Monday, 8:45am
(+/- 15 min? 30 min?)

The journey from atoms to assessed engineering *with quantitative confidence*: Purpose, principles, and (some) practice

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IMA Workshop: Uncertainty Quantification in Materials Modeling
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Why Uncertainty Quantification (UQ)?

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What's the point of multiscale materials simulation anyway?

To be insightful

identify, characterize, and assess crucial phenomena

To be predictive

move beyond forensics and pretty pictures (and papers)

To be meaningful

inform decisions (technical and programmatic)

Goal: establish credibility, quantitative confidence, in an evidence-based approach used to inform high-consequence decisions

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What kind of decisions?

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- Satisfy regulatory requirements in qualified assessment
- Support design choices for safety and performance
- Identify weakness&strengths, gaps in system analysis
- Inform resource allocation and investment strategy
- Inform technical program priorities

Credible quantitative measures are necessary

Meaningful UQ is means to establish quantitative confidence

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UQ alone is not enough

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- UQ is only meaningful within Verification and Validation (V&V) regime
  - Verification – are you solving what you think you are solving?
  - Validation – how well does what you are solving represent reality?
  - Uncertainties quantifies these questions
  - This also applies to experimental data!

- V&V and UQ only make sense in the context of an application
  - What are you solving for, precisely?

- Objective: acceptance of M&S "product"
  - (1) Internal: Process to identify and mitigate weaknesses in models
    - Make decisions – set priorities, allocate efforts
  - (2) External: Establish quantitative confidence in results
    - Make decisions informed by credible evidence

More questions than answers – defining a process, no clear answers

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Process: Perfection vs. provably good (enough)

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Goal: Establishing credibility, quantitative confidence

PCMM – Predictive Capability Maturity Model (Sandia)

Graded approach, greater risks => greater rigor

Rigor Level	Risk Level	Example Usage
0	Low consequence	Scoping studies
1	Moderate consequence	Design support
2	High consequence	Qualification support
3	Highest consequence	Qualification or certification decisions

Other, similar protocols: PMI (LANL), CAS (NASA) …

Process: approach that emphasizes every component in an assessment in a way balanced to maximize confidence in final output result

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Multiscale materials modeling UQ challenges

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Numerical UQ methods (relatively) well developed, but …

- Each application has unique multiscale sequence
  - custom UQ system every time?
- Physics/chemistry causalities not known *a priori*
  - define network of UQ assessment without causality?
- Upscaling challenge
  - electrons to atoms to chemistry to thermodynamics …
  - how to propagate UQ through scales? After calibration?
  - with undetermined roadmap to ultimate (assessed) quantities?
- Cultural
  - materials disciplines do not embrace/express UQ principles?

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Nuclear Waste Disposal

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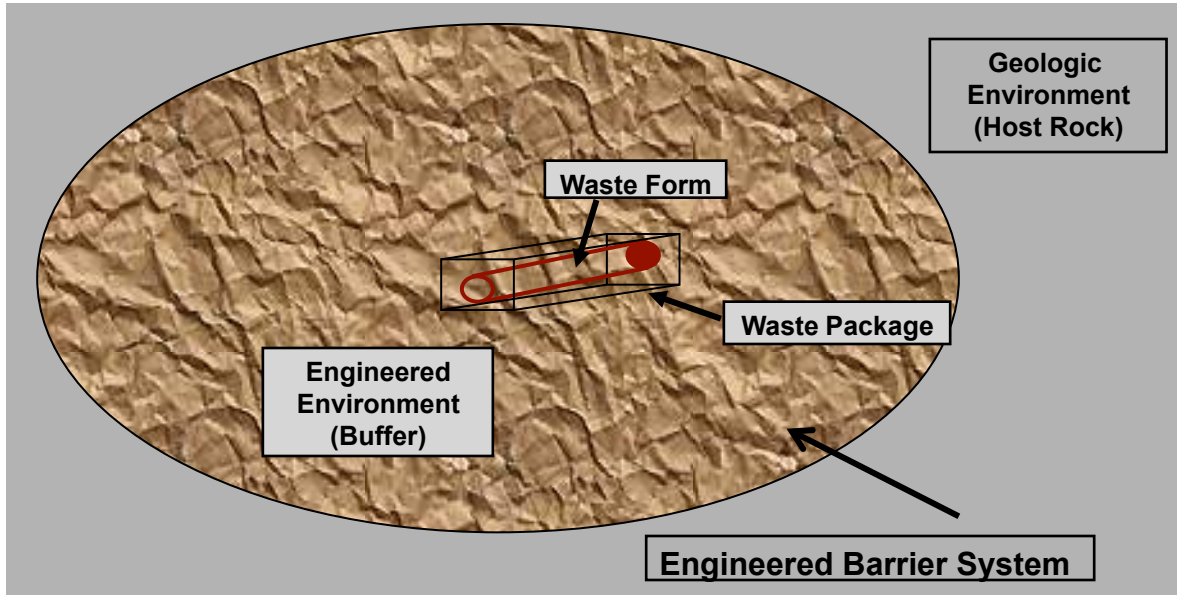
- **(now-retired NEAMS program) Long-Term (~10-year) Objective:**
  - Simulation of the long-term performance of waste forms in the engineered environment of a radioactive waste storage or disposal system
  - Simulate radionuclide movement to a specified receptor for a range of system designs (WFs, WPs, buffer/backfill, host rock) and conditions



Goal: assess waste form and long-term waste storage system for long-term disposal of nuclear waste subject to regulatory requirements.

