Thoughts on Modeling and Simulation in the DOE environment

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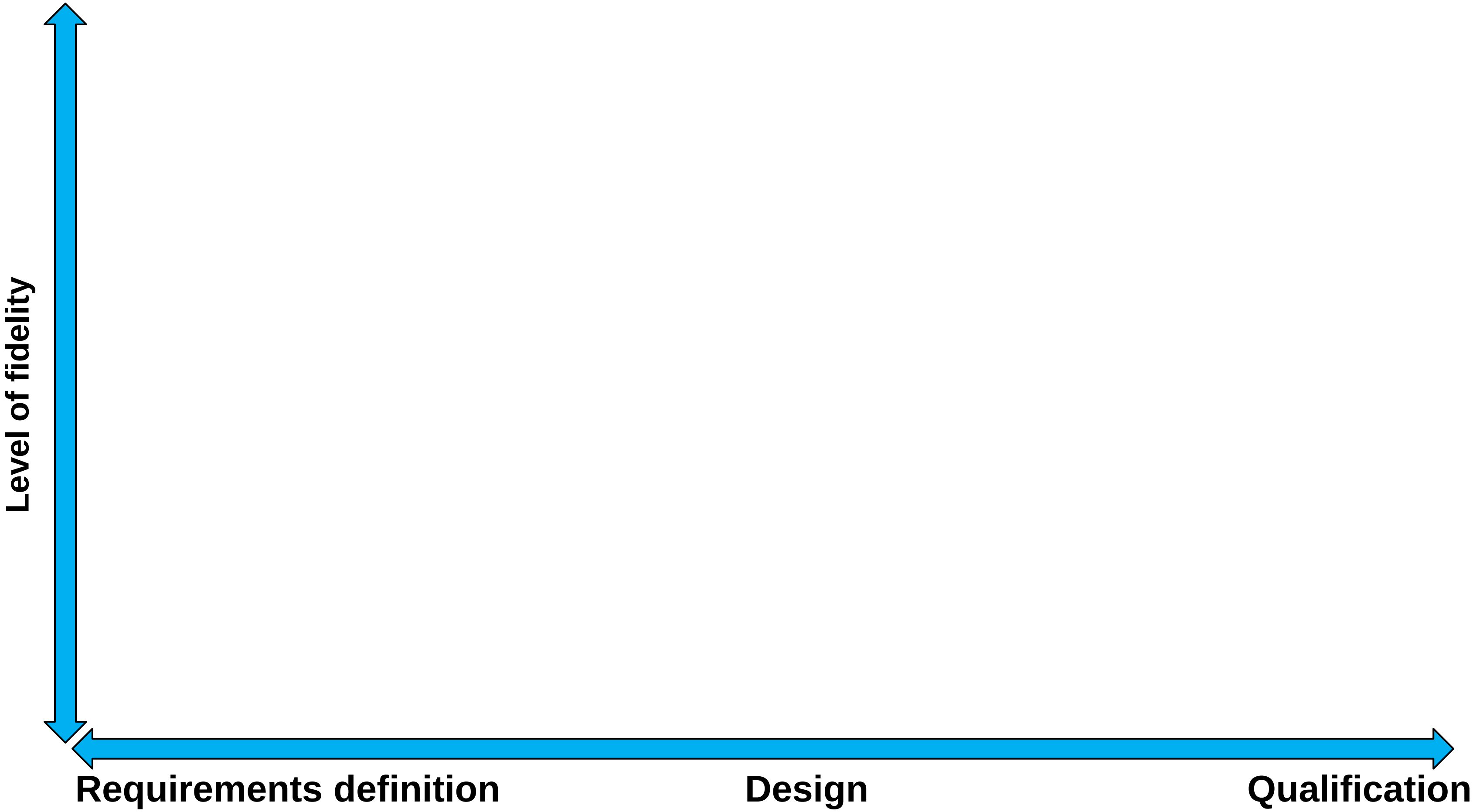
Three phases in the design cycle have different modeling requirements



