A Computable Approach to Validation

Roger Ghanem

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1. Objectives
2. Inspiration from Elementary Statistics
3. Characterizing Uncertainty
4. Validation Example
5. Panoramic View of My Research
6. Conclusion

Historical Perspective

Aristotle: Event is probable when the majority of the most intellectual persons deem it likely to happen.
Laplace: science of probability as the application of common sense.

Packaging of common sense for use by the most intellectual persons is a moving target that depends on the science and technology of the times.

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D'Alembert	Poincaré	Einstein	Feynman	Von Mises
Legendre	Kolmogorov	Wiener	···	

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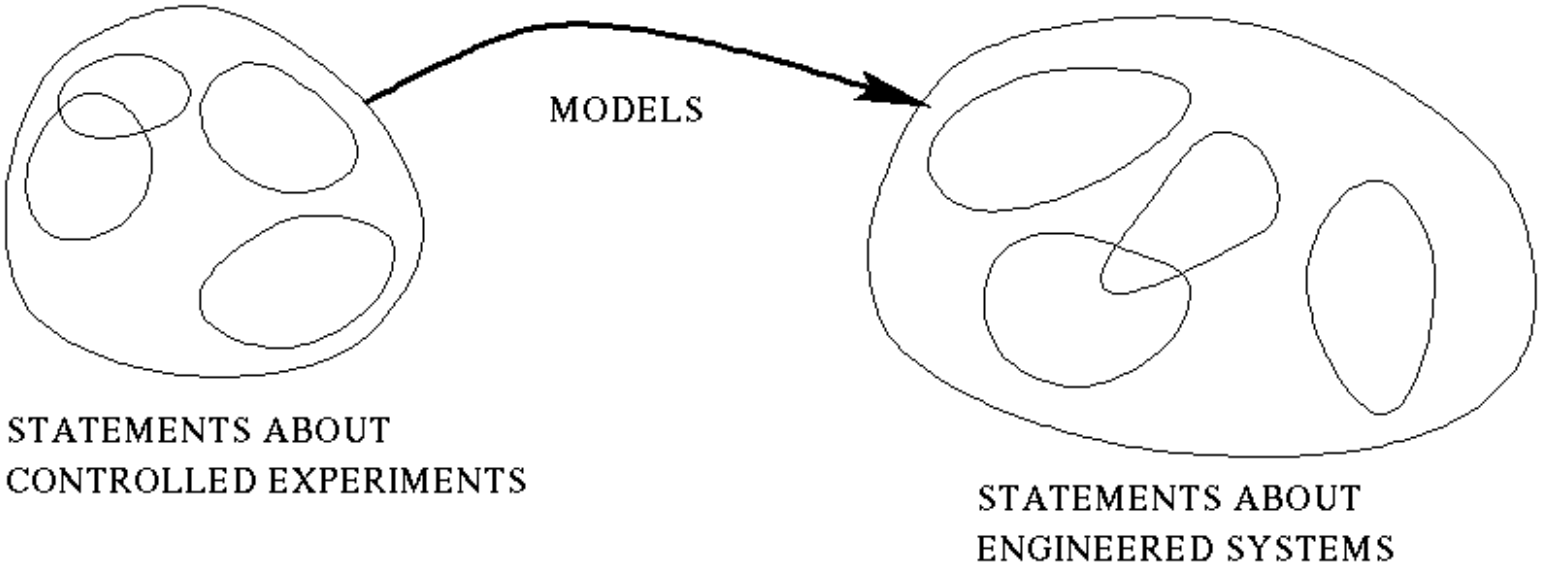
Current Perspective

Packaging of Information for Good Use



Four Components

1. Information
2. Inductive Models
3. Deductive Models
4. Quantities of Interest

- Experiments
- Calibration
- Propagation
- Decisions

Current Influences

- Multiscale Content
- Algorithmic
- Large Scale Computi
- Extreme Consequenc

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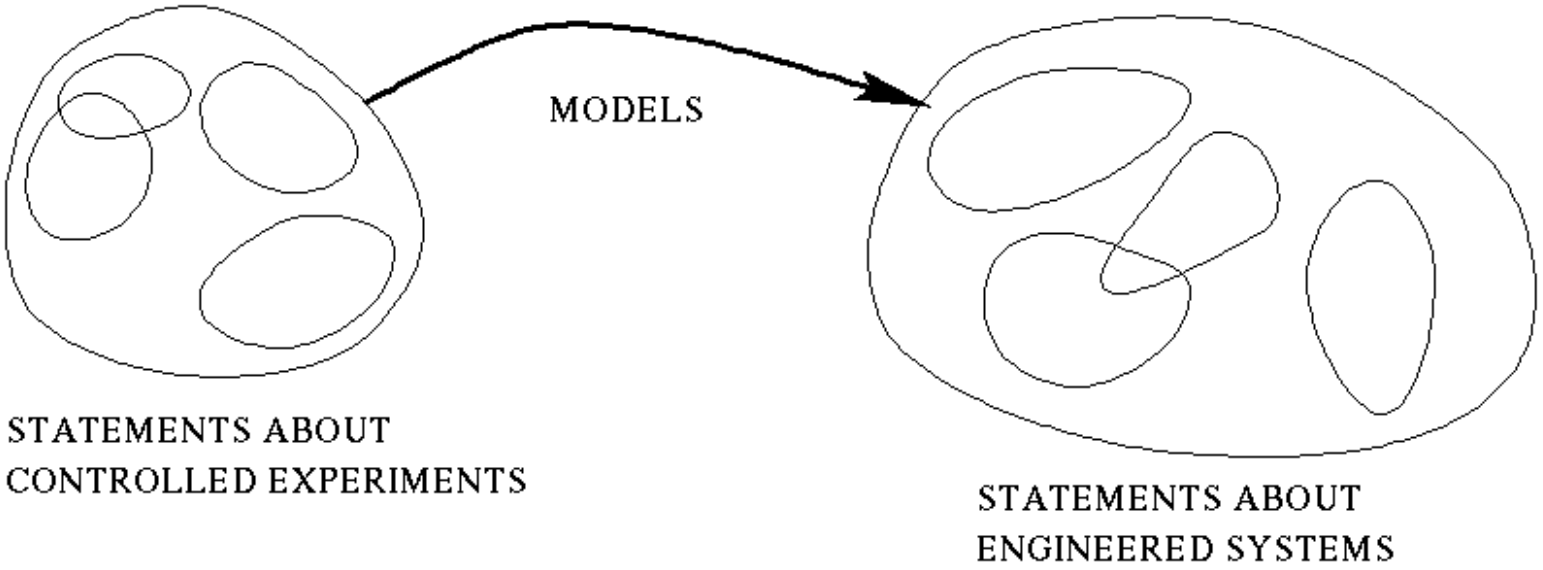

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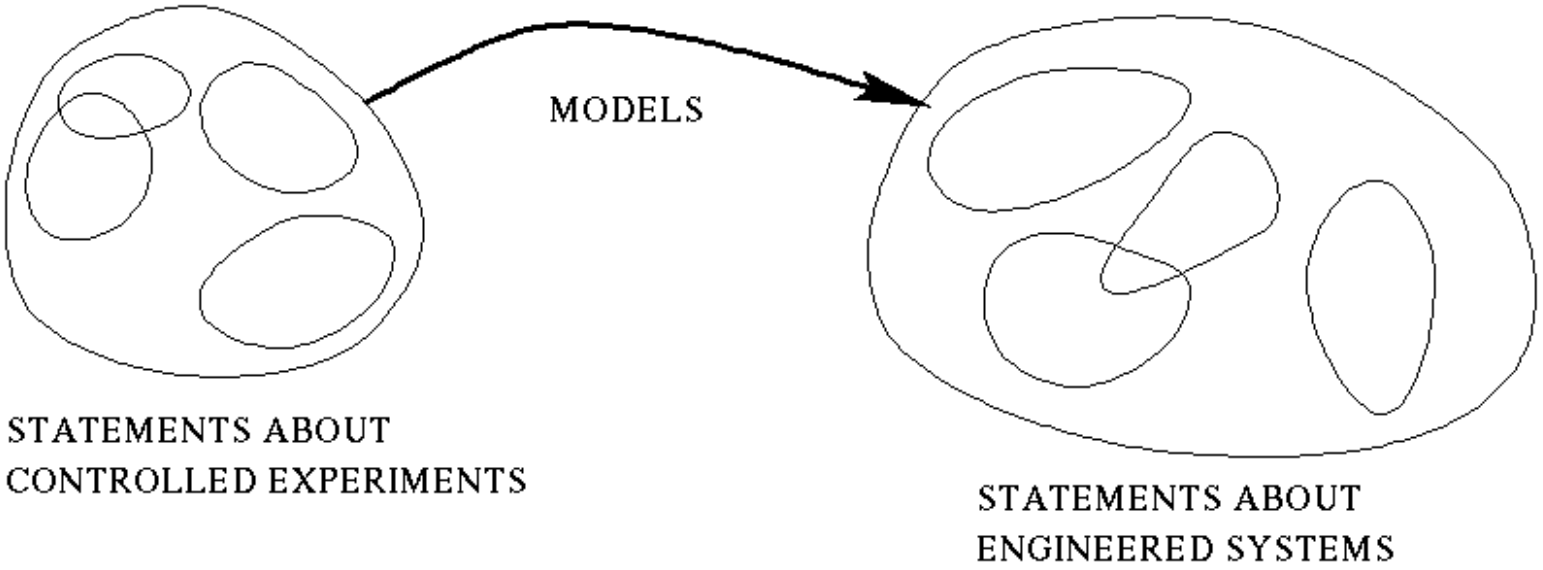

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VERY IMPORTANT !

- Probabilities of events are not properties of a physical system.
- They are conditioned on available information.
- Probabilities change as information changes.
- We want to find the set of knowledge and information required to achieve specified confidence in our prediction.

ALSO IMPORTANT !

- Probabilistic models provides a means to package information for good use.
- There is great freedom in chosing a mathematically consistent yet suitable packaging.

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Develop predictive capability that can be used as surrogate to reality.

Obstacles

- models are incomplete.
- data is incomplete.
- models are resolved with finite accuracy.
- reality itself is incompletely characterized.

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Obstacles

- models are incomplete. modeling error
- data is incomplete. data error
- models are resolved with finite accuracy. discretization error
- reality itself is incompletely characterized. ??

Error Budget

$$U = \hat{U}|_{h,d,p,m} + \underbrace{\epsilon_h|_{d,p,m} + \epsilon_p|_{d,m} + \epsilon_d|_m}_{\text{Limits on Predictability: Must be quantified}} + \epsilon_m$$

$\epsilon_h|_{d,p,m}$: can be reduced through better numerics.
$\epsilon_p|_{d,m}$: can be reduced through better statistics.
$\epsilon_d|_m$: can be reduced through better data.
ϵ_m : can be reduced through better models.

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Simple Example

$$\alpha \sim N(\mu, \sigma)$$

α can be reconstructed from estimates of μ and σ:

$$\hat{\alpha} = \bar{\alpha} + s\xi \qquad \xi \sim N(0,1)$$

Estimates are random variables:

$$\bar{\alpha} = \mu + \sqrt{\frac{\sigma}{n}}\eta \qquad \eta \sim N(0,1)$$

$$\frac{(n-2)s^2}{\sigma^2} \sim \chi^2_{n-2} = \sum_{i=1}^{n-2} \gamma_i^2 \qquad \gamma_i \sim N(0,1)$$

SO:

$$\hat{\alpha} = \hat{\alpha}(\xi, \eta, \gamma_1, \cdots, \gamma_{n-2})$$

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Upscaling:

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- random variables are typically substituted by a list of descriptors
  - statistical moments (discrete list)
  - values of PDF along abscissa points (continuous list)
- these lists have issues:
  - not easy to reproduce the random variable from knowledge of the list
  - items in the list cannot be interpreted in the context of approximation theory (for example as coordinates)
- polynomial chaos decomposition provides a representation for random variable using coordinates in a vector space.

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A Cameron-Martin Theorem

Let $x(t)$ be a Brownian motion, and let:

- $\{\alpha_i(t)\}$ is a CONS in $L^2[0,1]$
- $\Phi_{m,p}(x) = H_m\left[\int_0^1 \alpha_p(t)dx(t)\right] \quad m = 1, 2, \cdots \;\; p = 0, 1, \cdots$
- $\Psi_{m_1,\cdots,m_p}(x) = \Phi_{m_1,1}(x)\cdots\Phi_{m_p,p}(x)$

Then

$$\lim_{N\to\infty}\int_C^w \left| F[x] - \sum_{m_1,\cdots,m_N} A_{m_1,\cdots,m_N}\Psi_{m_1,\cdots,m_p}(x)\right|^2 d_w x = 0$$

The polynomial chaos decomposition of any square-integrable functional of the Brownian motion converges in mean-square as N goes to infinity.

For a finite-dimensional representation, the coefficients are functions of the missing dimensions. That is, the coefficients are themselves random variables dependent on the dimensions excluded from the representation.