Follow the radionuclides

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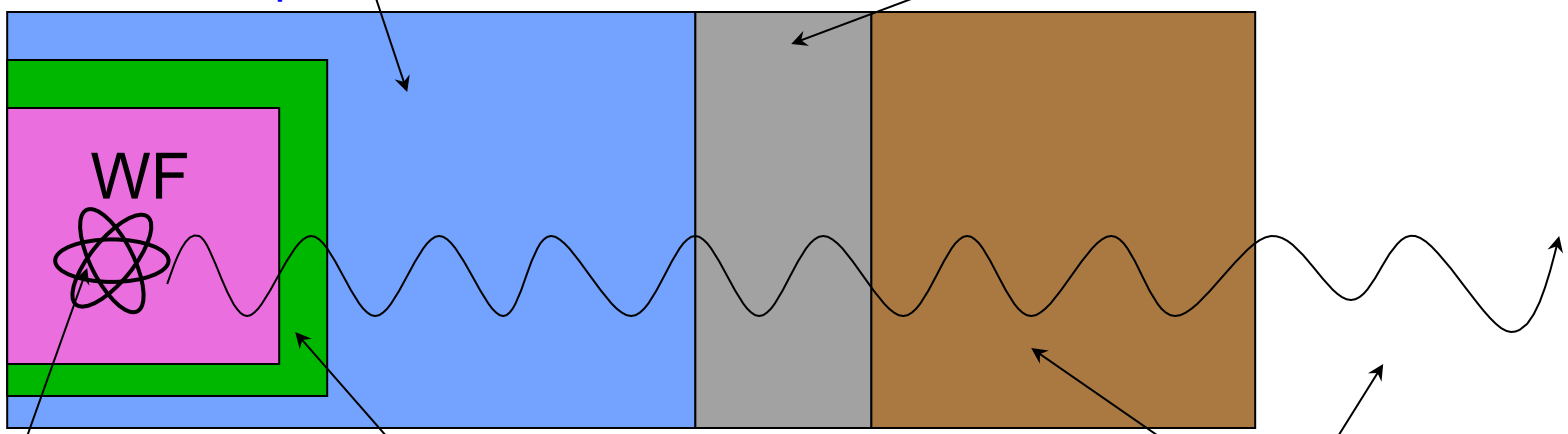
What happens at barriers?
- corrosion, cracking, sorption

What happens away from surface?
- transport, colloids, 2ndary phases
aqueous solution pH, redox, cations, anions

