Modeling and Simulation for Reactor Core Analysis

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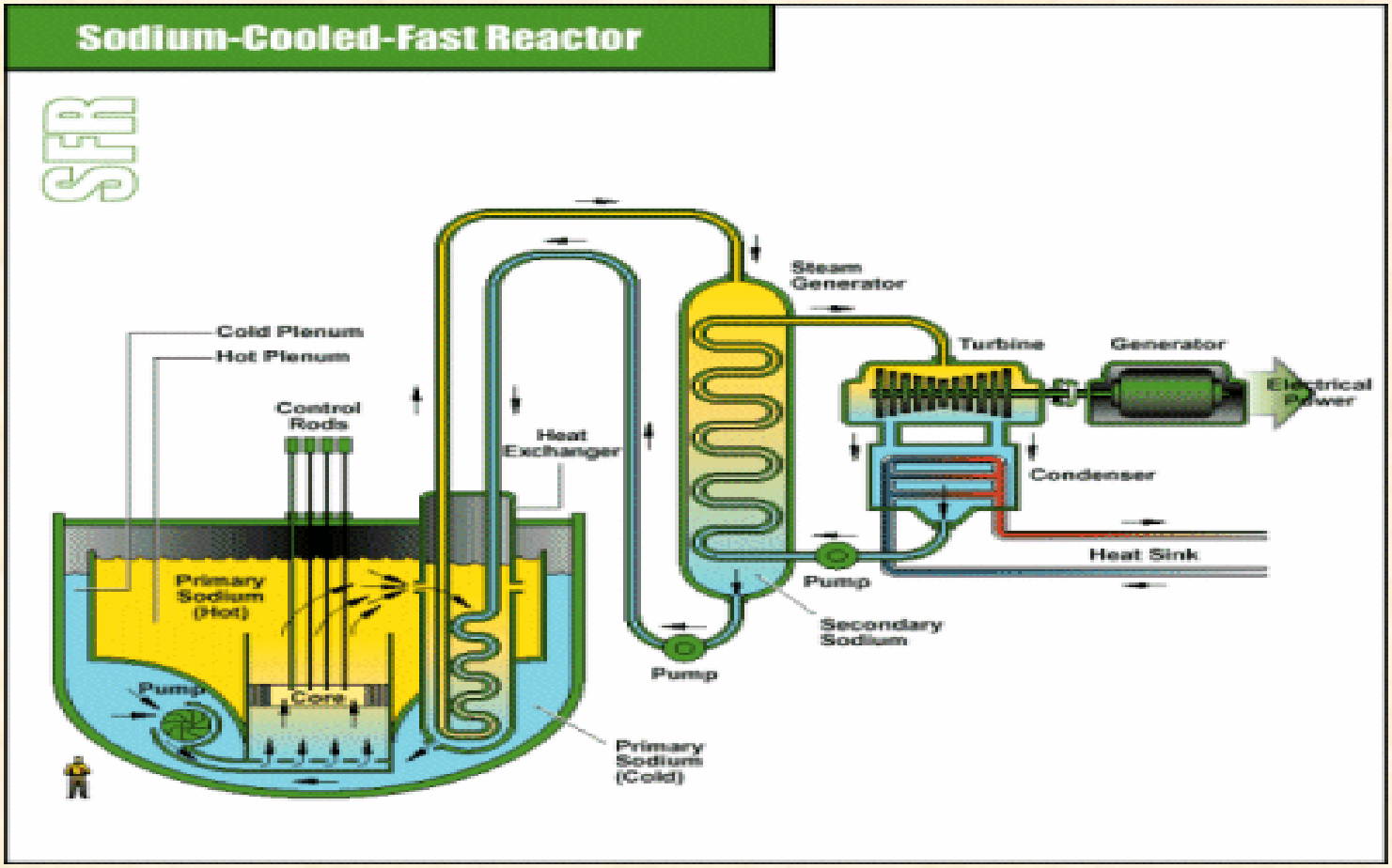
Reminder of 2015 Vision and Assumptions