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Polynomial Chaos

$$\alpha(x,\theta) \quad = \sum_{i=0}^{\infty} \alpha_i(x)\ \Psi_i(\boldsymbol{\xi}(\theta))$$

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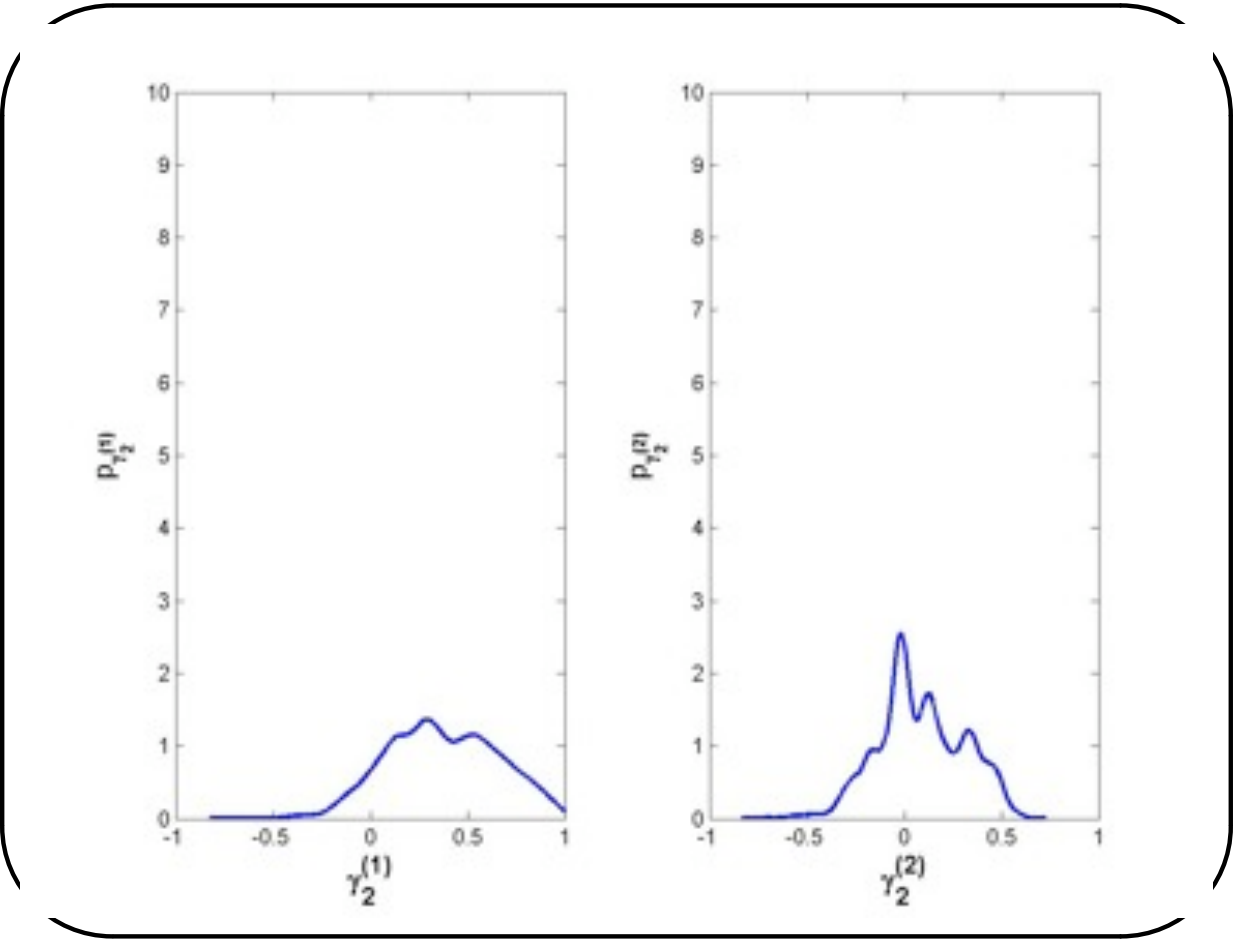
Note

- Must estimate α_i constrained by information:
  - experimental constraints:
    -$\boldsymbol{\xi}$ captures endogenous sources of uncertainty.
  - physics constraints:
    -α depends on $\boldsymbol{\xi}$ through a conservation law that must be honored.
- Dimension of $\boldsymbol{\xi}$ reflects complexity of the process α.
- Probability measure of $\boldsymbol{\xi}$ determines the geometry in which analysis and approximation are carried out.

$$\alpha(x,\theta) \quad = \sum_{i=0}^{\infty} \boxed{\alpha_i(x)} \Psi_i(\xi(\theta))$$



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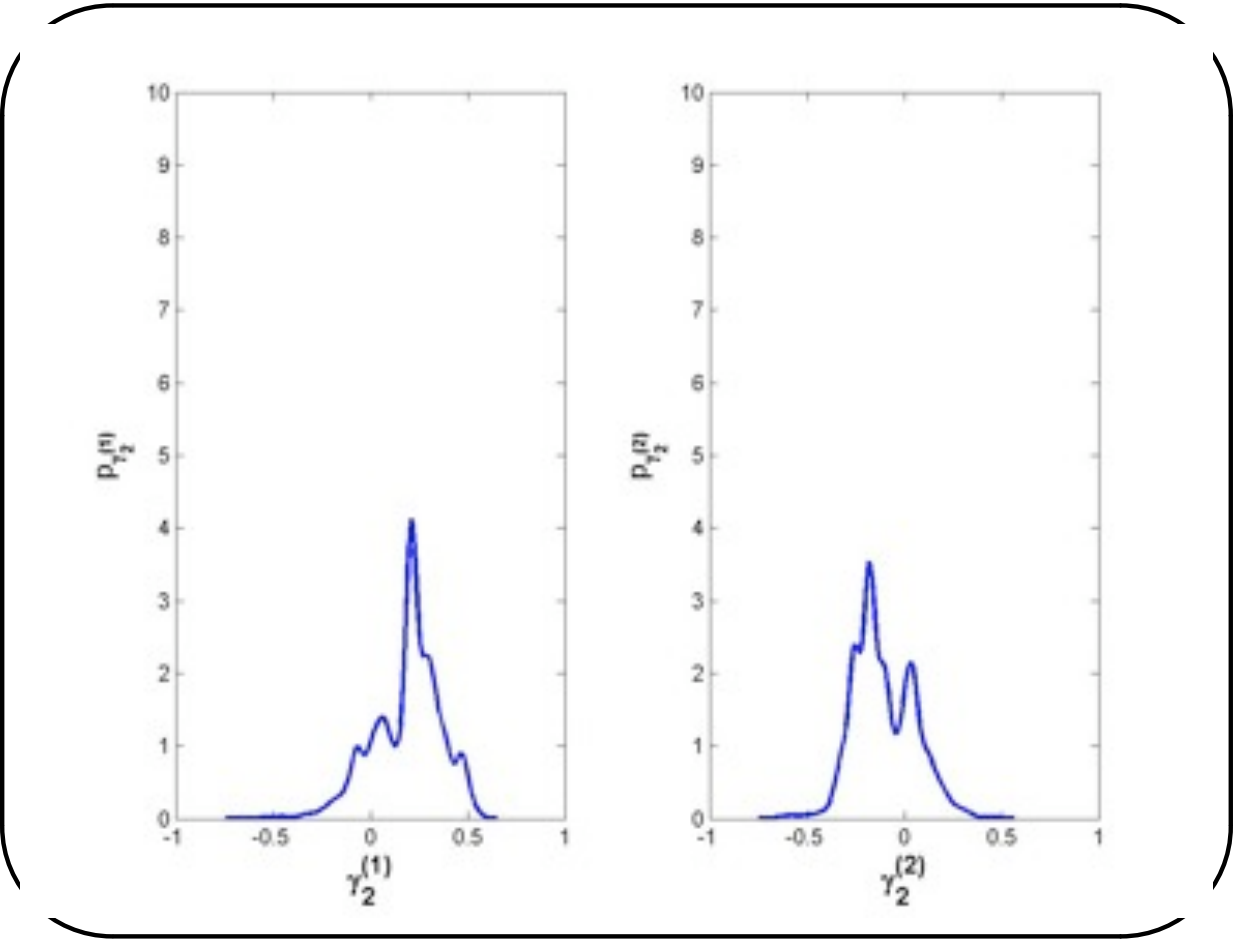

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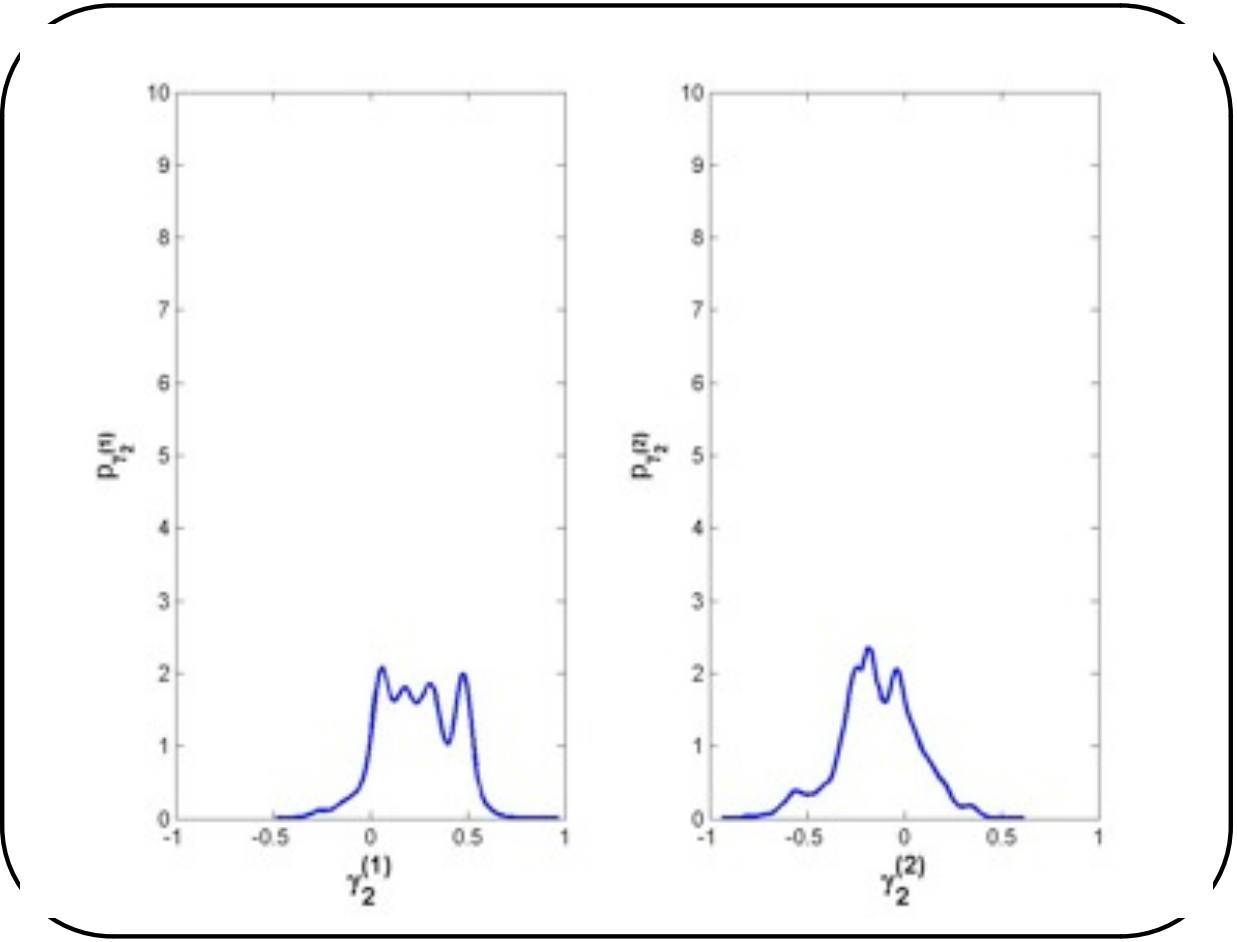