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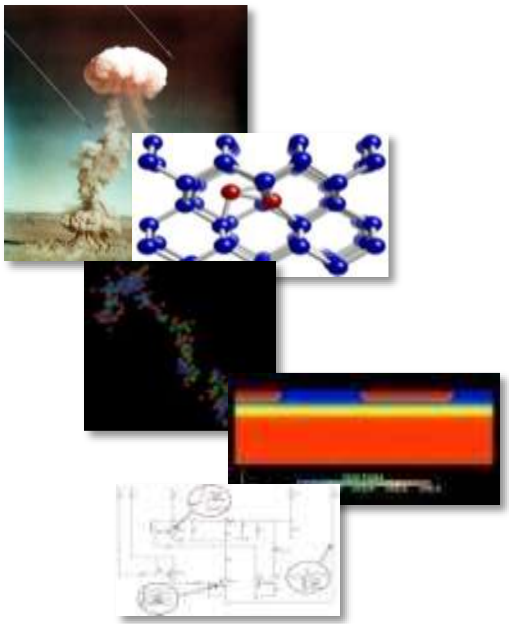
Level of fidelity



High fidelity
Multiple scales and physics
Full environment

Requirements definition | **Design** | **Qualification**

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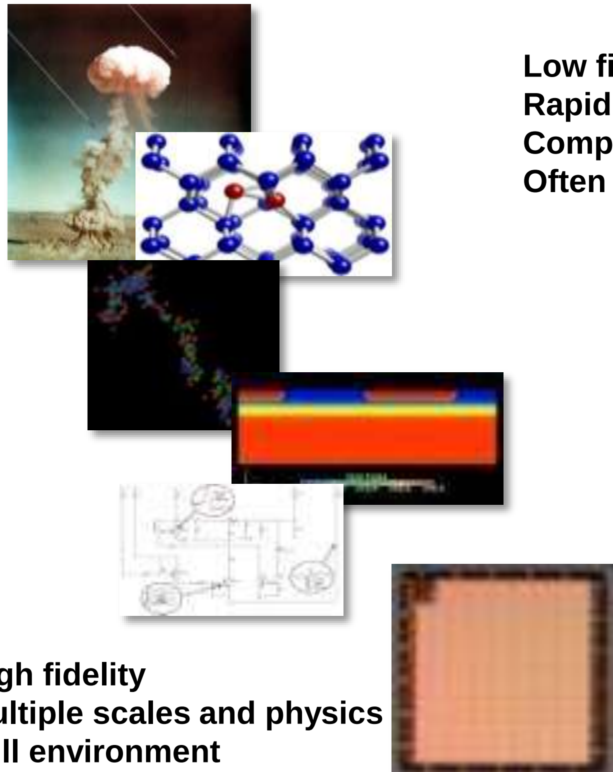

Low fidelity
Rapid turnaround design studies
Component level
Often single physics and scales

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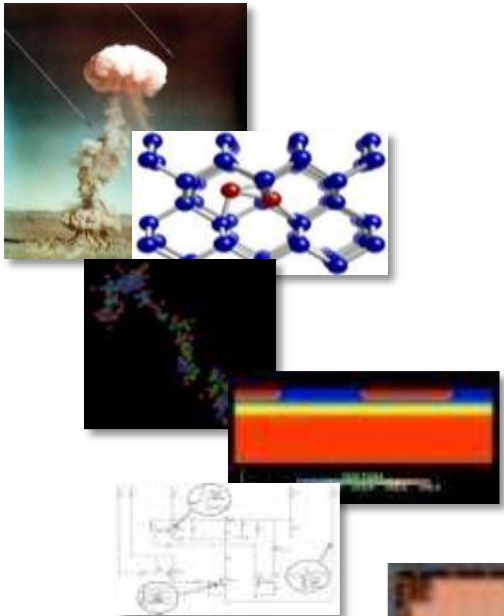

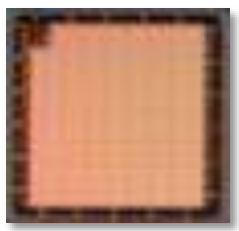

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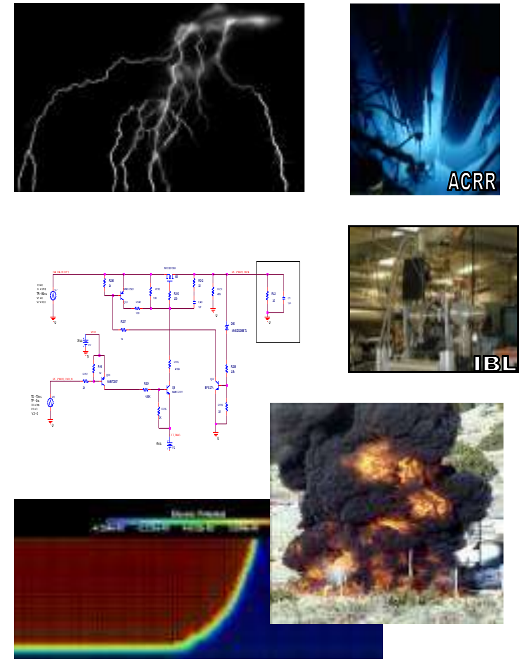