Cladding/canisters/package



glass, ceramic, metal

barrier layers, complexes, gels

EBS fill, geologic setting (salt, tuff, granite …)
- transport, sorption, …

what happens at the surface?
- leaching, transport, dissolution, …

what happens in the bulk?
-composition, phases, grains, cracking, …

Entire scenario might need to be modeled
Lots of coupled processes, unknowns

Waste disposal system model

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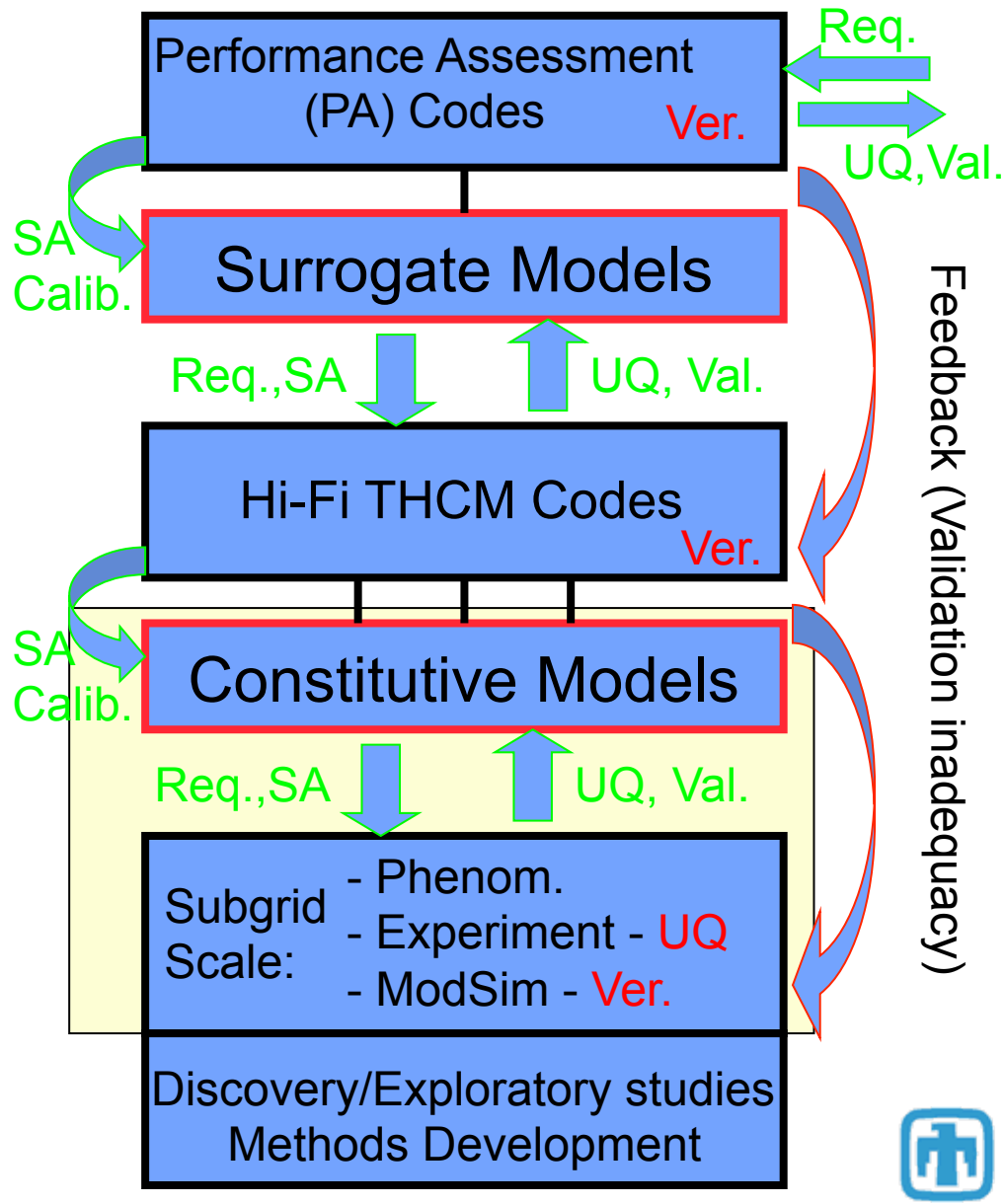
A System with well-defined process flows

Requirements-driven (PIRT)

Qualified applications (Verified)

VV/UQ'd data flow

Traceability, Reproducibility



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Anatomy of a model - two parts

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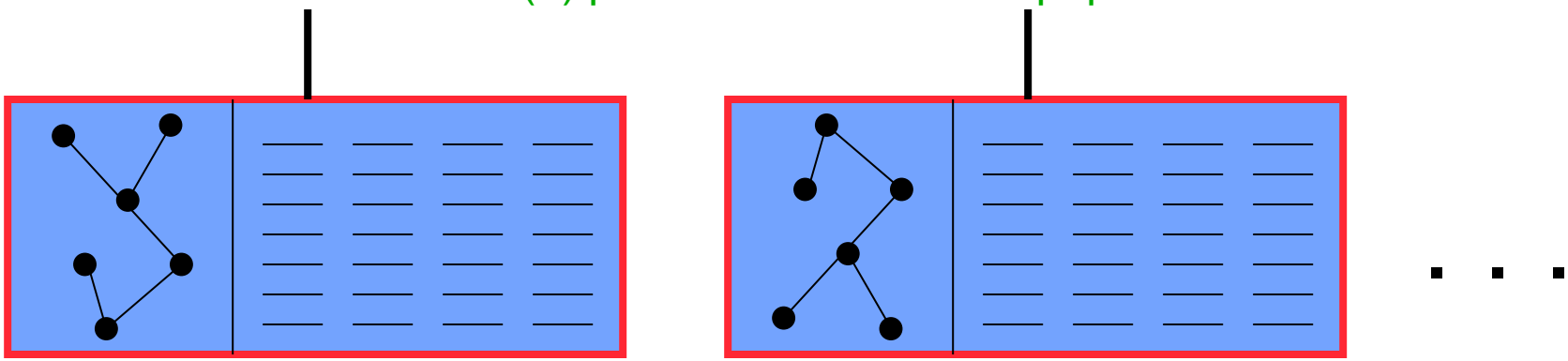
(1) a physics abstraction (e.g. coarse-grained model)
(2) parameter values that populate the model



Model (physics abstraction) | Realization (parameters) | Model (physics abstraction) | Realization (parameters) | . . .

- Phenomenological models - heuristic, irreducible
  - fit and calibrated to specific range
  - interpolative, not extrapolative
- Subgrid-physics-aware models - hand-off multiscale
  - potentially extrapolative (predictive)
  - experimental or mod-sim data
  - there is still fitting (calibration)

This duality a formal (and unsolved) challenge for UQ

Upscaling - "A miracle happens"

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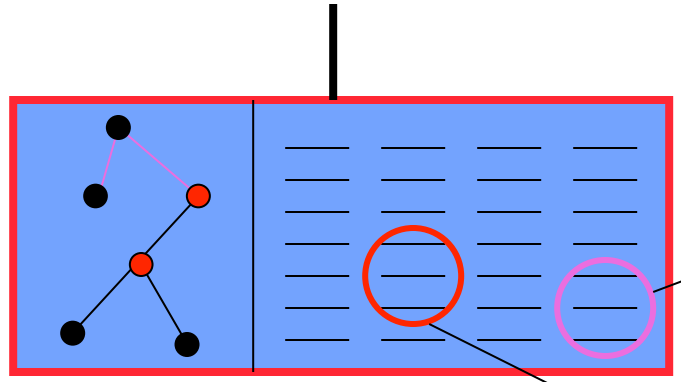