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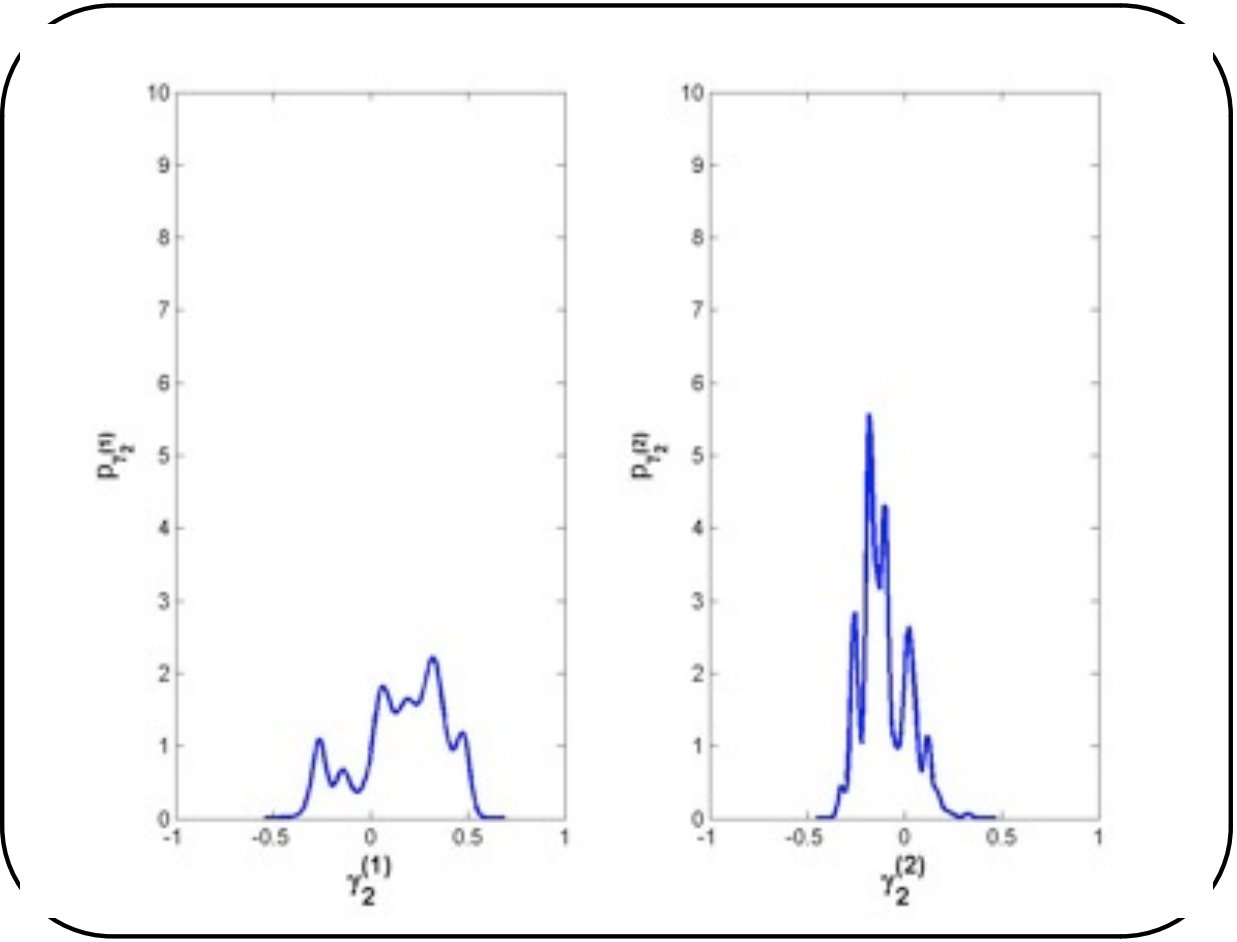

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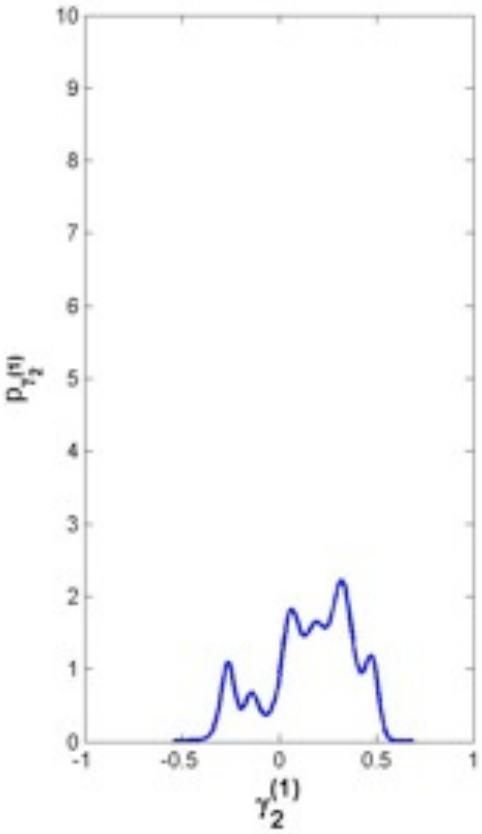

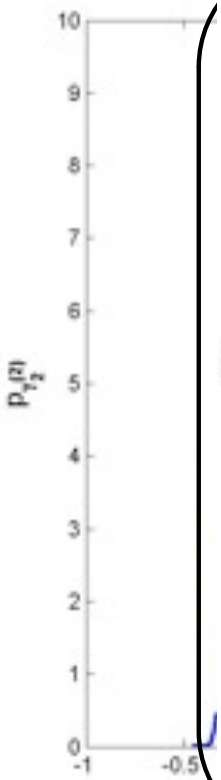

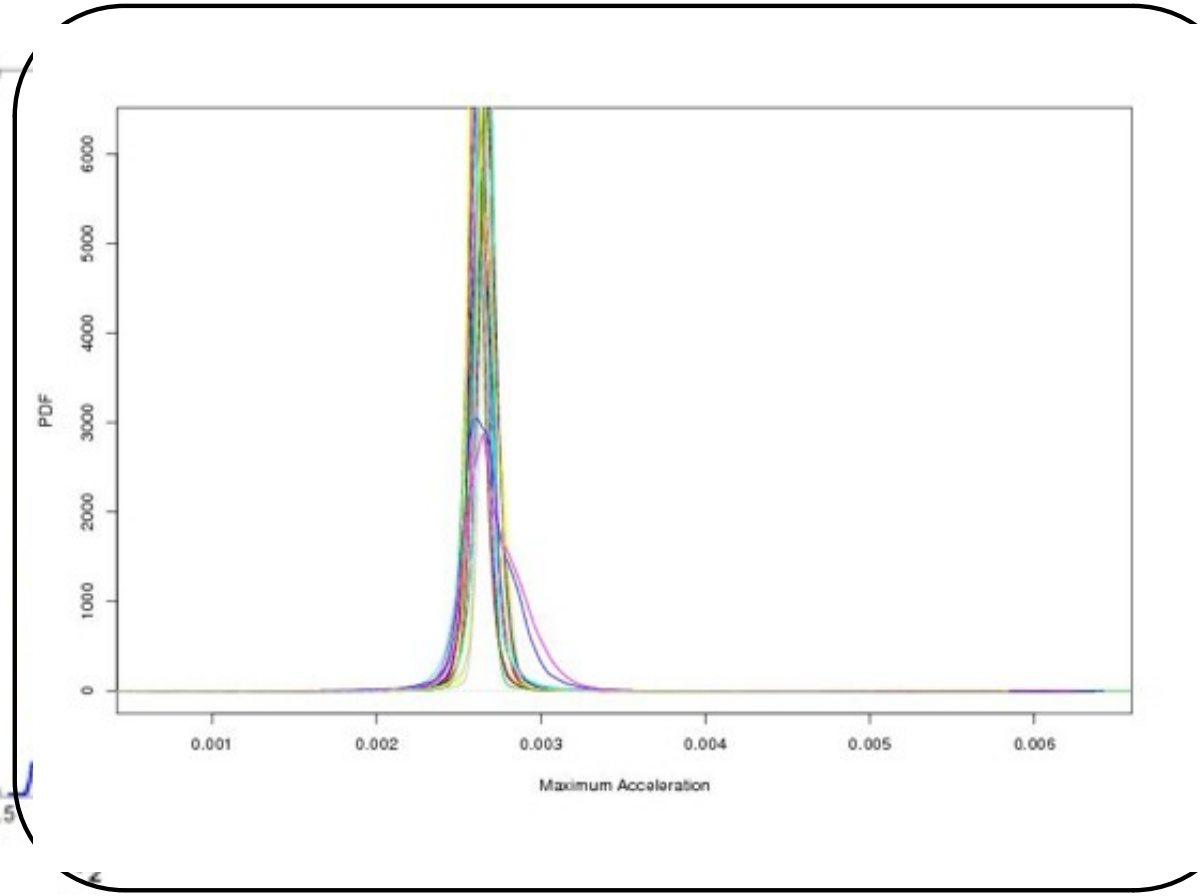

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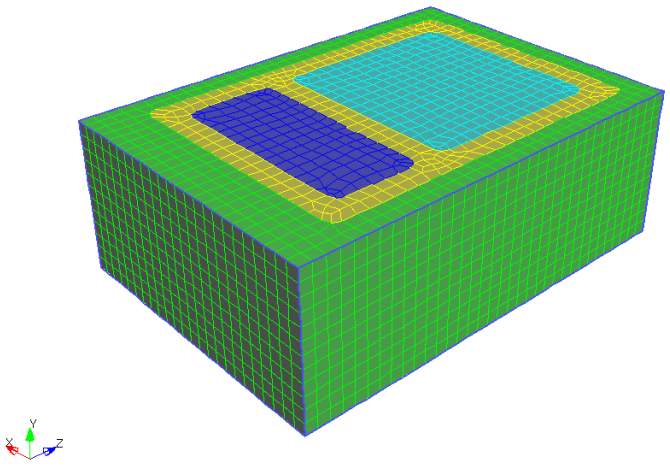

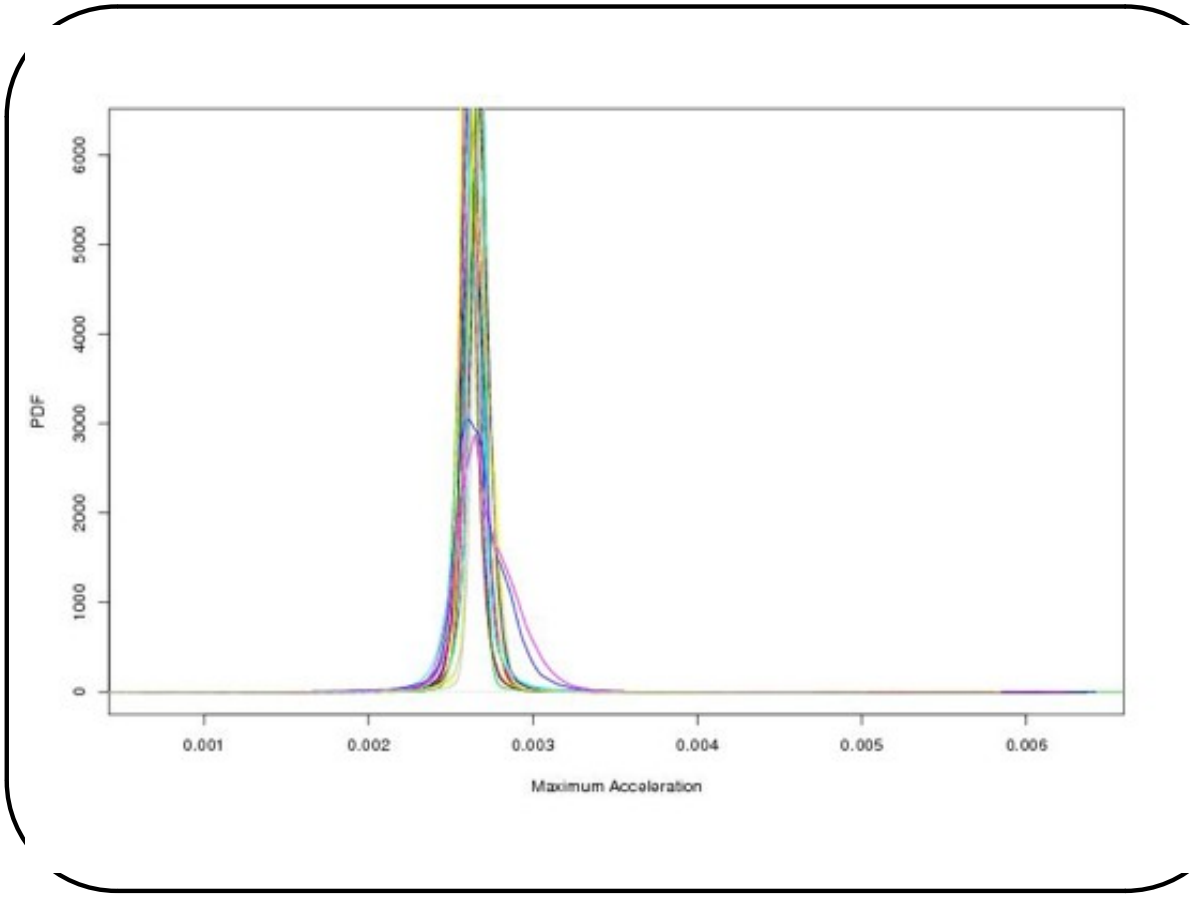

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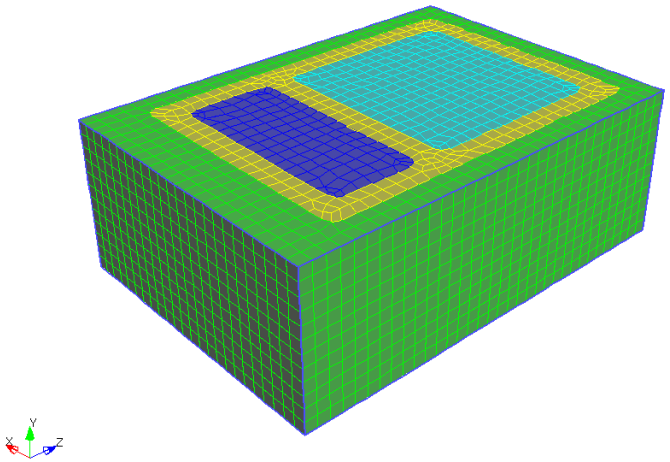