Level of fidelity

High fidelity
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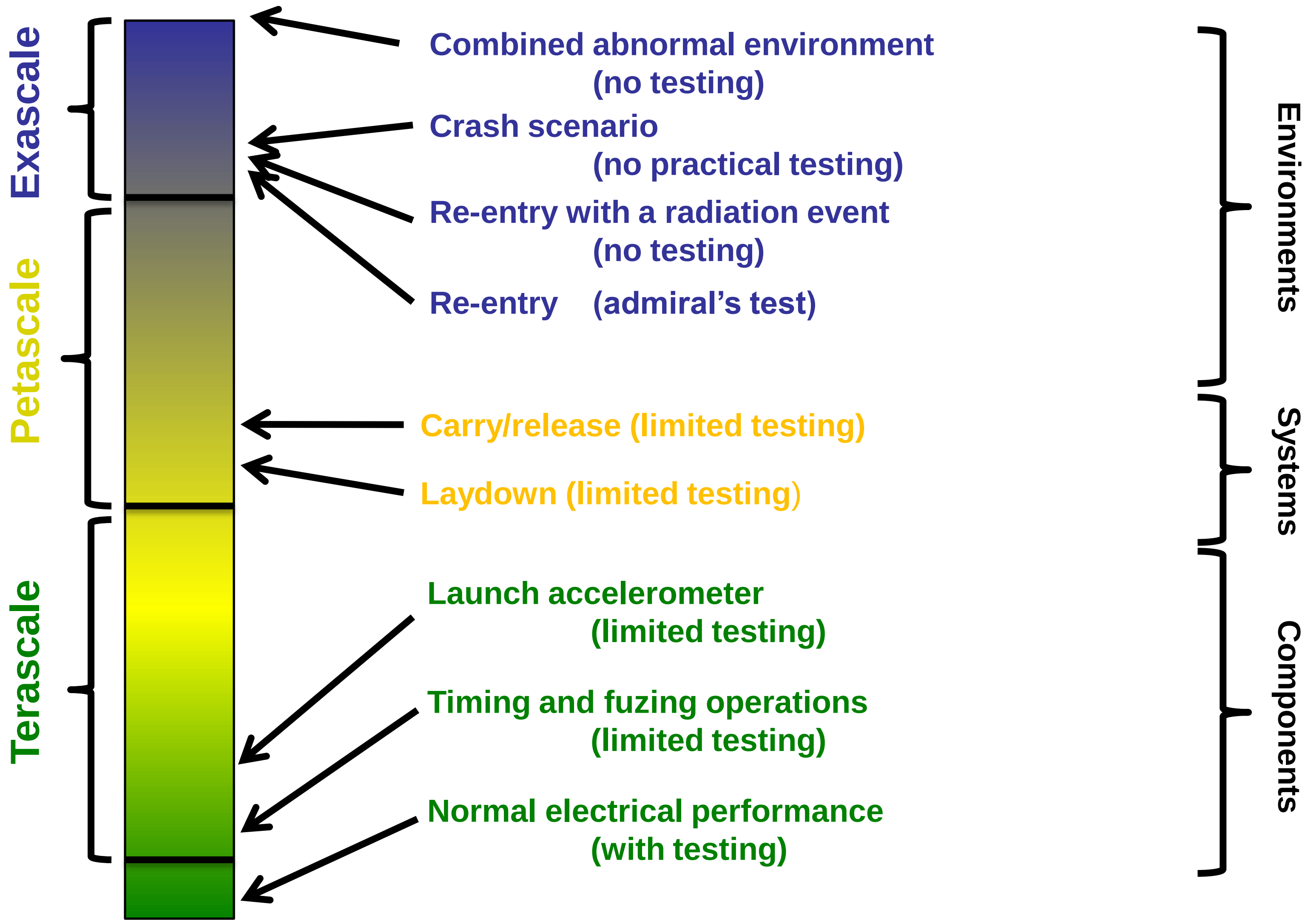
High fidelity
Multiple scales and physics
Rigorous V&V

Requirements definition | **Design** | **Qualification**

How much computing is required for different phases?