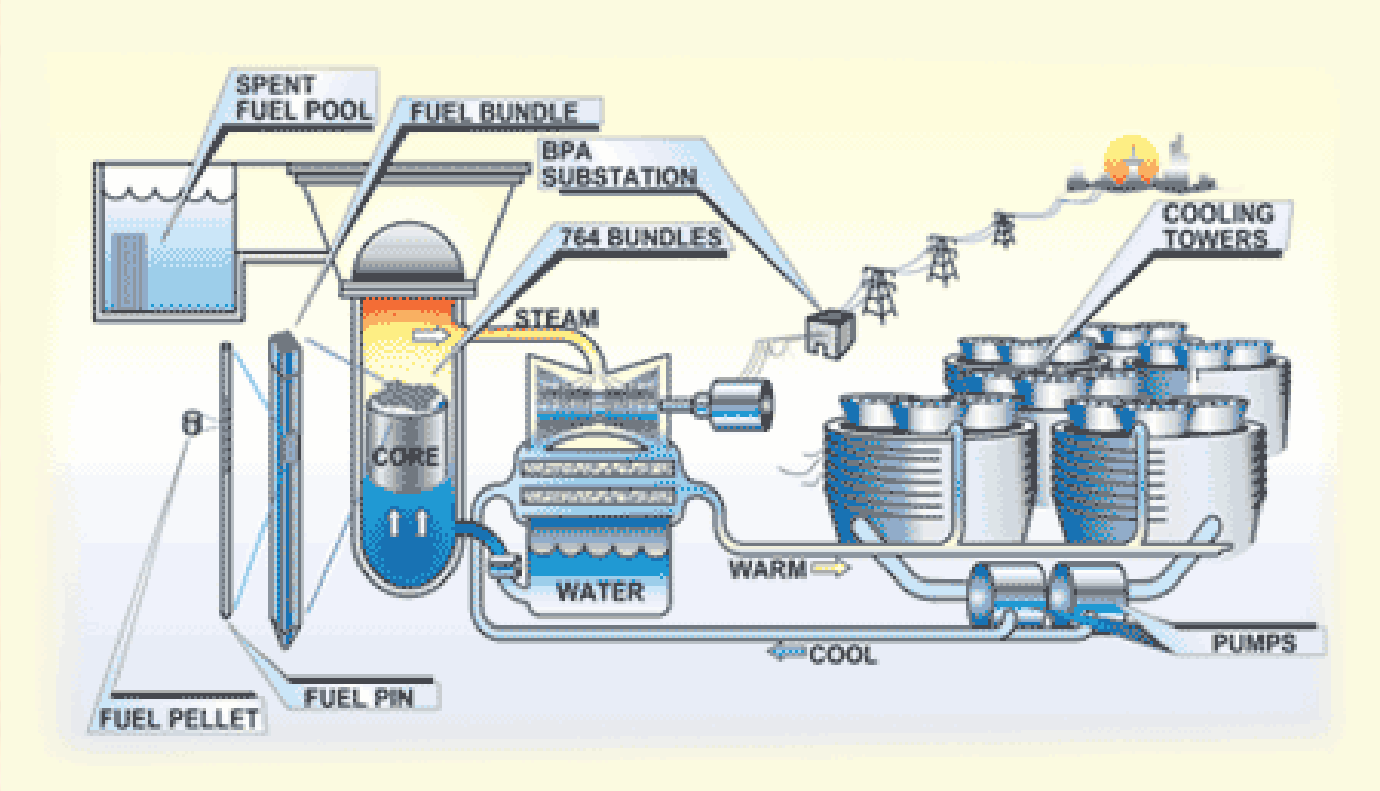
- **Nuclear energy simulation is "on par with experiment"**
  - **First-generation applications are deployed and being used to make mission-critical decisions that previously only experiments could make**
- **A closed fuel cycle solution is designed and being deployed (perhaps on a regional level)**
- **Regulatory agency accommodates new simulation capabilities**

- **An exaflops platform is successfully designed and deployed**
- **Next-generation nuclear energy simulation tools have had 8 full years of DOE program support for sustained research, development, deployment, V&V, and application**
- **Nuclear energy simulation capability requirements, roadmaps, and milestones are established and integrated with a validation experimental plan**

Nature of the problem – Fast Reactor (Advanced Recycling Reactor)



Nature of problem – Boiling Water Reactor



Is vision Correct and Attainable?