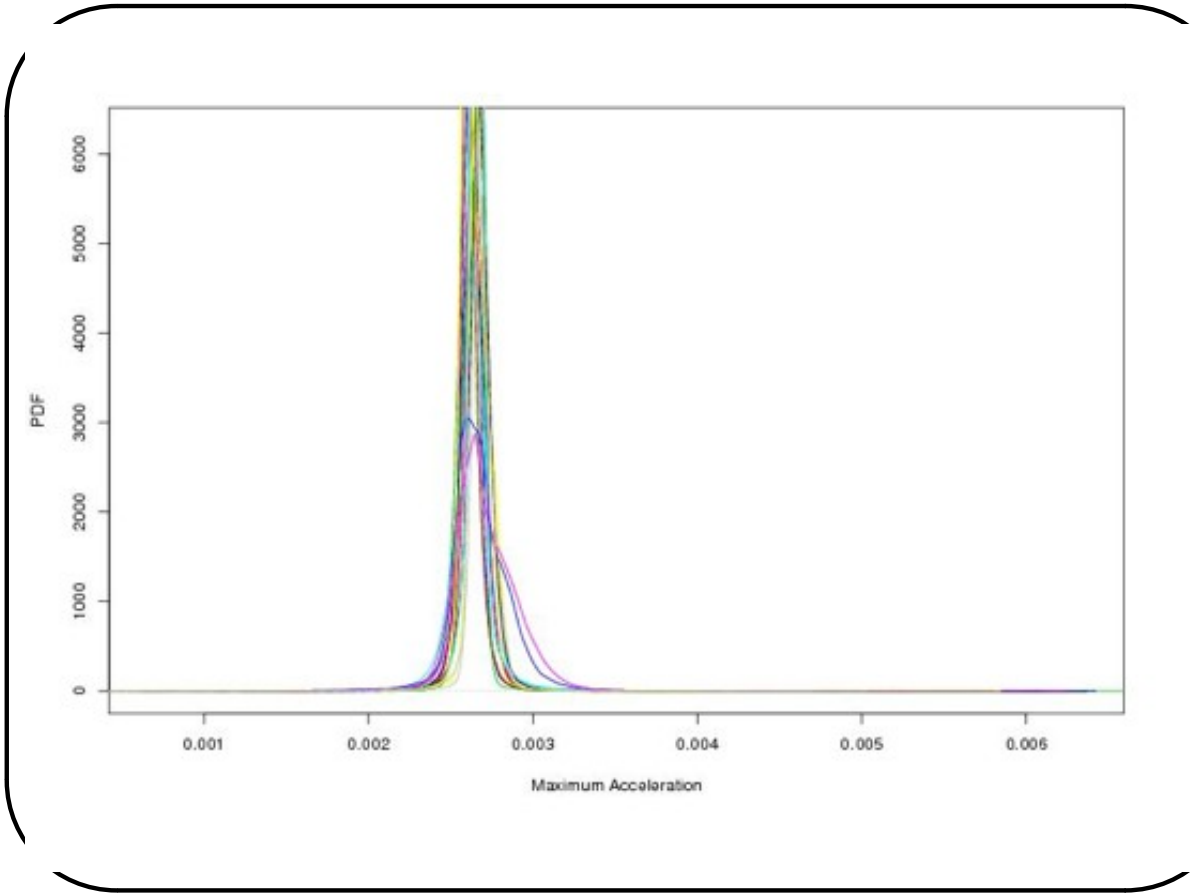

$$\boxed{\alpha_i = \sum_j \alpha_{ij}\Psi_j(\eta_i)}$$

$$\alpha(x,\theta) = f(x,\ \underbrace{\xi_1, \cdots, \xi_n}_{\text{Aleatoric Uncertainty}}\ ,\ \underbrace{\xi_{n+1}, \cdots, \xi_m}_{\text{Model/Data Uncertainty}}\ )$$

Estimating Chaos Coefficients:

- Galerkin projection - Gaussian Sampling distribution
- Maximum Likelihood - Asymptotic sampling distribution
- Maximum Entropy - Asymptotic sampling distribution
- Bayesian Inference - Posterior distribution of coefficients
- Ensemble Kalman Filtering - Point estimates.

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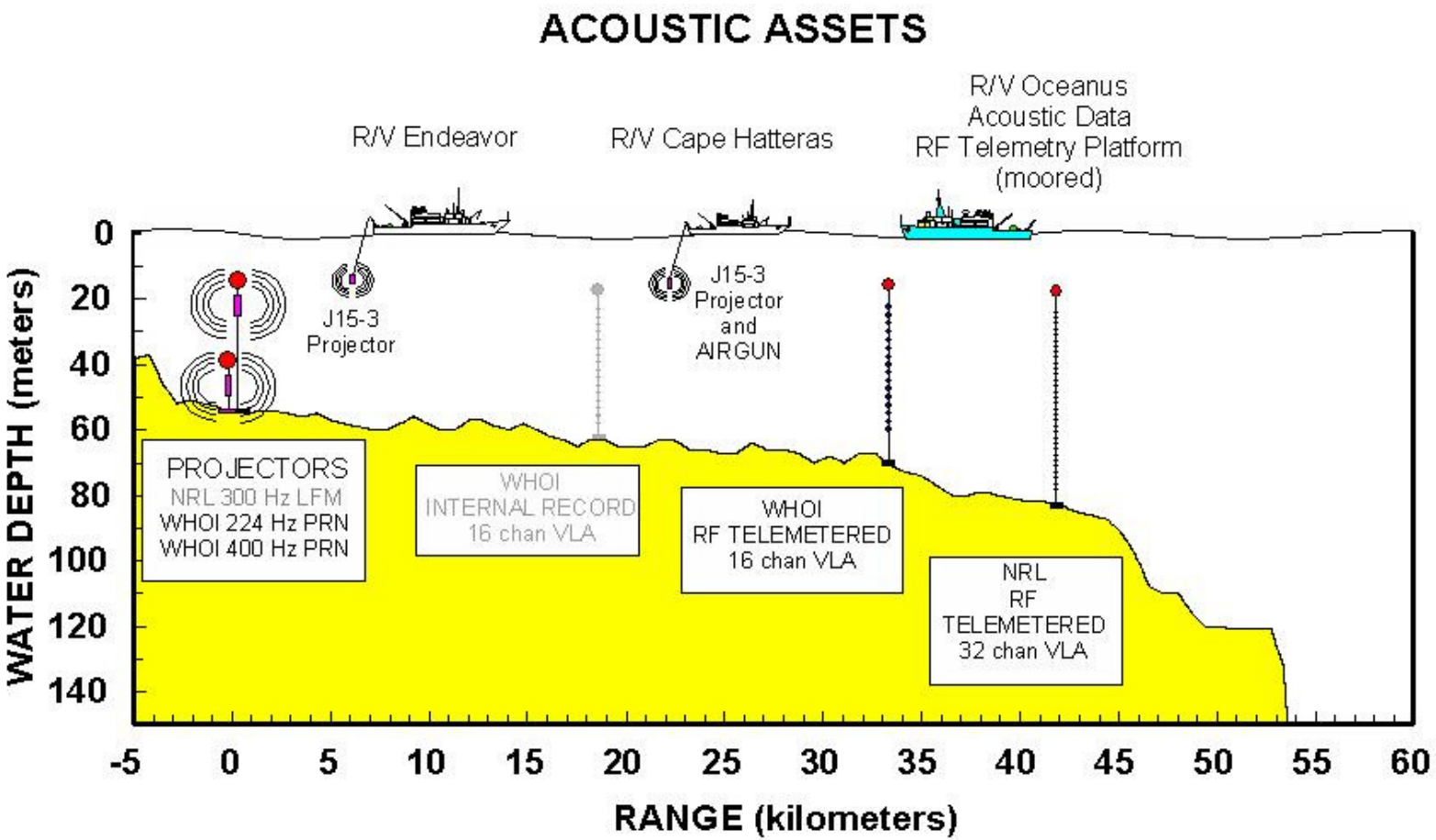
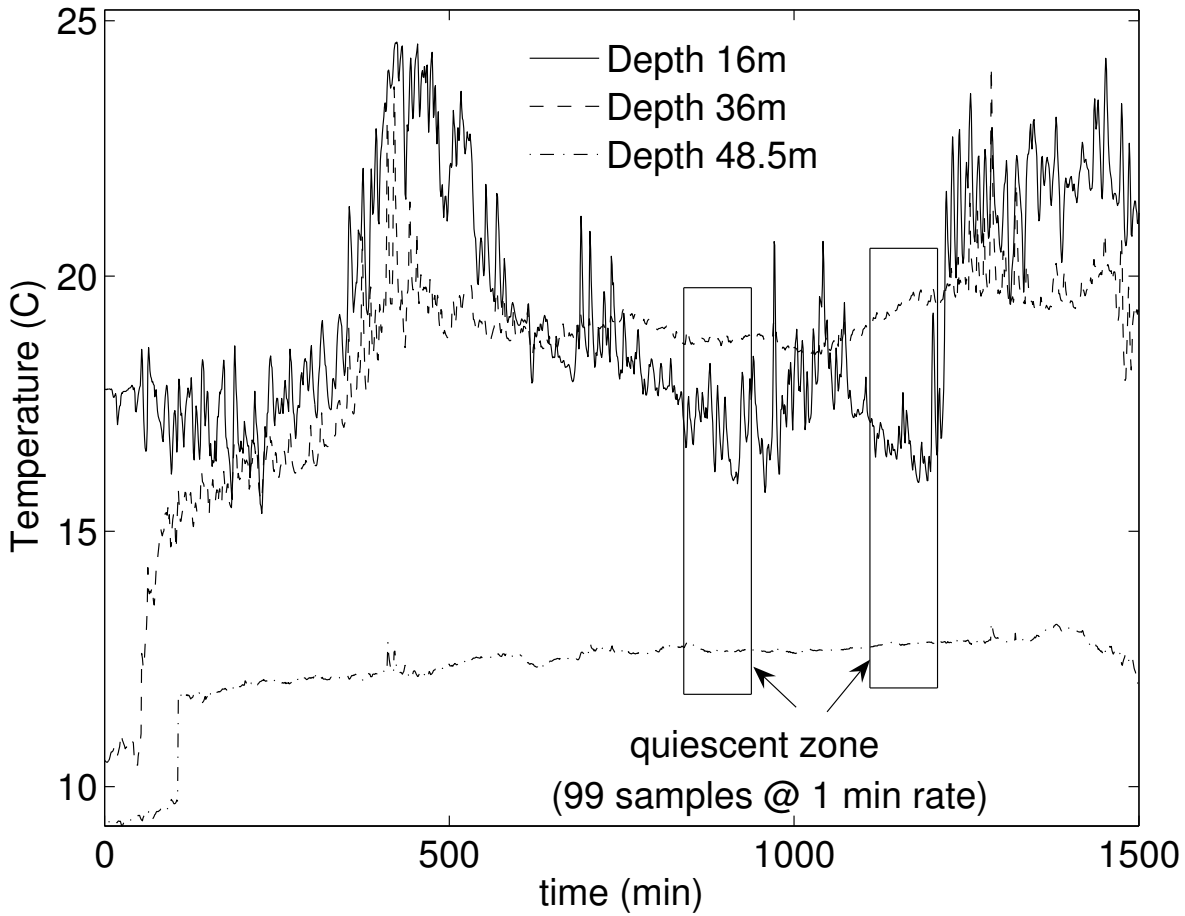
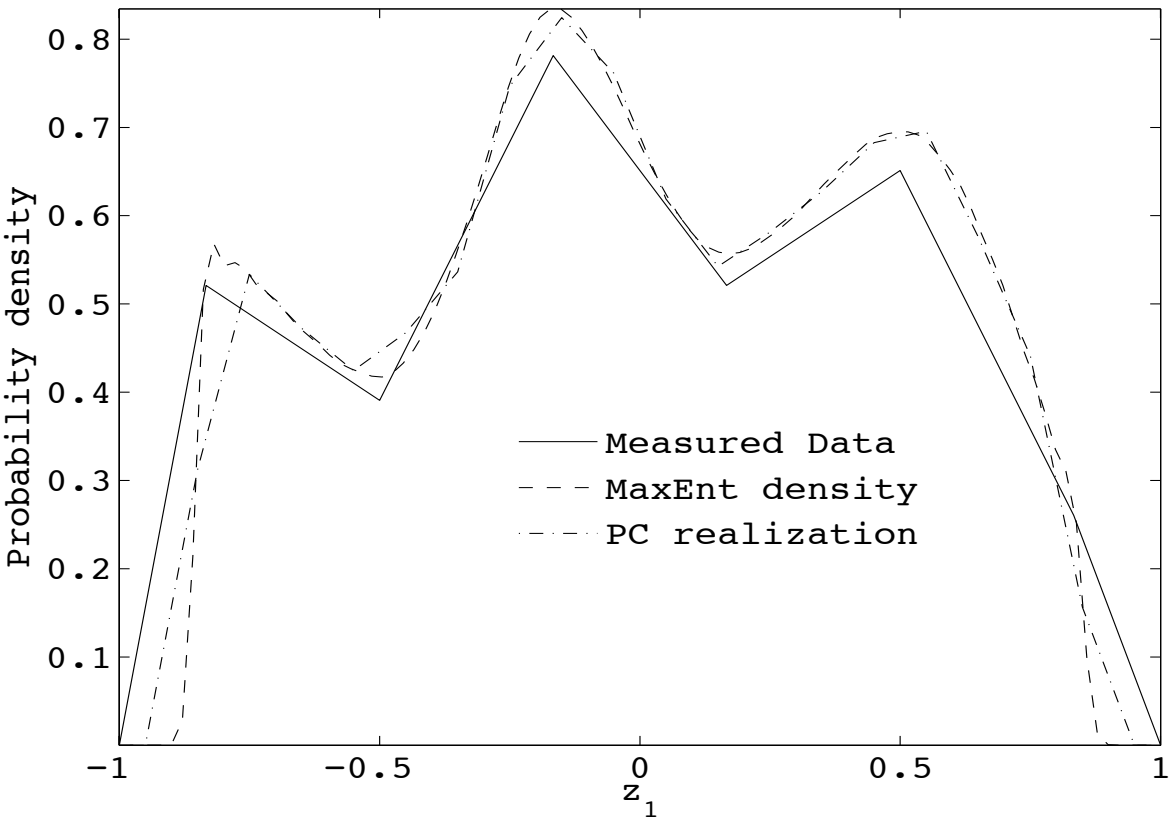