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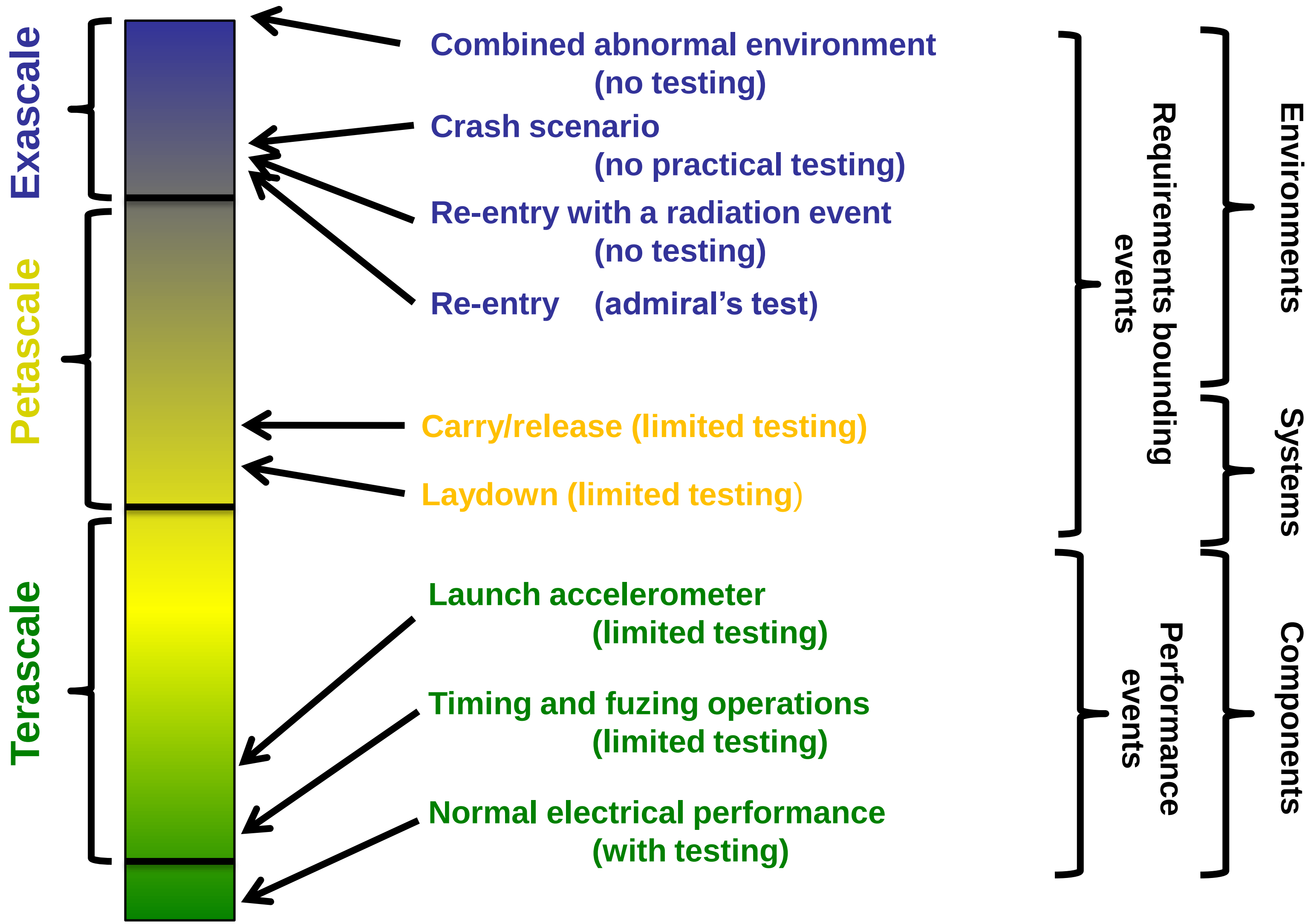