Replace phenomenological data with sub-scale data

Replace phenomenological data with sub-scale data

Two challenges:

1) accuracy of parameters
2) adequacy of physics abstractions (model form)

Model parameters usually refit (calibrated) for validation of application

Internal consistency (e.g. thermodynamic)
Model incompleteness

Physics abstraction mixes parameters (dependencies)

and may not be (quantitatively) reducible to sub-scale processes

Bridging this divide is unsolved challenge (both scientifically and UQ)
… more failures than successes (science), unclear process (UQ)

Requirements triage

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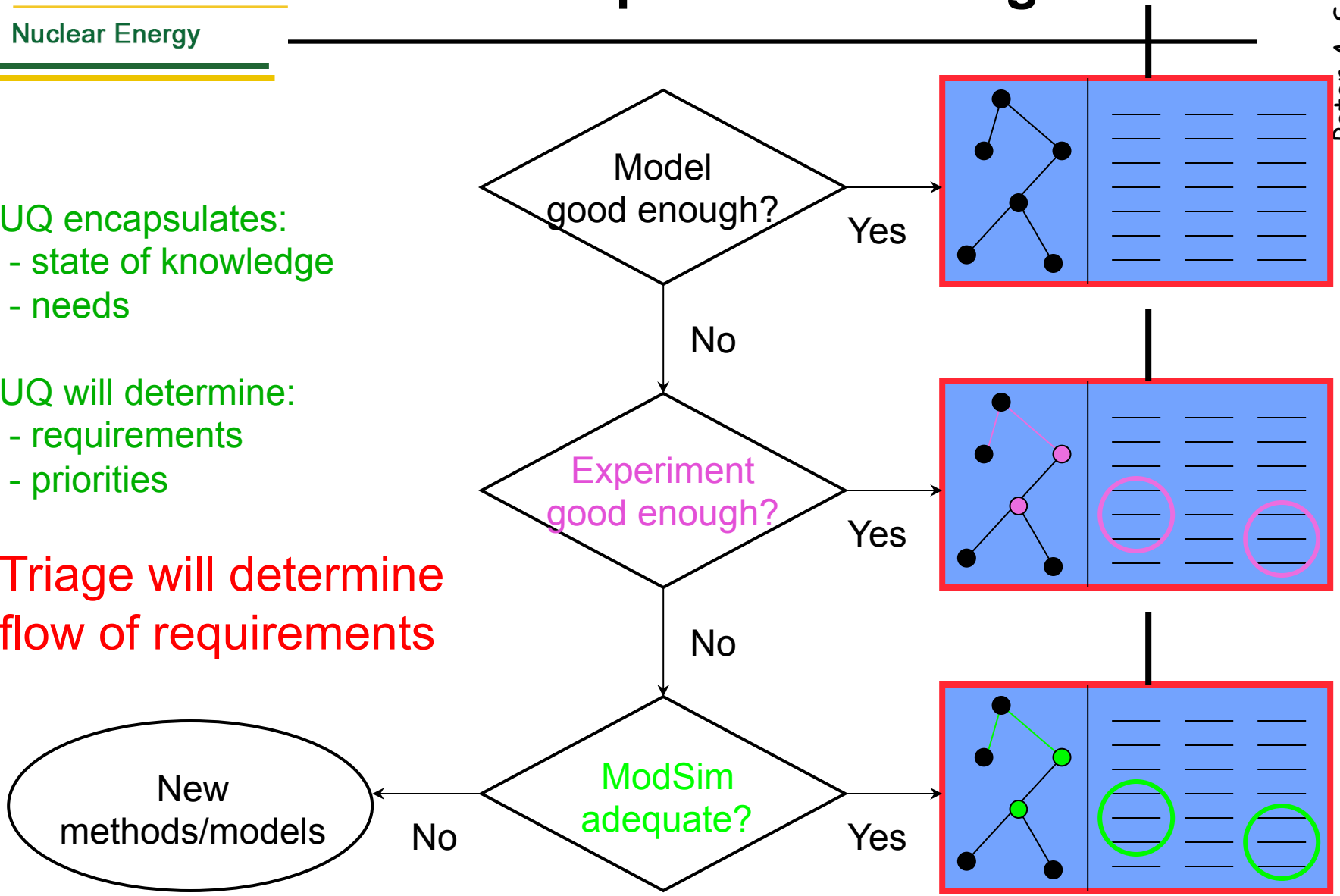
UQ encapsulates:
- state of knowledge
- needs