SWARM Data:


Depth 16m
Depth 36m
Depth 48.5m
quiescent zone
(99 samples @ 1 min rate)
Temperature (C)
time (min)
25
20
15
10
0
500
1000
1500

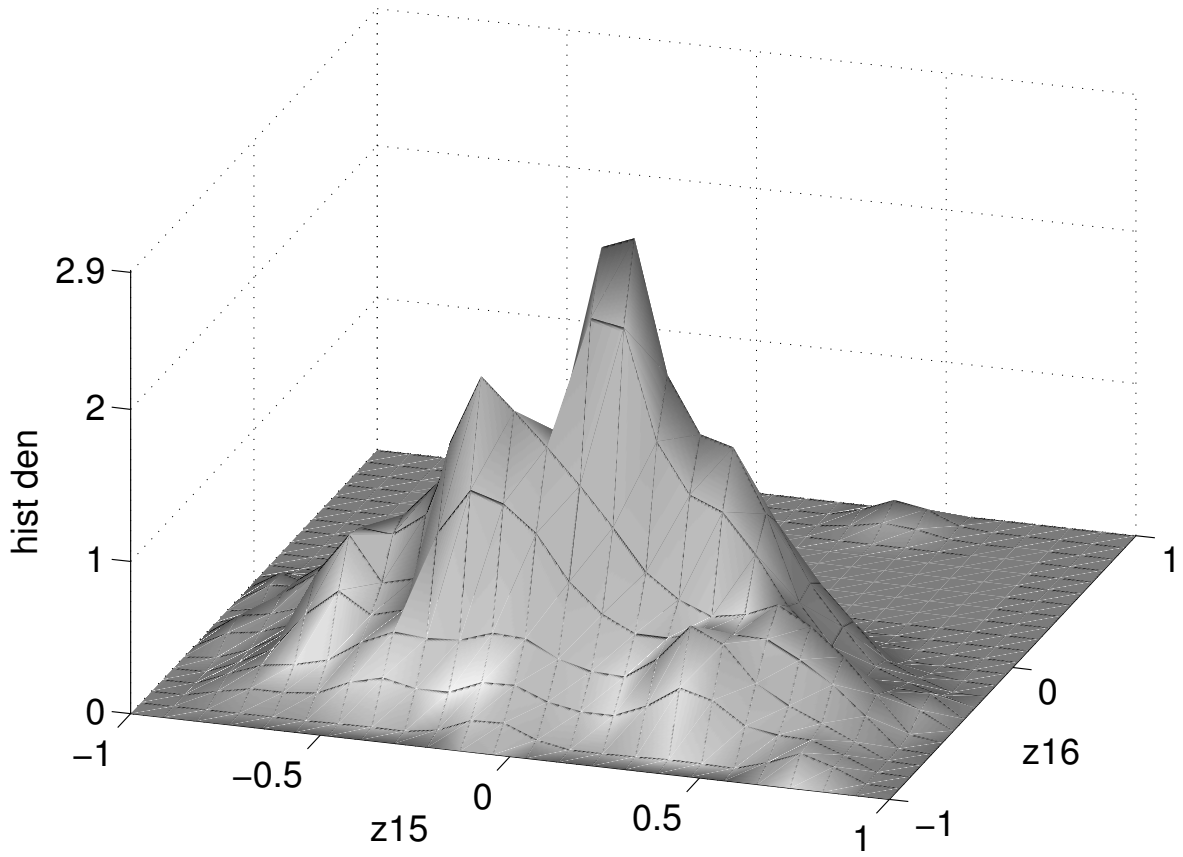
Marginal PDF for one KL variables

MaxEnt



Joint PDF for two KL variables

MaxEnt



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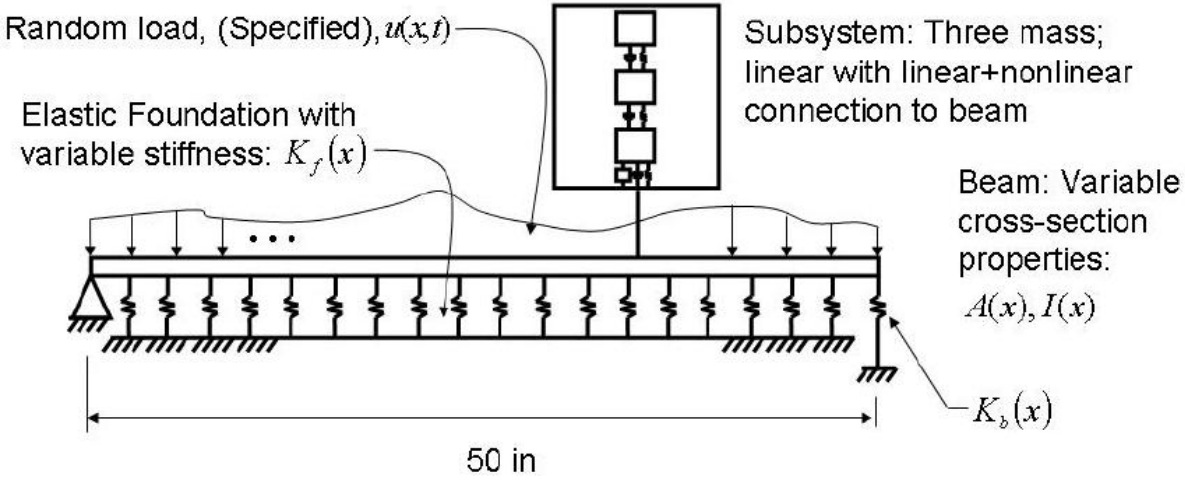
Sandia Validation Challenge

Problem Definition



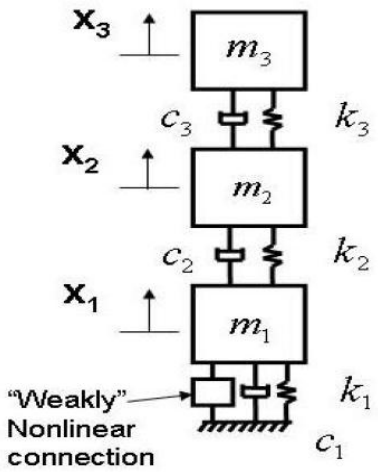
Certify a design without any full-system tests

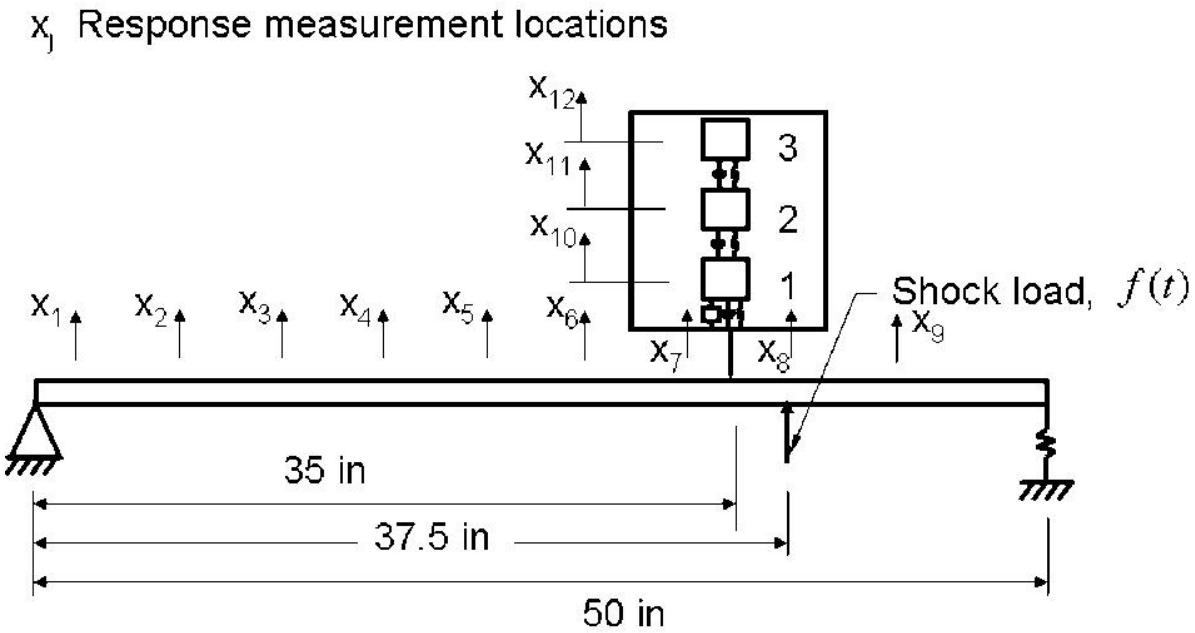
- use only linear models
- limited tests on subsystems
- certification criterion:

$$P_{am} := \mathrm{Prob}\{\max_{t>0} |a(t)| > 1.8e4 \mathrm{in}/\sec^2\} < 0.01$$

Sandia Validation Challenge

Test data on subsystems





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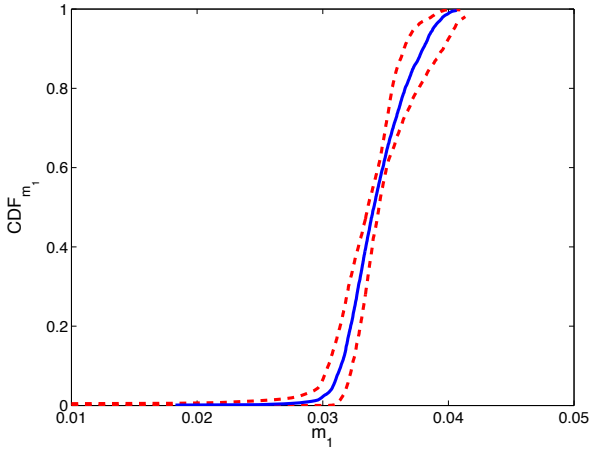
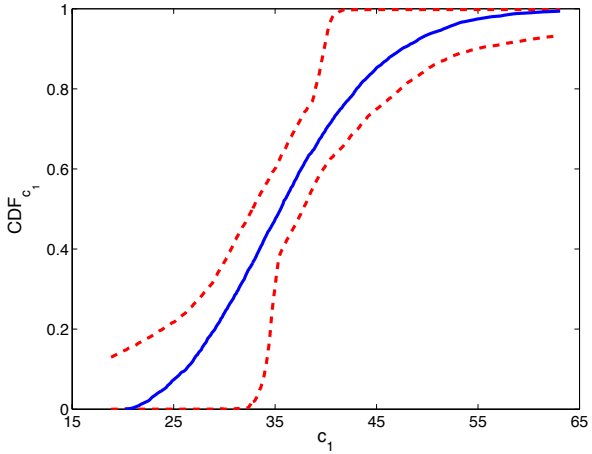
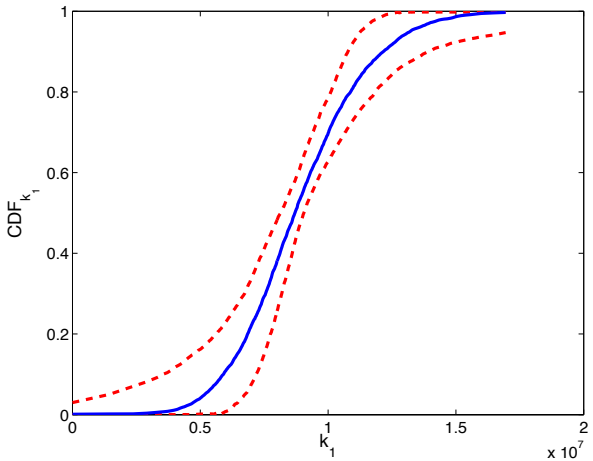
Statistical Calibration







Typical Mass, stiffness, damping estimates of CDF.