- **Nuclear energy simulation is "on par with experiment"**
  - **Known physics, reasonable data: certainly attainable**
    - **Transient reactor simulation with single-phase flow**
    - **Macro-scale transient fuel performance**
    - **Grand mathematics/computing challenge**
      - **Many physics spanning tremendous time/space/momentum scales**
  - **Unknown physics, insufficient of data: potential bottlenecks**
    - **Multi-phase, multi-material, chemically-reactive, turbulent flow**
    - **Macroscopic material properties**
    - **Radiation damage effects**
- **Regulatory agency accommodates new simulation capabilities**
  - **Requires tremendous technical work:**
    - **Advances in multi-physics sensitivity/uncertainty analysis**
    - **Wide-spread implementation of SQA, SQE, and verification tools**
    - **Many multi-physics verification experiments FOR EACH APPLICATION**
  - **Requires tremendous political work:**
    - **Requires completely independent software of comparable (or higher) quality for validation**
    - **NRC budget is 90% cost recovery; how involved can they be with the other 10%**

Is vision Correct and Attainable?

- **A closed fuel cycle solution is designed and being deployed (perhaps on a regional level)**
  - **Large number of challenges – many social/political**
  - **To build in 2015 requires qualified design in ~2010, requires submittal to NRC in 2009, requires qualified DOE software in 2007-8**
    - **New software will not contribute to a 2015 nuclear reactor or reprocessing center**
- **Key challenge to this vision in my mind is the extent at which modeling and simulation can replace (or supplement) experimental data**
  - **Past experience has always required experiment input for data and validation**
  - **Will be required in the future as well, but how much can this be reduced by modeling and simulation?**
- **Will our software be ready for exaflop in 2015?**

What are the Payoffs?

- **Existing Fleet**
  - **Simulation reduces margins increasing performance**
  - **100 reactors @ $1M/day, 5% power increase = $2B/yr for 20+ years**
- **Advanced new reactors**
  - **Optimized designs have no learning curve**
  - **Current fleet: 30 years @ 60% capacity; 10 years @ 90%**
    - **Unrealized potential equates to $328 billion in 2007 dollars over 30 years!!!**
- **GNEP**
  - **Recycling is financially viable**
    - **Fast reactors likely 50% more expensive than Advanced LWRs**
  - **Only one nuclear waste repository is required**
    - **Would strongly like to avoid or delay a 2nd repository**
- **Large potential payoffs from reduction in modeling bias and uncertainty on:**
  - **Improved assessment of safety margins**
  - **Favorable economics (enhanced operation of plants)**
  - **Reduction in the development time for advanced reactor technologies (new and improved fuels for reactors)**
  - **Improved optimization of plant designs**

Modeling/Simulation Importance to Facility Design

- To study fuel cycle and resource issues:
  - Once thru, Pu recycle, Actinide burning, waste disposal, etc.
- To develop and optimize nuclear plant/facility designs
  - Systems design, physical layout, materials requirements, cost, economics
- To demonstrate fundamental safety issues
  - Defensive systems, passive safety, establish licensing basis
- To avoid (reduce) costly prototype construction and operations
  - Critical assemblies, prototypes, intermediate scale plants
- To accelerate optimum fuel selection
  - Fuel irradiation (in addition to simulation) is almost certainly required
- To characterize spent fuel related requirements
  - On-site storage and criticality
  - Shipping cask designs
  - Repository requirements

Simulation Importance to Plant Operation

- To optimize performance in a mixed utility electrical grid
  - Cycle length, fuel resource requirements, economics, outages
    - Analyze 100,000's of core loading options
- To demonstrate cycle-specific safety requirements
  - Static and transient calculations
    - 10,000's of coupled neutronics/thermal-hydraulic/systems computations
- To provide reactor operator support
  - Optimize startup and power maneuvers,
    - 1,000's of calculations per cycle
- To provide on-line monitoring functions
  - Real-time surveillance of safety margins
    - 1000's of calculations per cycle
- To enhance operator training
  - Real-time simulation on full-scope simulators
    - Continuous simulations from cold shutdown to hot operations

Who are the stakeholders?