UQ will determine:
- requirements
- priorities

Triage will determine flow of requirements



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VV/UQ required throughout

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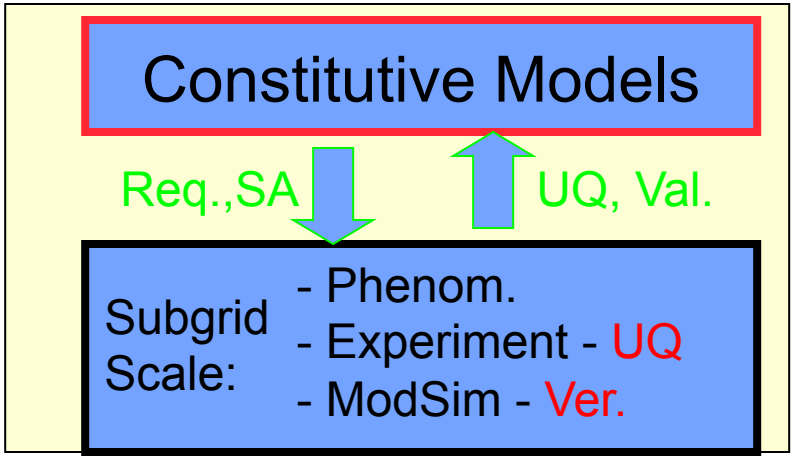
Into high-consequence decisions:
All data/process flows must be …

Traceable - provenance recorded
Reproducible - by others
With quantified confidence - VV/UQ



Required elements from all simulations feeding the system:

1) Necessary - Line-of-sight into system requirements

2) Verified - codes/solutions/models - (confidence in methods)

3) Validated - quantified errors and uncertainties (numerical and model)

4) Documented - sufficient to be reproducible (by others, 10 year later)

Materials Problem: Glass dissolution

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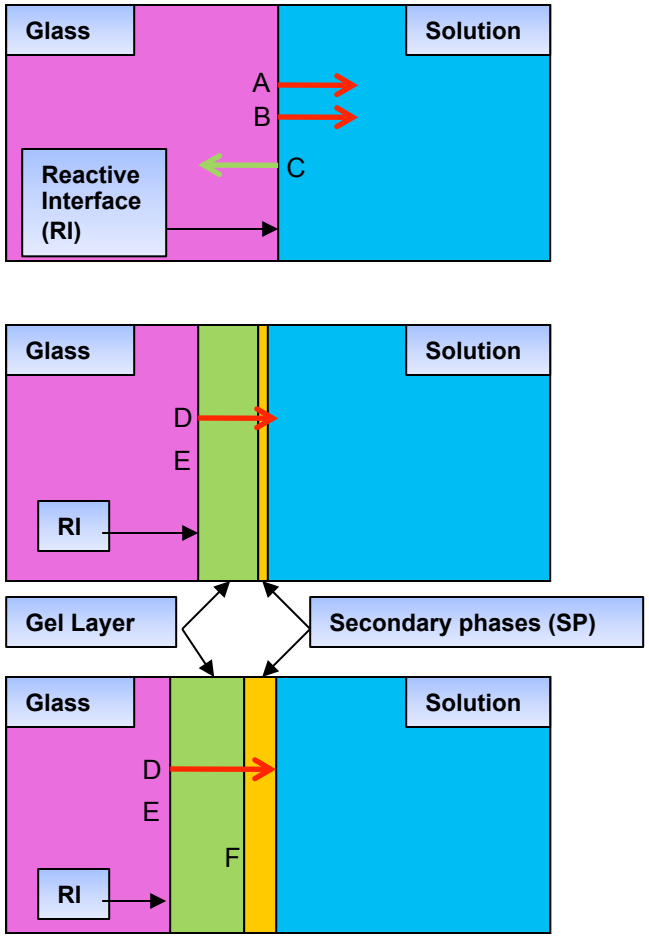