Red Scatter indicates dependence on further data.

Sandia Validation Challenge

Outcome

Certification Criterion:

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Estimated as random variables - Variability comes from small sample size

Sample Mean of P_{am}	Sample Variance of P_{am}
0.0835	0.000830

C.O.V. = 34% !

Sandia Validation Challenge

Outcome

Certification Criterion:

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Outline

1. Objectives
2. Inspiration from Elementary Statistics
3. Characterizing Uncertainty
4. Validation Example
5. Panoramic View of My Research
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Applications

- Prognosis for material integrity
- Carbon Sequestration
- Nuclear safety
- Stochastic networks
- Uncertainty in agent-based models
- SmartGrid
- Urban Sustainability

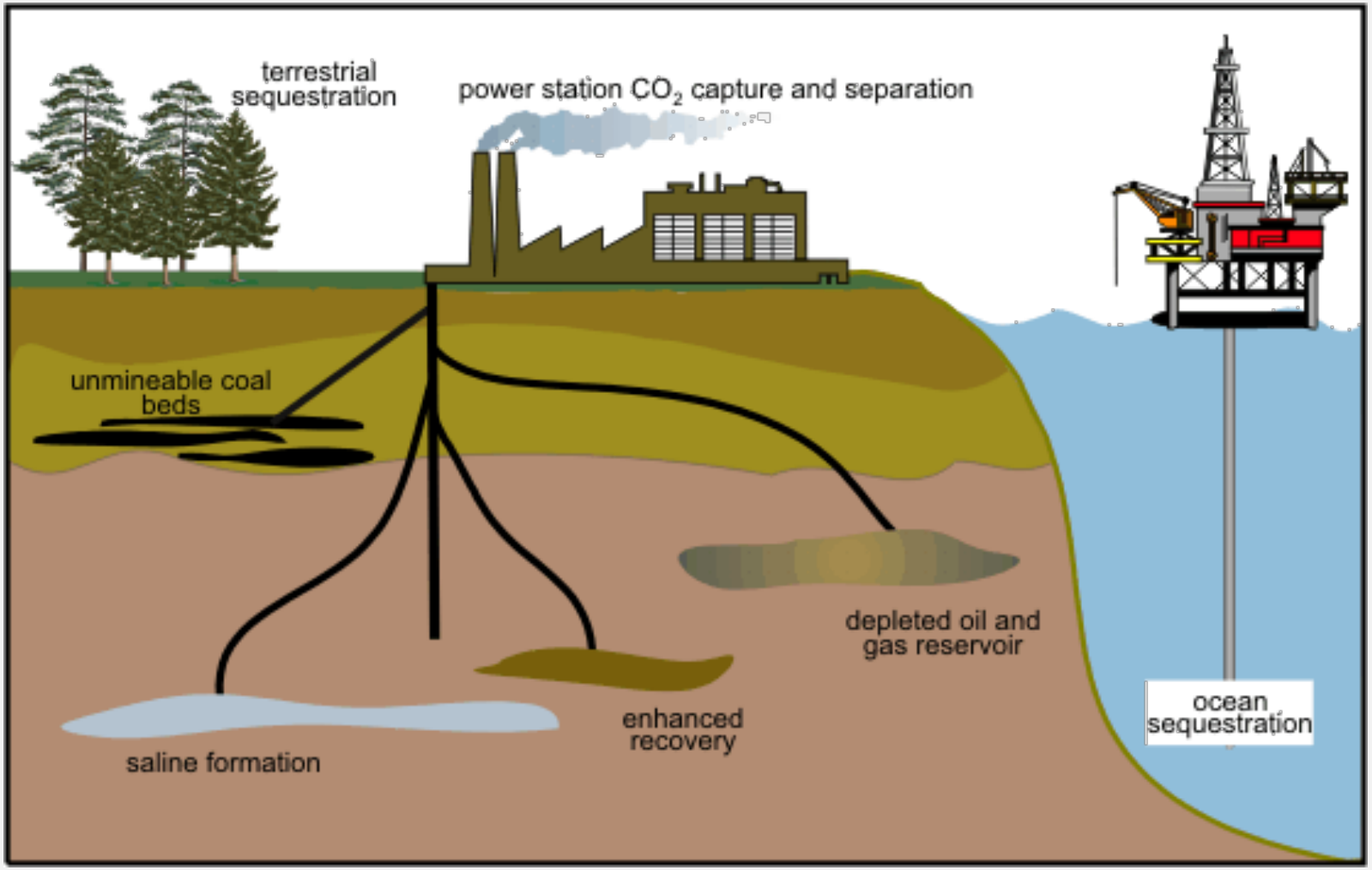
Prognosis

anticipate damage in microstructure and recommend pre-emptive actions:

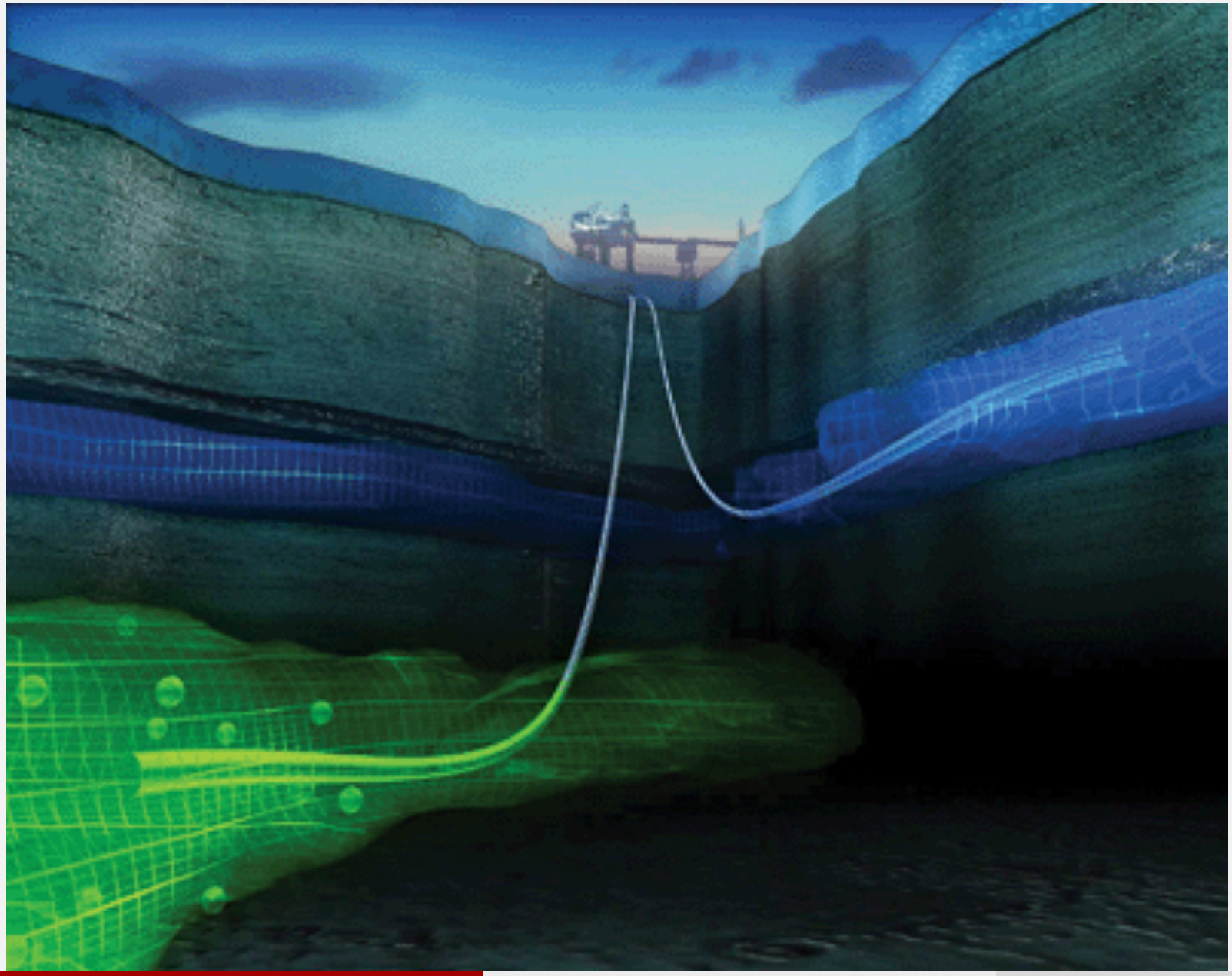
Multiscale Models: Transfer information from calibration scale to prediction scale.

- New multiscale constitutive behavior using random matrix theory and stochastic Green's functions.
- New stochastic models for microstructure.
- New decision tools and sensor placement algorithms.