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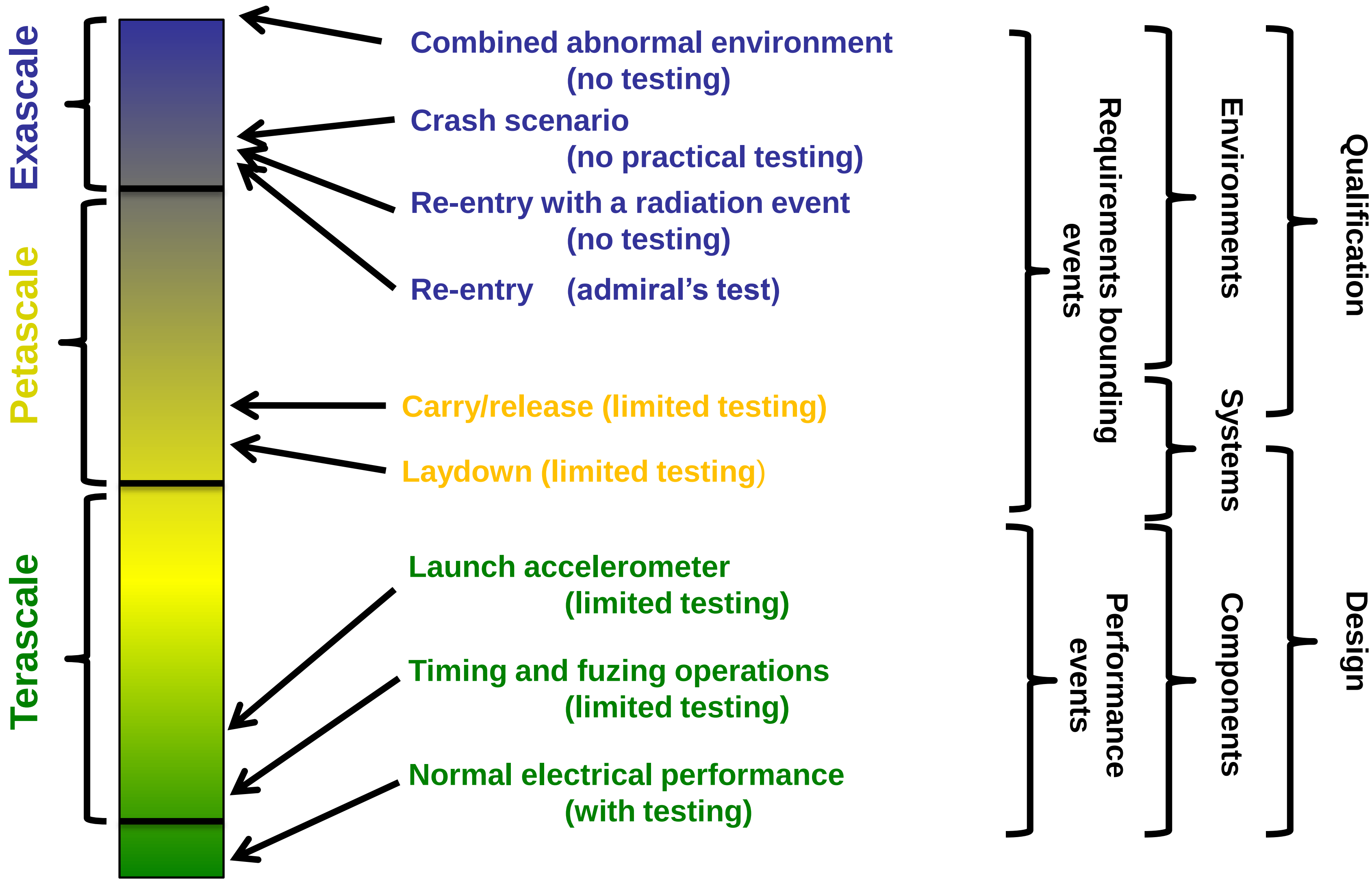
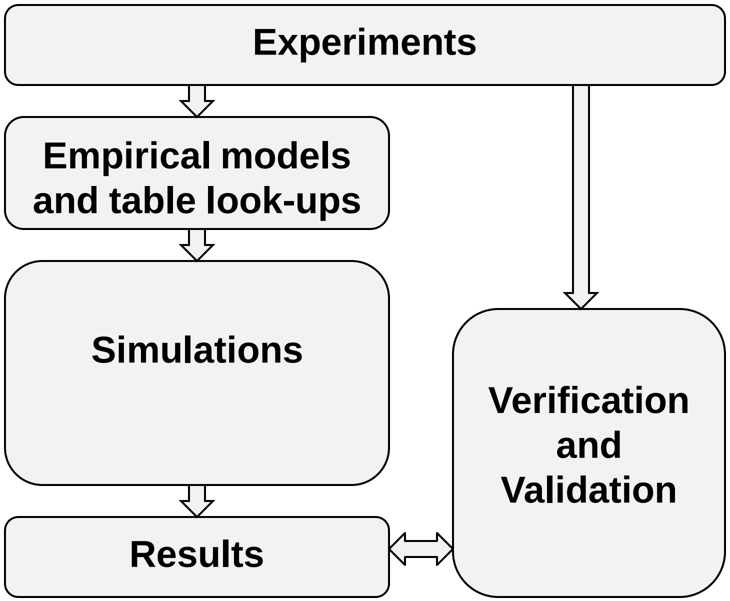