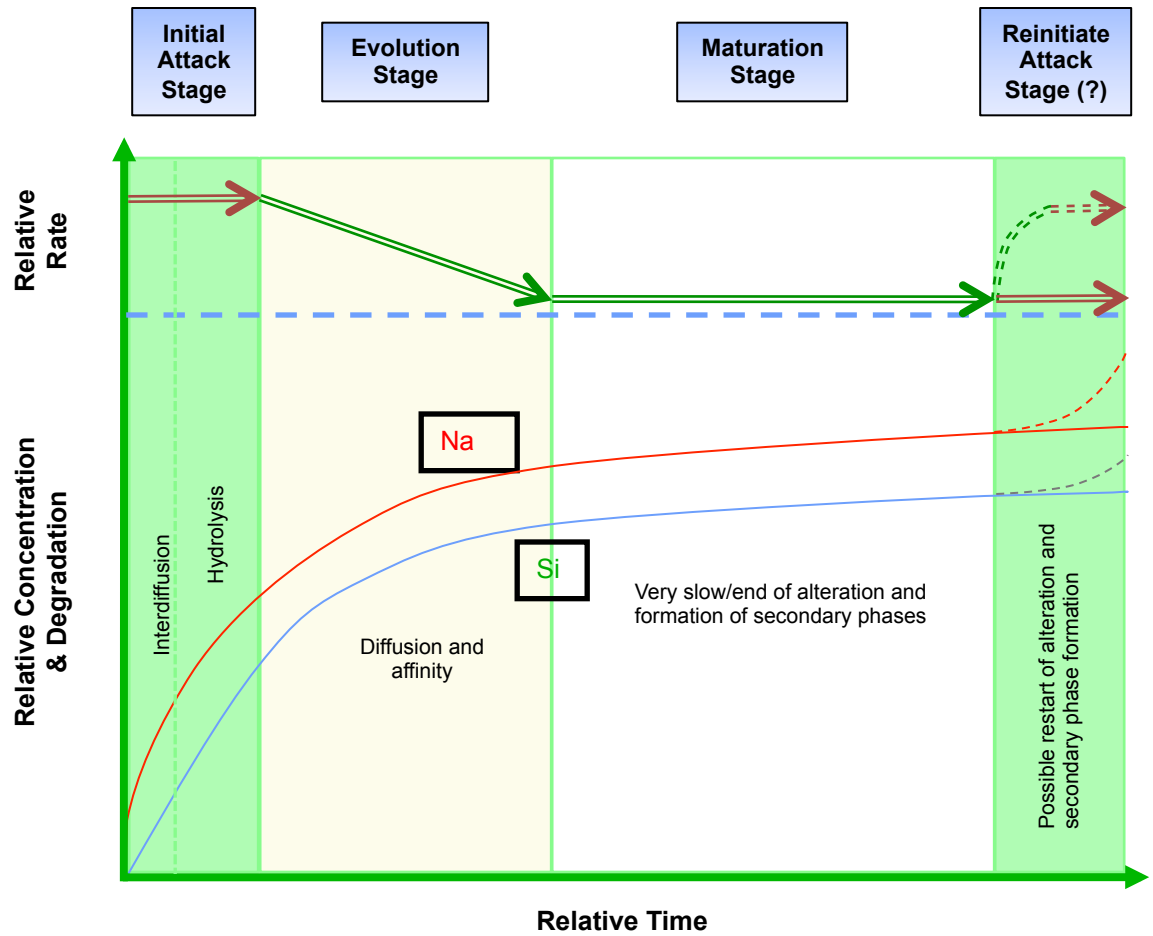

A – rate of alkali surface release
B – rate of Si, Al surface detachment (tends to be limiting)
C – rate of H_2O diffusion into glass

D – rate of silica diffusion through the gel (± SP) layer (at least partially limiting). Other constituents mass transport rates may also be important.
E – the aqueous composition at the RI is not the same as the Solution (aqueous silica concentration especially) and the surface area of the RI may be reduced by glass-gel contact area.
F – the gel and secondary phase layers may be acting as a mantle, in part isolating the fresh glass from the Solution.

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Materials bulk phenomena

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- Structure and chemistry of radionuclide-bearing phases and corrosion products

  - structure and phase stability as function of composition
  - volumetric and conductivity changes
  - cascade simulations, amorphization and recrystallization
  - point defects formation energies (*v*, *i*, anti-site, Frenkel, etc.)
  - point defect migration energies
  - nucleation and growth of gas bubbles, secondary phases, and cracks
  - volume diffusion of chemical constituents (esp. radios) to surfaces
  - grain boundaries, grain structure, microstructural evolution
  - diffusion along grain boundaries
  - surface free energies - exposed surfaces and cracks
  - microcracks, surface charges
  - indiffusion of water, reactions, and mechanical effects