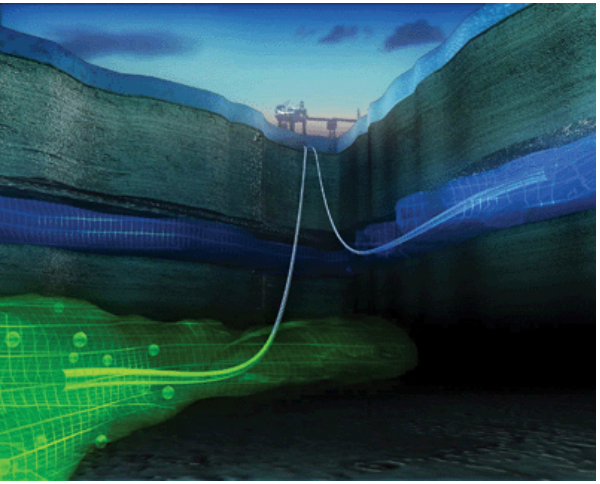
Safe Carbon Sequestration

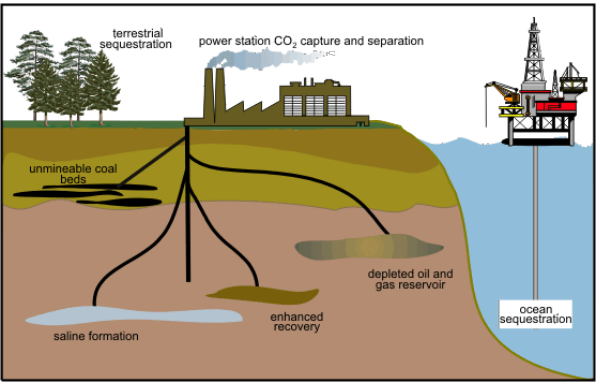


Safe Carbon Sequestration



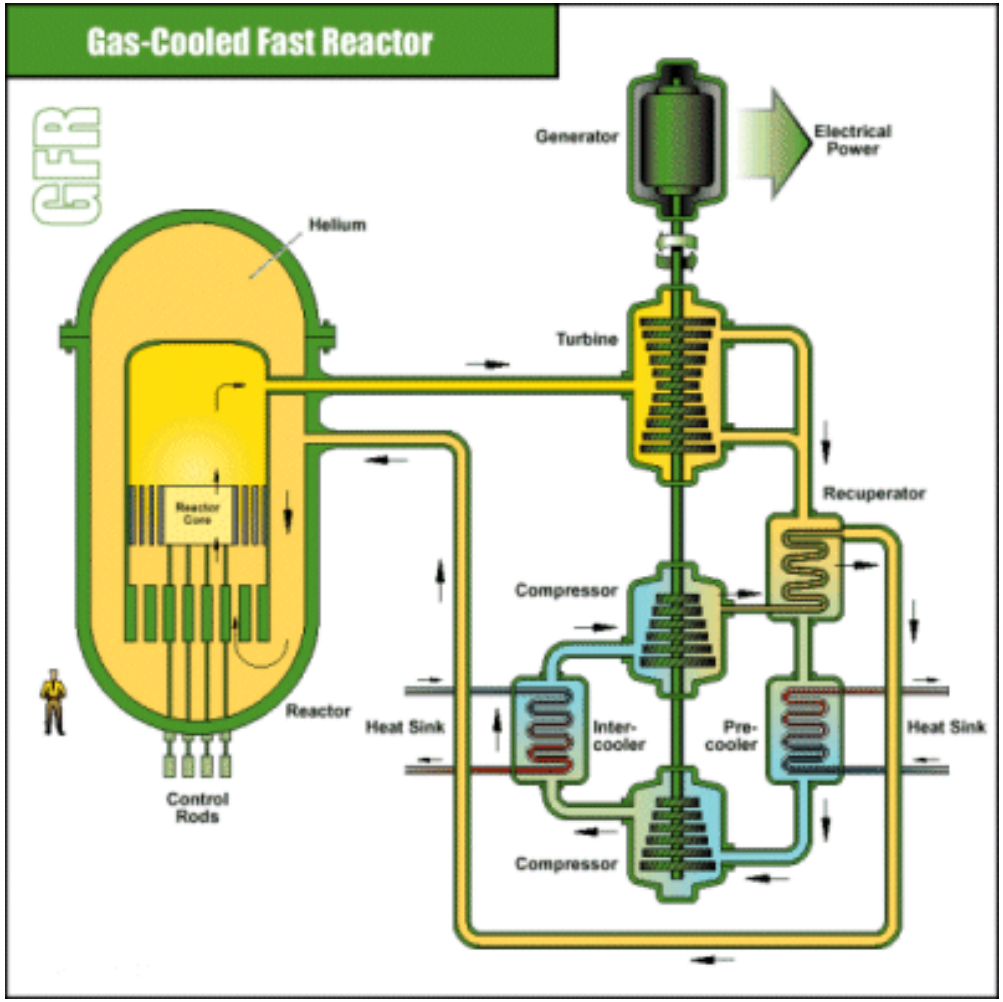
Safe Carbon Sequestration

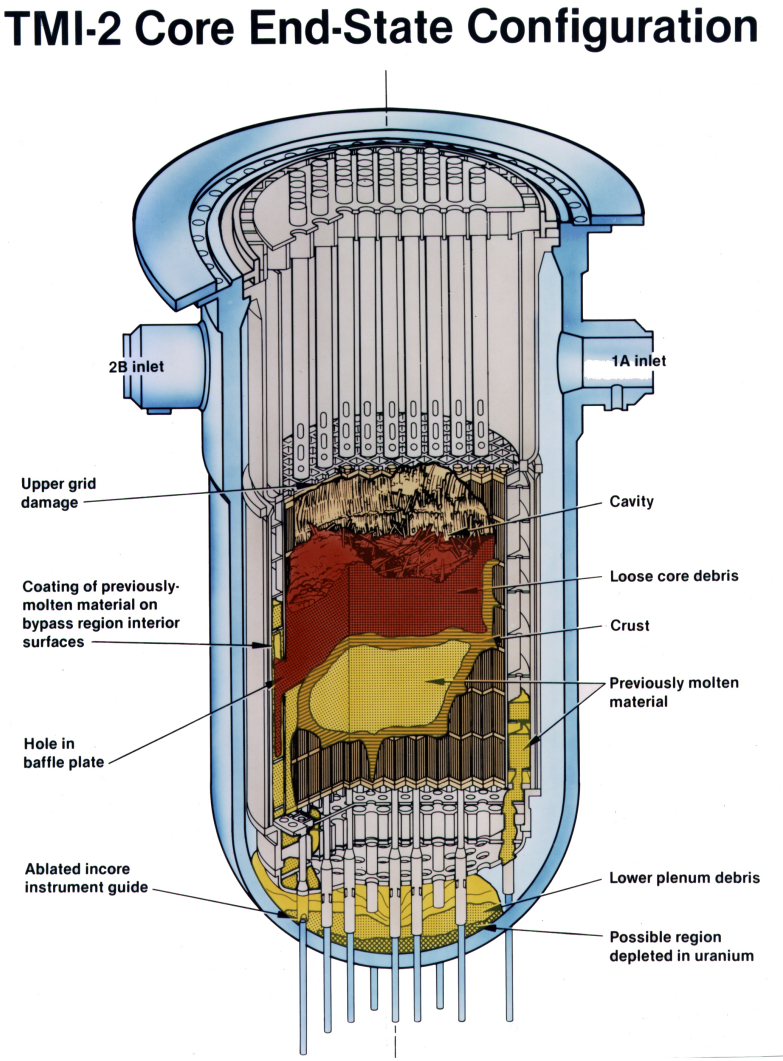




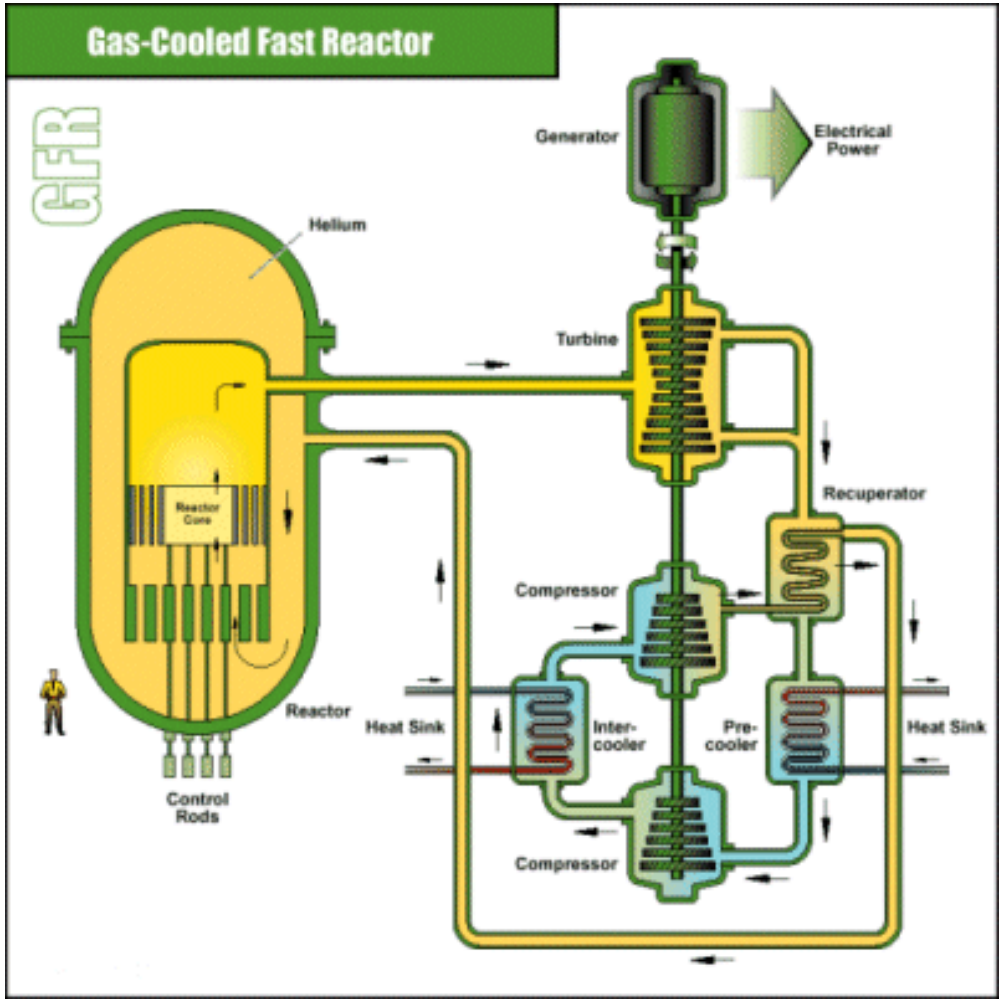
- Reactive flow in uncertain subsurface formation.
- Leakage with chemistry from caprock (stochastic upscaling of caprock interface with formation).
- Algorithms for Petascale computing.

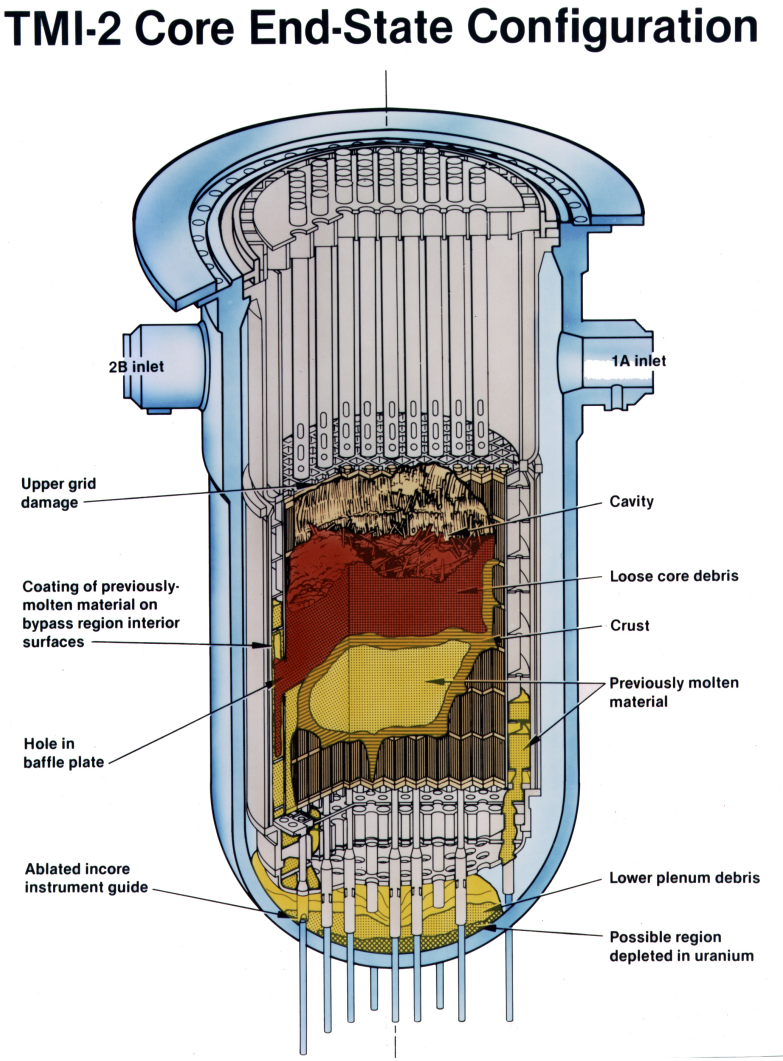
Risk analysis of next generation fast nuclear reactors





Risk analysis of next generation fast nuclear reactors





Risk analysis of next generation fast nuclear reactors

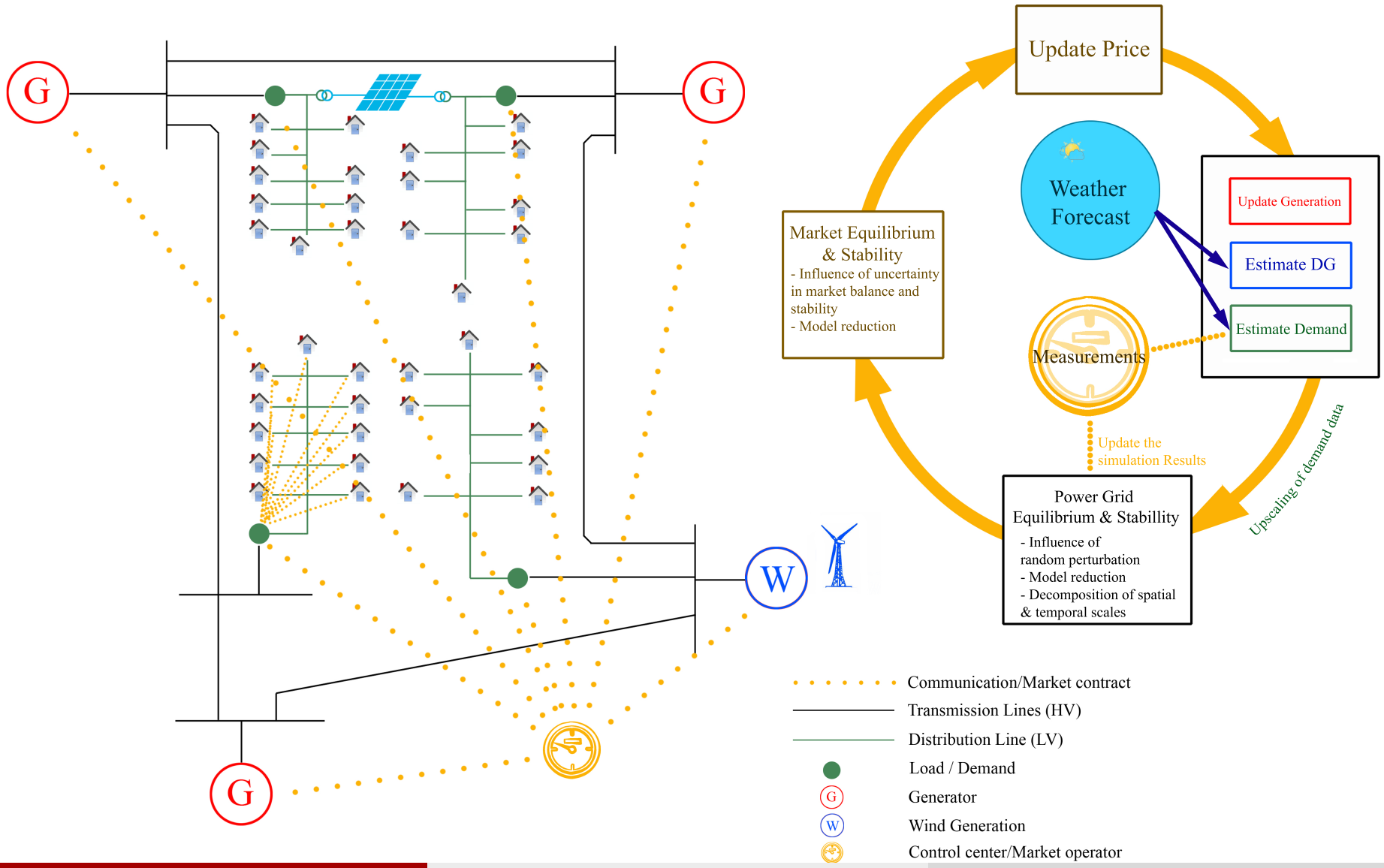
UQ with Multiphysics/ Multiscale/ Multimodel:

- Understanding the interplay between neutron transport, thermo-mechanical properties and failure of reactors.
- Theory to characterize stochastic dynamics of coupled system.
- Stochastic upscaling to describe the effect of neutron transport on safety of reactor system.