- **Nuclear reactor vendors – improved tools for development and assessment of advanced reactor designs**
- **Nuclear plant operators/utilities – improved designs and tools to enhance operations of reactors**
- **Department of Energy - improvement in meeting key mission goals (e.g. GNEP)**
- **Nuclear Regulator Commission – better tools for licensing assessment and safety analysis**

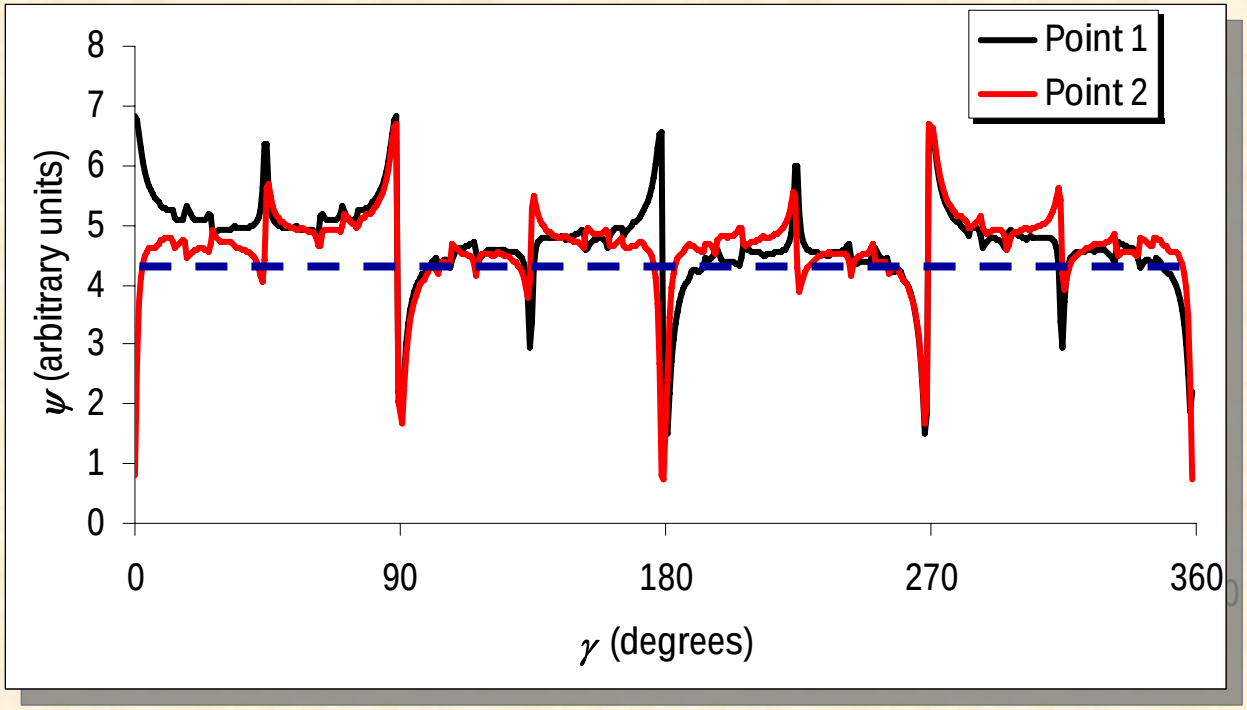
What are the critical timelines?

- **Facility is operational in 2XXX**
- **Construction starts in 2XXX-5**
- **NRC receives license in 2XXX-7**
- **All software has been qualified in 2XXX-9**
- **If software is available in 2015 impact would be on reactors starting up in ~2024.**
- **Complete multi-physics V&V in 2013 & 2014**
- **Single physics V&V completed by 2013**
- **Regular use of developmental multi-physics software by 2013**
- **Regular use of single-physics software by 2011**