Interface phenomena

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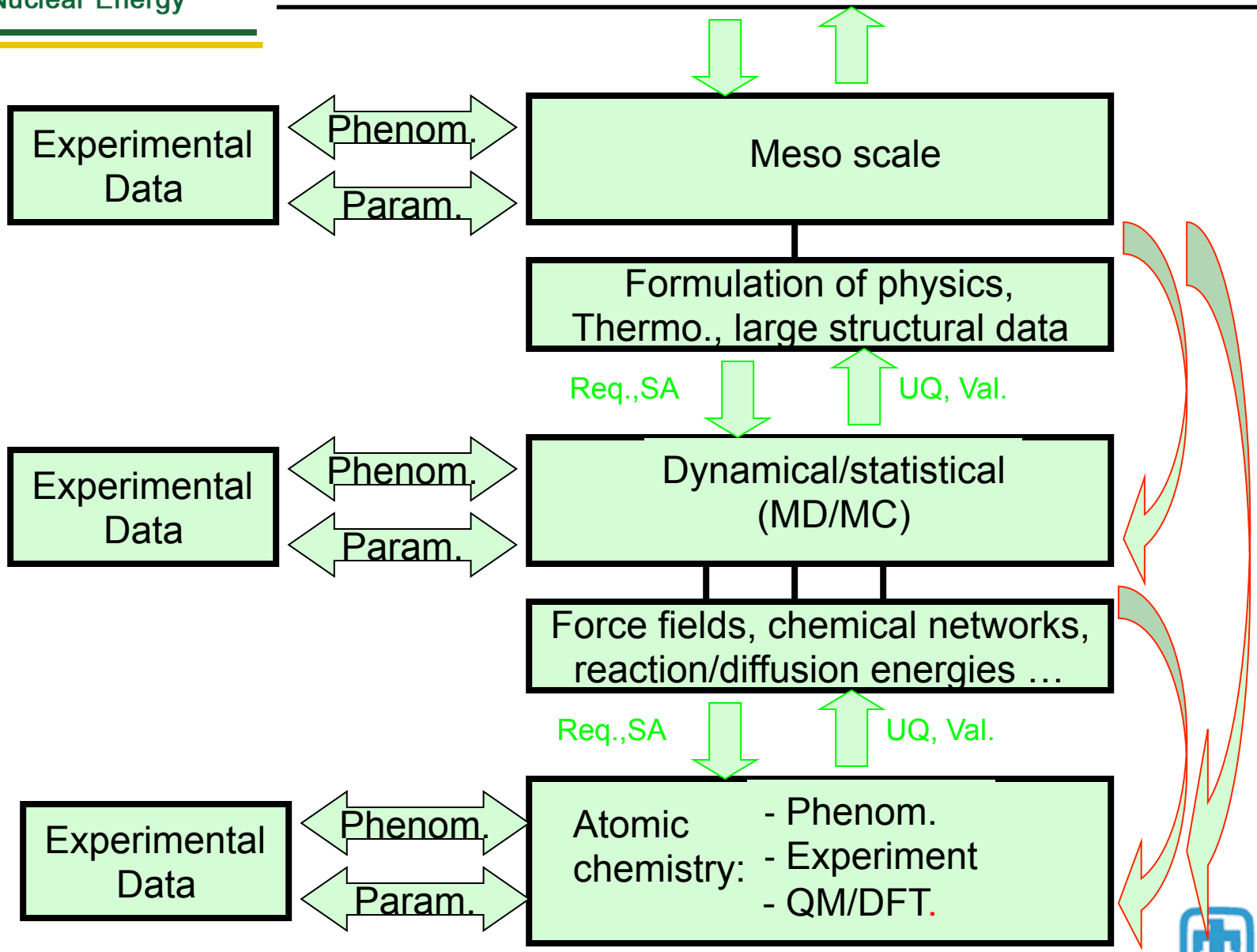
- Chemistry of solid-aqueous interactions: corrosion, dissolution, reprecipitation, (as function of composition, oxidizing or reducing, pH, temperature, …)

  - surface/interface free energies
  - surface site energies and densities
  - energies of surface chemical processes, elemental attacks
    (WF degradation products, H_2O, O_2, H^+,OH^-, H_2O_2, …)
  - migration/diffusion of chemical species along surfaces
  - out-/in-diffusion energies and rates of chemical species
    (water, bulk vacancies, ion exchange, radionuclide redox)
  - surface layer precipitation or dissolution: formation energies and rates
  - microbial effects
  - electrochemical corrosion
  - radiolysis effect on the chemistry
  - fugacities (partial pressures) of species in gas phase
  - equilibrium AND kinetic treatments of each of these

Upscaling within subcontinuum



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Assembly into upscaling: Need for piecewise V&V, UQ

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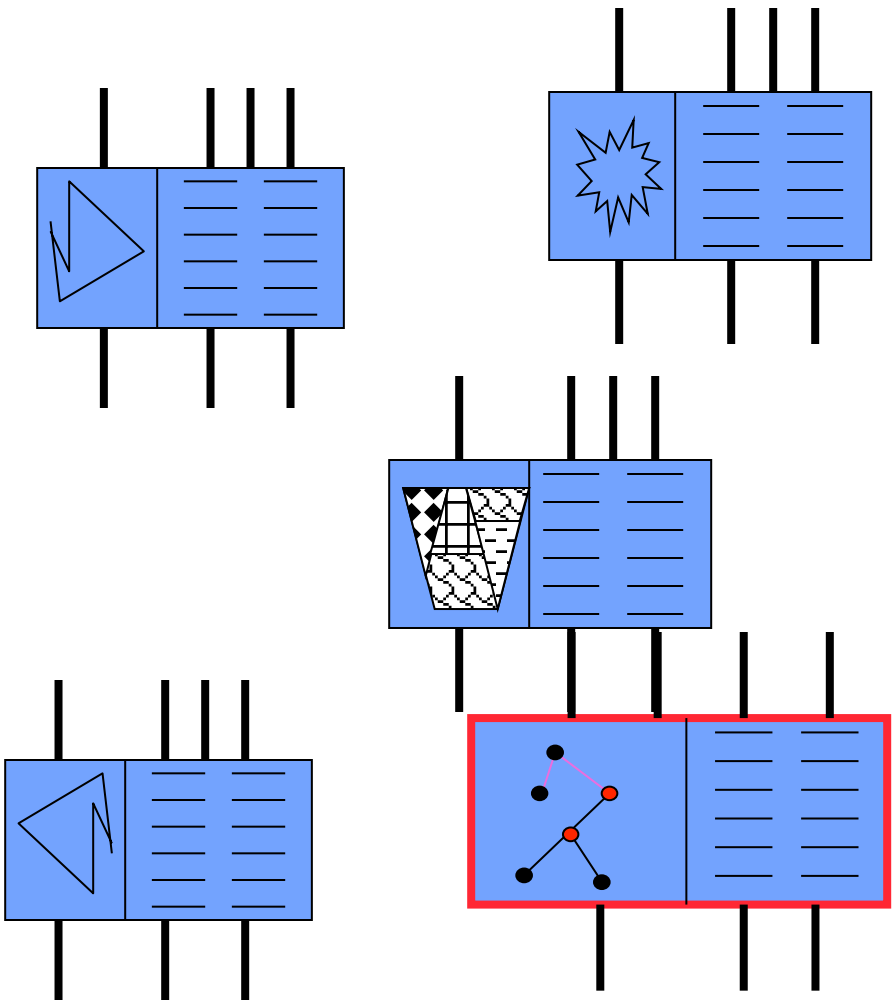

What simulation are you really doing?