Stochastic networks and hybrid systems

- Interface between network models of infrastructures, discrete models of humans and continuum models of environmental effects.
- Reaction kinetic networks: upscaling from molecular chemistry.
- Stability and dynamics of hybrid systems.

Smart Grid


G
G
G
W
Update Price
Weather Forecast
Update Generation
Estimate DG
Estimate Demand
Market Equilibrium & Stability
- Influence of uncertainty in market balance and stability
- Model reduction
Measurements
Update the simulation Results
Power Grid Equilibrium & Stabillity
- Influence of random perturbation
- Model reduction
- Decomposition of spatial & temporal scales
Upscaling of demand data
Communication/Market contract
Transmission Lines (HV)
Distribution Line (LV)
Load / Demand
Generator
Wind Generation
Control center/Market operator

SmartGrid at USC

News: Thursday, December 3, 2009

LADWP Receives $60 Million For Smart Grid Project

[back] [comment]

The Los Angeles Department of Water and Power (LADWP) earlier this week was awarded over $60 million in smart grid demonstration funding-the most of any other municipally-owned utility in the country-to develop, deploy, and test advanced smart grid technologies in partnership with a consortium of top Southern California research institutes including USC, UCLA, and CalTech/Jet Propulsion Laboratory.

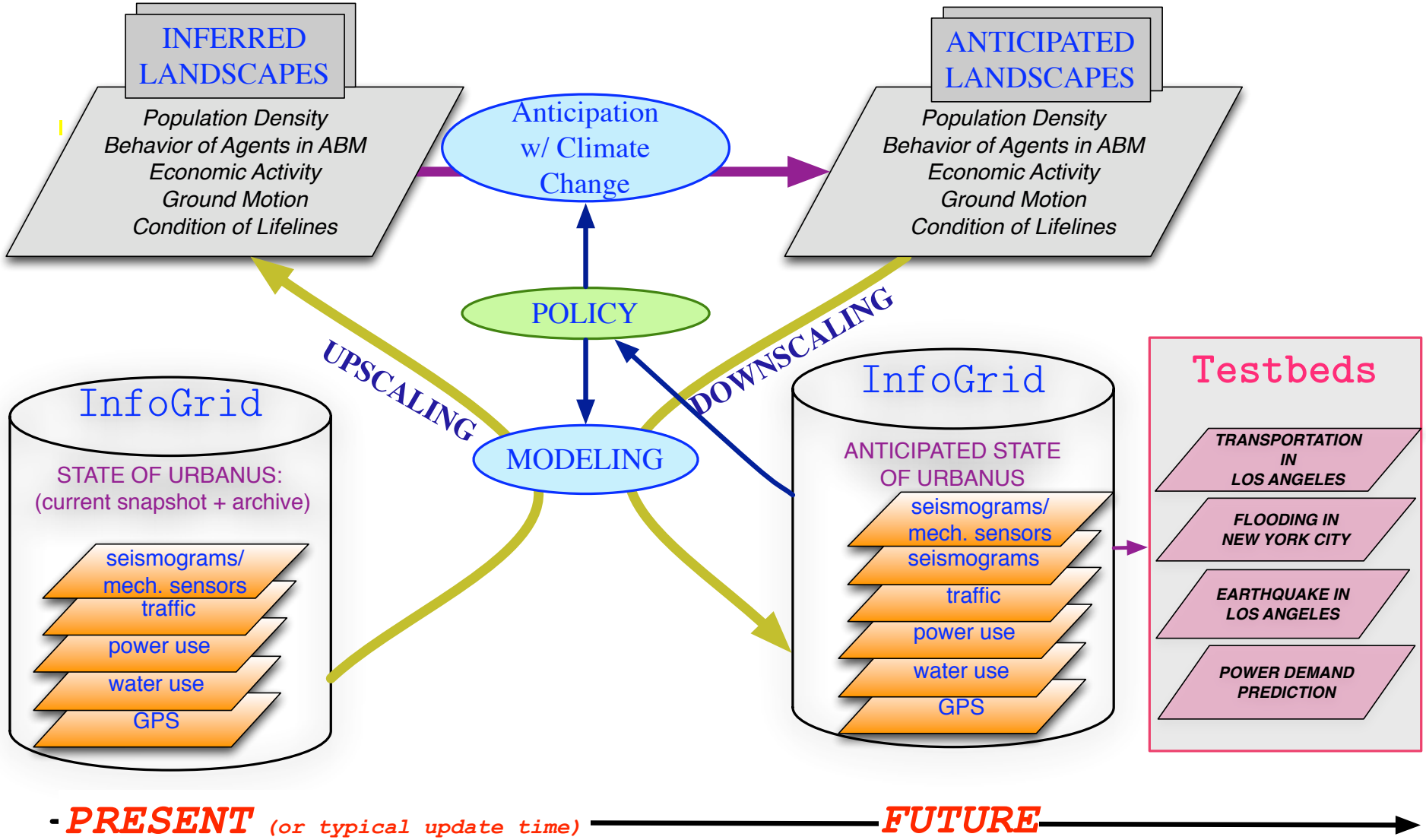
The program will use the USC and UCLA campuses as testing grounds for innovative technologies to prove the viability of the demonstration technology. Through a number of demonstration projects, LADWP and the research institutes will gather data on how consumers us energy in a variety of systems, testing the next generatio of cyber-security technologies, and cutting-edge method of integrating a significant number of plug-in hybrid elect vehicles onto the grid. This work will provide invaluable data on the benefits and cost-effectiveness of various technologies, which will save time and money down the road.

The universities will serve as microcosms of the entire ci providing an innovative "micro-grid" where to carry out testing in real-time within each campus environment.

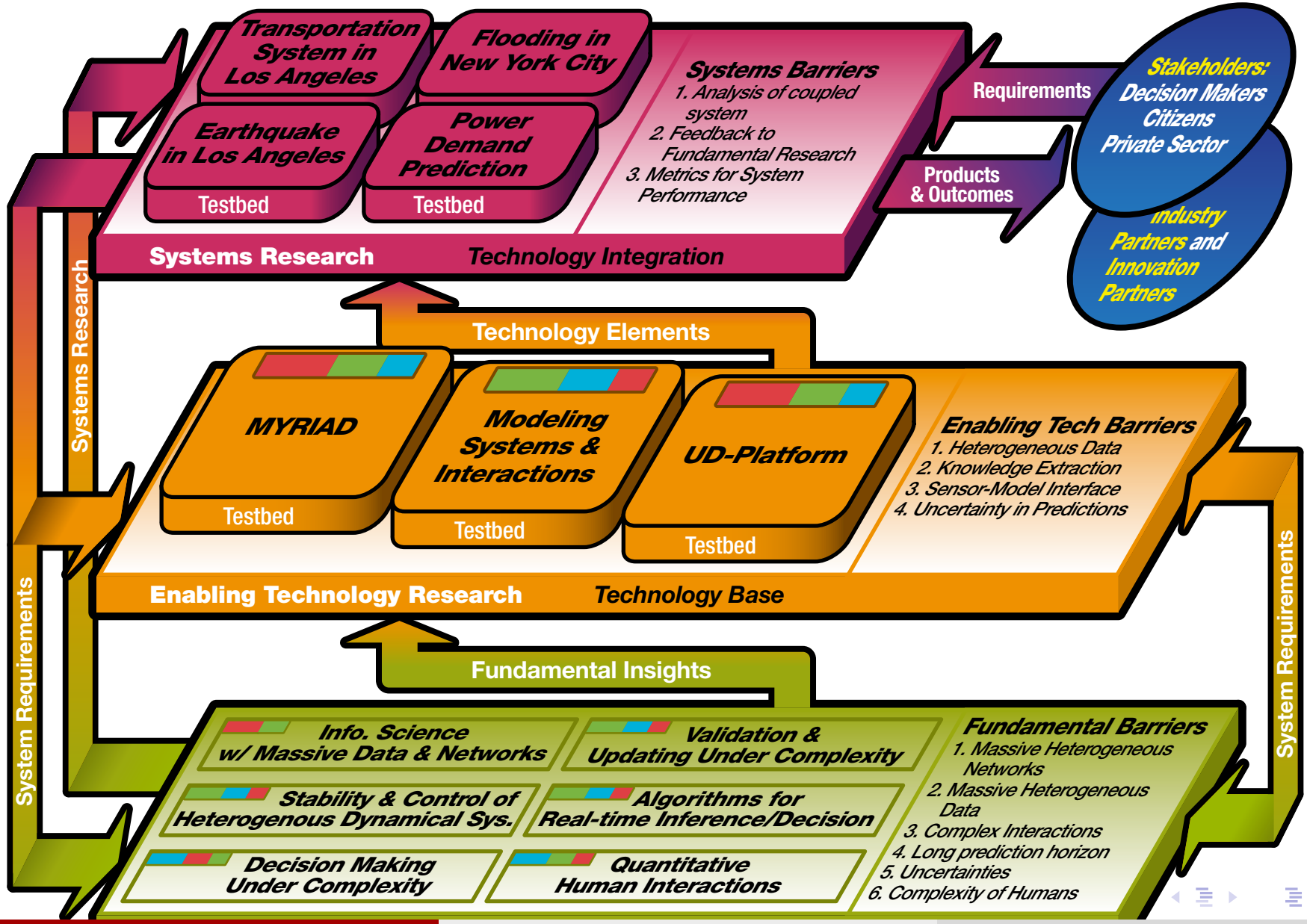
Sustainability by Design

- Quantitative analysis of interactions, between human dynamics, environmental factors, and policy.
- Multiscale models of forests to manage natural-urban interface (fires, wildlife sustainability ...)
- Sensor placement for disaster avoidance in urban water distribution systems.

Sustainability by Design



Big Picture


Transportation System in Los Angeles
Flooding in New York City
Earthquake in Los Angeles
Power Demand Prediction
Testbed
Testbed
Systems Barriers
1. Analysis of coupled system
2. Feedback to Fundamental Research
3. Metrics for System Performance
Requirements
Products & Outcomes
Stakeholders:
Decision Makers
Citizens
Private Sector
Industry Partners and Innovation Partners
Systems Research
Technology Integration
Systems Research
Technology Elements
MYRIAD
Modeling Systems & Interactions
UD-Platform
Testbed
Testbed
Testbed
Enabling Tech Barriers
1. Heterogeneous Data
2. Knowledge Extraction
3. Sensor-Model Interface
4. Uncertainty in Predictions
Enabling Technology Research
Technology Base
System Requirements
System Requirements
Fundamental Insights
Info. Science w/ Massive Data & Networks
Validation & Updating Under Complexity
Stability & Control of Heterogenous Dynamical Sys.
Algorithms for Real-time Inference/Decision
Decision Making Under Complexity
Quantitative Human Interactions
Fundamental Barriers
1. Massive Heterogeneous Networks
2. Massive Heterogeneous Data
3. Complex Interactions
4. Long prediction horizon
5. Uncertainties
6. Complexity of Humans

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Challenges

Philosphical

- meaning of life and happiness.

Logical

- e.g. dependence on new information.
- Can underlying hypothesis be tested ?

Mathematical

- Construct a mathematical structure that permits the articulation of the logical and philosophical imperatives.
- Describe the problem within that mathematical structure.

Technological

- Instruments to achieve requisite resolution of physical phenomenon.
- Computers to achieve requisite numerical resolution for mathematical

Challenges/ Opportunities

Critical

- understand the significance of enhanced predictive power.
  - new quantities of interest.
- understand the nature of added requirements:
  - human: who sets confidence limits
  - physical: is a coin toss random ?

Technical

- explore new packaging of information.
- move away from labeled probability models.
- develop error estimation methods for the various components.
- resolve the computational burden: error estimation.
- develop stochastic reduced-order models: eg. curse of dimensionality.
- optimize and design.