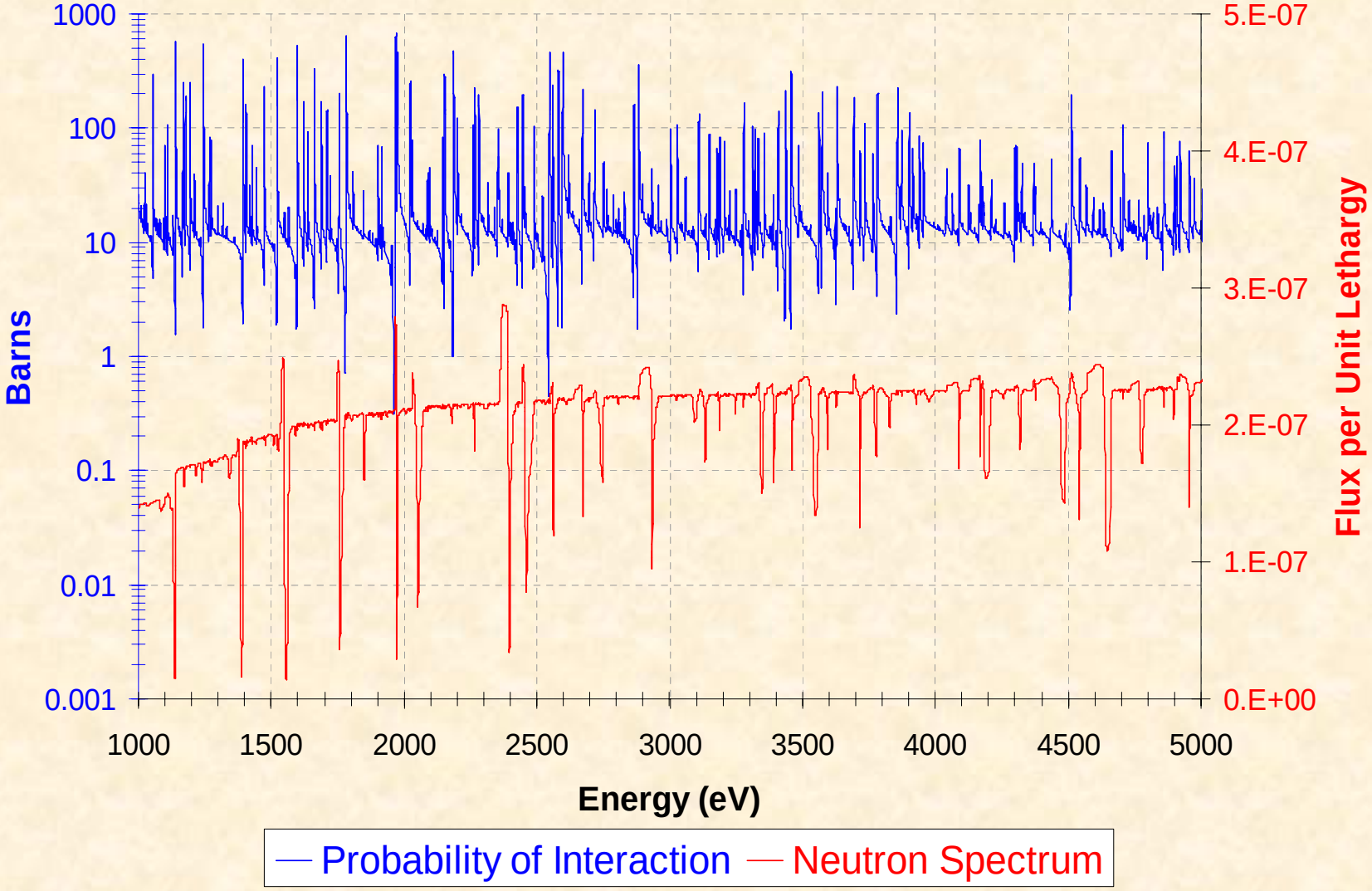
What are the Technology Barriers and Facilities?