Line-of-sight

What are the inputs (looking down)?
- model form/assumptions?
- parameter dependencies?
- how good are they?
- how good do they need to be?

What are the outputs (looking up)?
- what is the output quantity?
- what upscale needs this?
- how well does it need it?
- how good is the output?

Every scale must be up/down-scale-aware
VV-UQ are measure of awareness

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Mapping V&V and UQ onto subcontinuum

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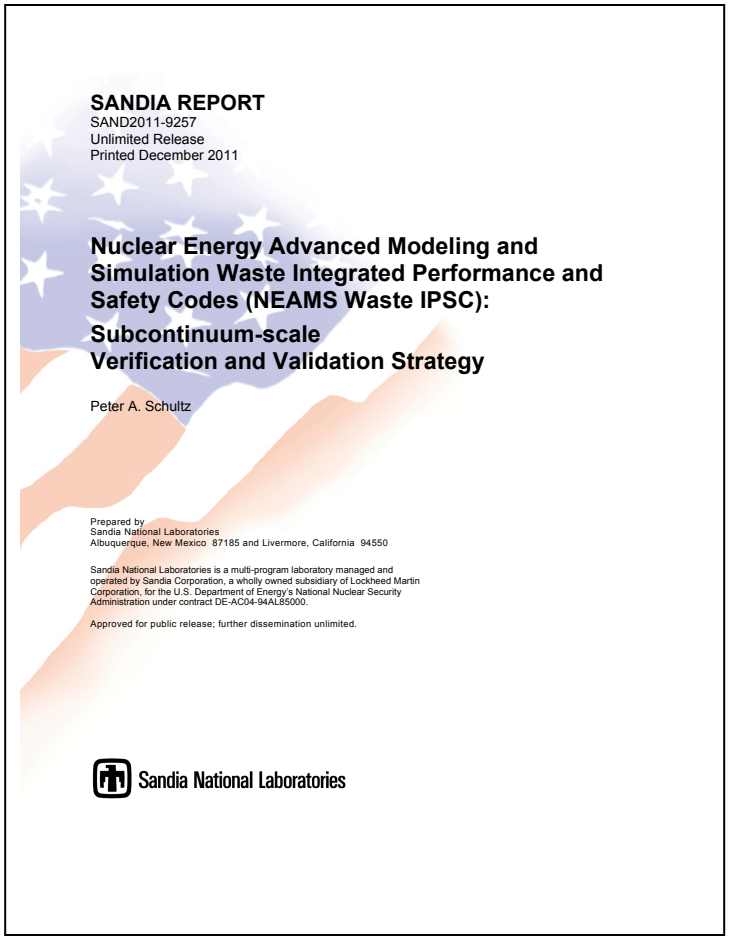

SANDIA REPORT
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Nuclear Energy Advanced Modeling and Simulation Waste Integrated Performance and Safety Codes (NEAMS Waste IPSC):
Subcontinuum-scale Verification and Validation Strategy

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- Presumptive line-of-sight
- Subcontinuum-adapted PCMM

Rigor Level	Risk Level	Example Usage
0	Low consequence	Scoping studies (discovery)
1	Moderate consequence	Design support (development of model form)
2	High consequence	Model qualification (parameterization and validation)
3	Highest consequence	Quantified impact on continuum scale simulation

- Traceability, reproducibility, assessability
- Verification – code, numerics, models
- Validation
- UQ & SA
- Deliberate awareness of numerical vs. physical uncertainties

A start of a conversation, not a solution

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Challenges

- Tyranny of engineering timescale (see: Becker 3:55pm)
  - Most project are 3-5 years (at most) – "physics freeze" even shorter
  - Need for model development/validation data (not just engineering data)

- Upscaling challenge (e.g. several MD talks here)
  - How to propagate UQ through opaque barrier (calibration, model v. numerics)
  - How to define meaningful UQ with undefined physical causality networks
  - How to deal with every-UQ-is-a-custom-UQ analysis?

- Avoiding the drunk-(mathematician)-under-a-streetlamp UQ approach
  - Errors (uncertainties) in materials more model form and unknowable
  - Often too easy to do "simple" numerical analysis and ignore real risks

- Science v. engineering culture - Establish principles of VV&UQ in science
  - Incremental approach that enables credible piecewise VV&UQ
  - Presumptive line-of-sight as organizing principle
  - Articulate/enforce protocols for quantitatively meaningful simulations
  - Graded approach – rigor reflects sensitivity/importance
  - Promote culture of quantitative-confidence science for engineering
    - deliberate and explicit recounting of due diligence

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