Is physics-based predictive?
Is predictive physics-based?



Observational M&S
- Models derived from observation
- Not predictive
- Cannot validate

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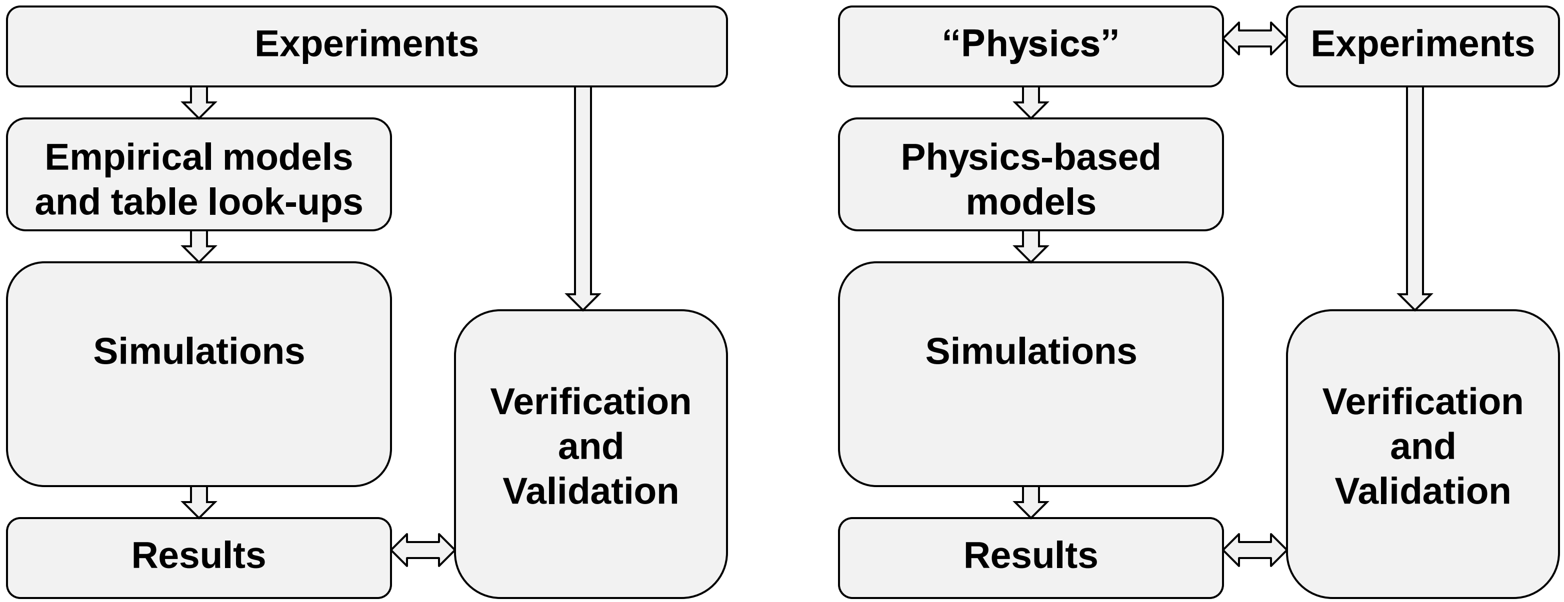