- **Time-scales**
  - **um (neutron transport, turbulent vortices), ms (nuclear kinetics, conduction, rad. heat tfer), sec (convection), days (nuclear decay), weeks (nuclear transmutation , fuel restructuring), years (material degredation)**
- **Length-scales**
  - **Molecules (material properties), crystals (nuclear data, material properties), um (fuel restructure, turbulent vortices, bubble formation)… pressure vessel (10 m^3), containment (100 m^3)**
- **Momentum-scales**
  - **Nuclear resonances**
  - **Angular dependence in neutron transport**
  - **Turbulent flow**
- **We are far behind… we are likely missing important physics that we don't even yet realize!**
- **Key technology barrier is that reactor-specific analysis tools are not being developed on a large-scale for the larger, parallel computing systems.**
  - **Some relevant work performed under ASC and for standard engineering tools (CFD, structural)**

Example neutron angular direction distribution



The Fine Energy Resolution of the Solution is the Weighting Function to Create a "Multi-Group Cross Section Set"



Remember Limitations to Simulation Accuracy

- **Mechanical knowledge:**
  - **Manufacturing fluctuations/uncertainties (e.g., IFBA coatings)**
  - **Mechanical changes (e.g., BWR channel bowing)**
  - **Crud buildup (e.g., axial offset anomaly)**
  - **Fuel cycling history (e.g., fission gas migration)**
  - **Fuel pin thermal conductivity degradation (e.g., burnup degradation)**

- **Feedback modeling**
  - **Where is the coolant? (e.g., flow anomalies)**
  - **Local hydraulic information (e.g., bubble level of detail?)**

- **Data uncertainties**
  - **Measured data (ENDF/JEF) cross section uncertainties**
  - **Unresolved resonance models**
  - **Bound thermal scattering models**
  - **Energy yields from fission, gamma yields, capture gamma production**
  - **Knowledge of reactor power and flow operational conditions**

What is the Technology Roadmap?

- **Development needed for:**
  - **Basic Science – Fuel/Materials fundamental properties**
  - **Reactor Core – Neutronics/Thermal/Structural/ Fuels Simulation**
  - **Reactor System – Seismic/Balance Of Plant**
- **Likely represents 4-6 major code development projects, many of which will need to be coupled**
- **Incorporation of codes into licensing basis, design and analysis procedures, and operations support**

What are the major annual program gates?

- **Learn what we're missing (2008)**
  - **Couple "low"-fidelity solvers with all the physics**
  - **Set requirements for new software tools**
- **Get each physics package right (2011)**
  - **Robust SQA, SQE, validation, verification on day 1**
  - **Increase phase-space fidelity and resolution**
  - **Designed for multi-physics coupling and HPC**
  - **Propagate all data and computational uncertainties**
- **Analyze the full system (2013)**
  - **Determine sensitivities, discover missing physics/data/**
- **Fill in the holes and first available, production ready tools (2015)**

What are the management and technical risks?

- **A key management risk is that the distribution of technology experts across various laboratories, commercial enterprises, and universities**
- **A technical risk is not including an appropriate experimental program to provide data needed for modeling and sim program**
  - **Quantification of simulation methods accuracy and precision is important if we are going to increase our reliance on them.**
  - **How are we going to accomplish this is a way that will meet regulatory requirements?**
- **Another technical risk is that there are multiple methods and approaches that are suitable for these problems, Funding only one approach will introduce risk – diversity is needed.**
  - **Diverse modules that are interoperable**
- **New policymakers = new "goals" for the project. Commit to 4+ year funding cycles (SciDAC-like)**

What are the budget estimates?

- **For each multi-physics code team:**
  - **15-30 FTE in FY08 with 10% annual increase**
  - **Diverse technical expertise on each team should include at least…**
    - **3 “computational physics” expert for each “physics”**
    - **2 “math/CS” expert for each “physics”**
    - **2 “experimental” experts for each “physics”**
    - **2 software quality experts**
    - **2 multi-physics experts**
    - **1 computer hardware expert**
- **Experiments and experimentalists**

Discussion

- **We'll will always need experiments (perhaps at a smaller scale or a fewer number)**
- **Regulated environment**
  - **We need the ability to put error bars on our results (all inputs have uncertainties and we will have modeling errors and methods inaccuracies)**
  - **A case will need to be made that the simulation accuracy is sufficient to ensure public safety**
- **Need to add fidelity/resolution – but will have to handle all of phase space + multi-physics detail**
- **Coupling and scaling of multi-physics algorithms is an issue.**