing with computationally intensive model simulations

- Employ more tractable mathematical/model representation (use an emulator)
  - continuous ←—→ discrete
  - mean behavior ←—→ individual behavior
  - use (very) complicated (not complex) modeling approach

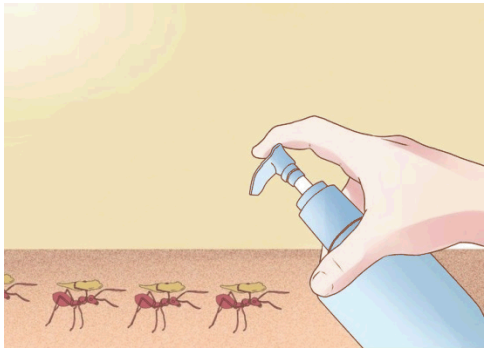


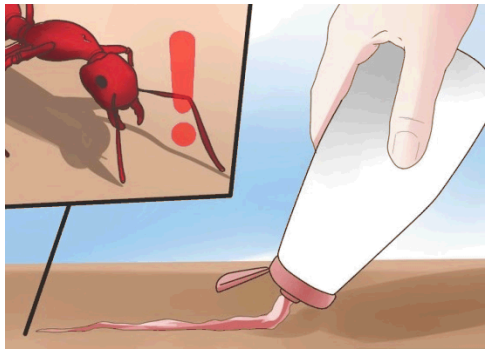
- Buy a bigger/faster computer

Modeling Interventions

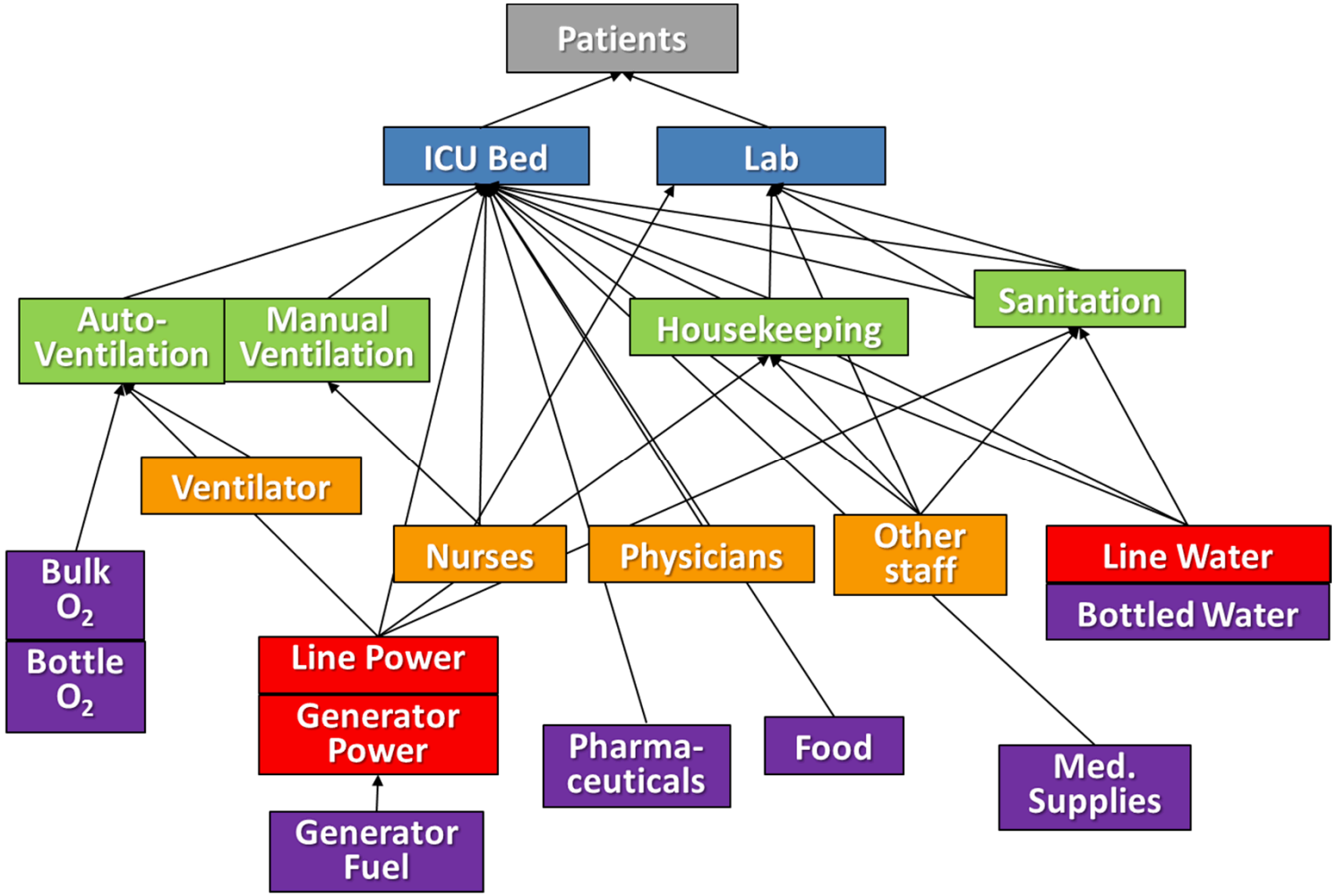
Example:

- Want to keep ants outside
- Possible interventions
  - Attempt to kill them
  - Build a barrier
  - Entice them to stay outside
  - …
  - Combinations
- How detailed does the ant model need to be?
- Can it be validated?





Hospital ICU resilience




Verification
Validation
Credibility
Uncertainty Quantification


Verification
Validation
Credibility
Uncertainty Quantification
Distinguisher