Observational M&S
- Models derived from observation
- Not predictive
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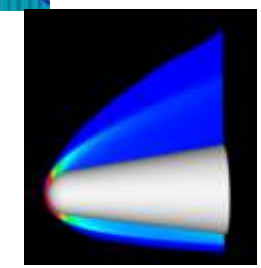
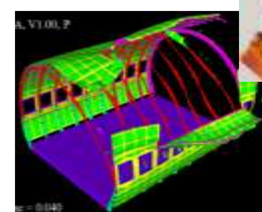
Physics-based M&S
- Models based on "science"
- Can be predictive
- Incorporates multiple scales
- Can validate

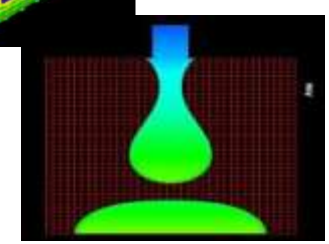
Predictive modeling and simulation must be physics-based and validated

There are many engineering challenges that will rely on predictive modeling and simulation

- **Large Scale/Complex Structural Response:** Structural response due to severe mechanical insult including shock and penetration
- **Predictive Flight Test Simulation:** Simulated re-entry body flight environments including structural load propagation to internal component mechanical response
- **Engine design on a laptop:** Turbulent reacting flows in combustion, predictive simulation code for high-speed mixing & fluid jet break-up
- **Thermal Mechanical Failure:** Abnormal thermal environments with applicability to ship fire, plane fire, …
- **Energetic Material Initiation:** Predictive capability for simulating explosives
- **Electromagnetic Effects:** Lightning with EM coupling
- **Aging:** Predictive capability for physical effects such as hardening, embrittlement, degradation
- **Manufacturing:** Including flows, coating with the ability to predict as-built performance



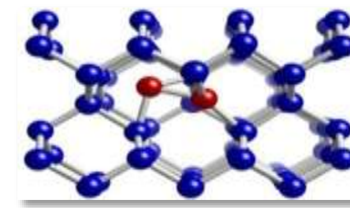


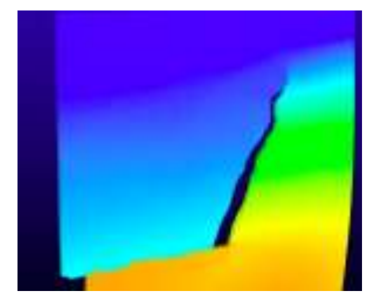


There are many research challenges needed to support a predictive engineering capability

Driven by engineering challenges

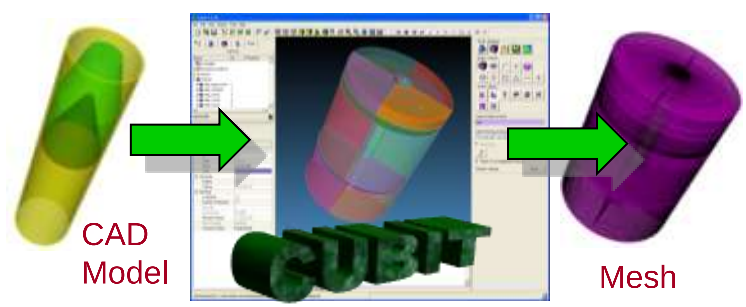
- Validated, predictive modeling approach(es) for ductile material crack initiation, propagation and fracture
- Determining pressure and velocity field turbulent aerodynamic flow fluctuations with structural dynamic load coupling models & testing (e.g. 6-degree of freedom shaker)
- Improved high resolution, time resolved diagnostics: i) imaging fluid break up, ii) characterizing explosive initiation, iii) measuring spatial and temporal plasma properties
- Computationally tractable approaches for multi-scale (10 m – 10 μm) mechanics simulations (e.g. shock/blast to structural dynamics)
- Coupled thermal-mechanical simulation with time/temperature dependent materials properties
- Determining operative lightning-induced failure mechanisms in weapon systems
- Rapid problem set up for large models with different levels of detail





Further out

- Computational design of engineered materials/structures at the continuum scale – with materials science
- Inverse analysis capabilities for failure assessments – algorithm development with computer sciences
- Community geomechanics model that couples thermal/mechanical/hydraulic/chemical response – with geosciences



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V&V should be an intrinsic part of all elements of modeling and simulation

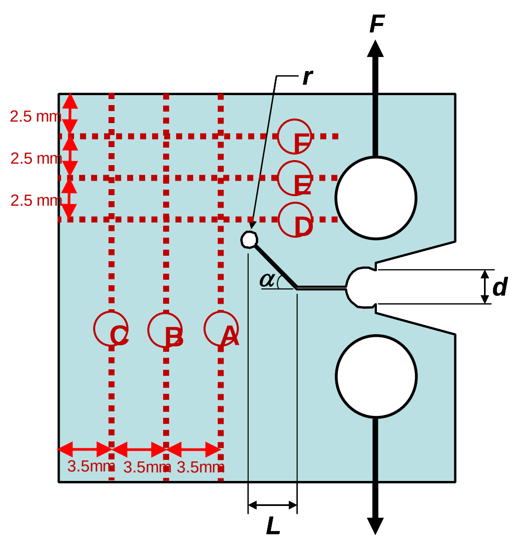
- **V&V/UQ is a part of every analysis**
- **Aspects of "intrinsic V&V" include**
  - SQA standards and rigorous testing methodology
  - Automatic code and feature coverage reports in each log file
  - Dynamic test suites designed around key applications
  - Support for solution convergence for various quantities of interest by users
  - Embedded sensitivities and UQ where possible linked to sample-based UQ
  - Integrated workflow that includes support for computing margins
  - Support for DoE and coupling to validation experiments
  - Code expects models and input to include uncertainties and propagates these uncertainties through simulations
  - Integrated post-processing (e.g., visualization) includes techniques for understanding and presenting uncertainties and margins
- **Customers demand it, analysts perform it, scientists, engineers and developers enable it**

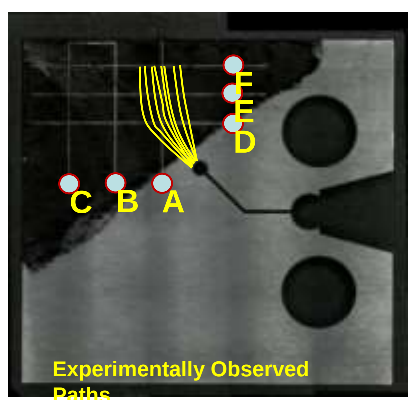
Sandia's X-Prize is an attempt to test to predictivity of fracture and failure modeling and simulation capabilities

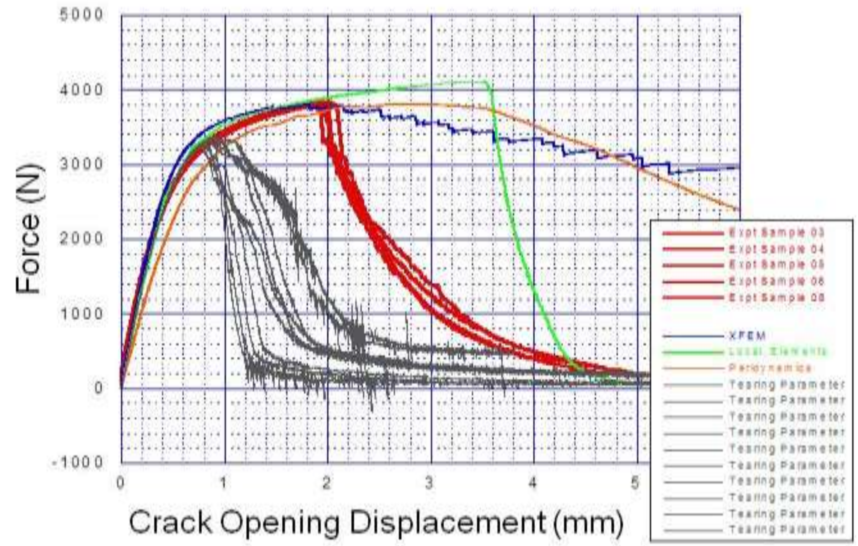
Three challenge problems were defined to assess failure initiation and crack propagation methods

4 Modeling Paradigms Were Used

- XFEM – diplacement and discontinuities embedded in elements
- Peridynamics – meshless method
- Tearing Parameter – plastic strain evolution integral
- Localization Elements – focused on element interfaces







Summary

- Predicting ductile failure initiation and crack propagation remains an extremely difficult problem.
- Wide variation in modeling results suggest our methods are not yet predictive.
- Limits in experimental capabilities were also observed

Closing Thoughts

- Modeling and simulation can impact all phases of the design/qualification cycle, but computing needs are very different.
- "Predictive" simulation is a high bar.
- The goal is really to be able to use modeling and simulation as the basis for decisions.