A Random Walk Toward Advanced Modeling & Simulation Capabilities in Nuclear Engineering

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Drivers for Nuclear Energy Advanced Modeling and Simulation Needs

- Economics
- Licensability
- Security & Safety

Key Areas To Model

- Materials
- Fuels
- Thermal-hydraulics
- Neutronics
- Structures
- Separations & Safeguards
- Waste Form

Common Attributes Desired of Nuclear Energy Advanced Modeling and Simulation (NEAMS)

- Multiphysics capability
  - FRR simulation requires coupling of T-H, neutronics, structures and fuels
- Multiscale capability
  - We will not be able to nor need to model every phenomena at the fine scale
- Higher-order phase space treatments
  - To achieve fidelity within computational resources
- Exploitation of leadership class computing
  - Introduction of parallel constructs and clever memory management

Common Attributes Desired of Nuclear Energy Advanced Modeling and Simulation (NEAMS)

- Verification & Validation
  - As part of code development plan
  - Driver for experimental results required
  - Incorporating Uncertainty Quantification
- Automated Data Assimilation
  - Data adjustment (along with posterior uncertainties) based upon new experimental results
- User Friendly
  - Robustness, visualization, and automation, e.g. optimization

Where Are We At?

- Multiphysics
  - Have tightly coupled core neutronics/T-H capability, with limited coupling to fuel thermo-mechanical model and other physics phenomena
  - Most significant challenges are likely in fuel modeling, e.g. current codes may have eight different physics packages loosely coupled and heavily based upon correlations
  - Such coupling will lead to additional complexities, e.g. strong nonlinearities, well posedness of solution, and moving material interfaces.

Where Are We At?

- Multiscale
  - ❖ Space scales difficult/Time scales **super** difficult
  - ❖ Have always used approach in neutronics
    - ➢ Evaluate Nuclear Data => Preprocessing (NJOY) => Resonance Treatment => Lattice Physics => Core Simulator
    - ➢ Approach: Start with great energy, angular and spatial detail for small spatial subdomains and end with little energy, angular and spatial detail for the large spatial domain.
    - ➢ Trouble: One-way street problem!
      - ✓ Some interesting ideas exist using subspace methods to formulate a two-way street approach while achieving consistent closure.
      - ✓ The curse of resonances, which are approximately treated.
  - ❖ Evolving capabilities in thermal-hydraulics (DNS to Components) and materials (ab initio to fracture mechanics).

Where Are We At?

- Higher-order Phase Space Treatments
  - Temporal: Abandoning operator splitting approaches for multiphysics problems to utilize higher-order treatments
  - Energy: Expert judgement on energy group structure still prevails. There has to be a better approach!
    - Now can calculate scattering kernels using ab initio code to get classical potential function followed by use in molecular dynamics code. But we still cannot calculate cross-sections without considerable approximation, e.g. optical models, except for simplest nuclei.
  - Spatial: Lots of alternatives with higher-order methods.
    - Many times mesh refinement is preferred approach due to material heterogeneities. However, continued mesh refinement may invalidate physics captured in model being used, e.g. diffusion theory and fluid flow.
  - Angular (neutronics): Several alternatives developed to address, e.g. quasi-diffusion theory & generalized equivalence theory.

Where Are We At?

- Exploitation of leadership class computing
- Nuclear energy enterprise used to lead in using latest high-end computing resources, but now other enterprises lead, e.g. aeronautics, pharmaceutical, automotive, and weather forecasting.
- Lots to learn from other activities, e.g. ASC & SciDAC
- Needed at least in research phase, many times in support of developing understanding & coarser-scale models, and supporting V&V.

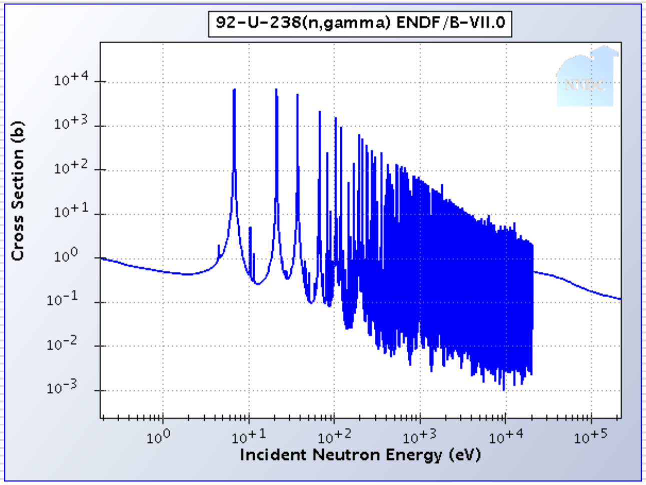
Where Are We At?

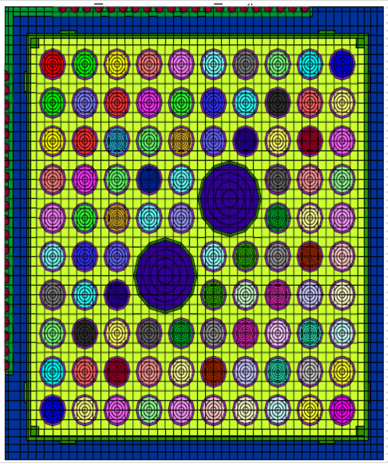
- Verification & Validation

- ❖ Without industry and regulatory acceptance is doomed.
- ❖ Error & Uncertainty Quantification: Desire knowledge of errors & uncertainties based upon source, i.e. numerical treatment, modeling, epistemic uncertainties (e.g. data including correlations), aleatory uncertainties (random phenomena), and initial & boundary conditions.
- ✓ Until recently could address data uncertainties only if data field small (forward perturbation [DAKOTA] or Perturbed PDEs [SUNDIAL]) or response field small (adjoint based method for linear problems). Now via Efficient Subspace Method (ESM) can address simultaneous large data and response fields.
- ✓ Data uncertainties (including correlations) dependence on state condition needs further attention.

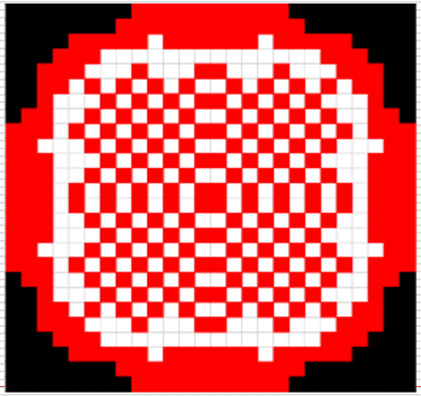
BWR Calculational Sequence

ENDF Library
XS processor
Multi-Group Library
Lattice Physics
Few-Group Library
Core Simulator
Core Observables

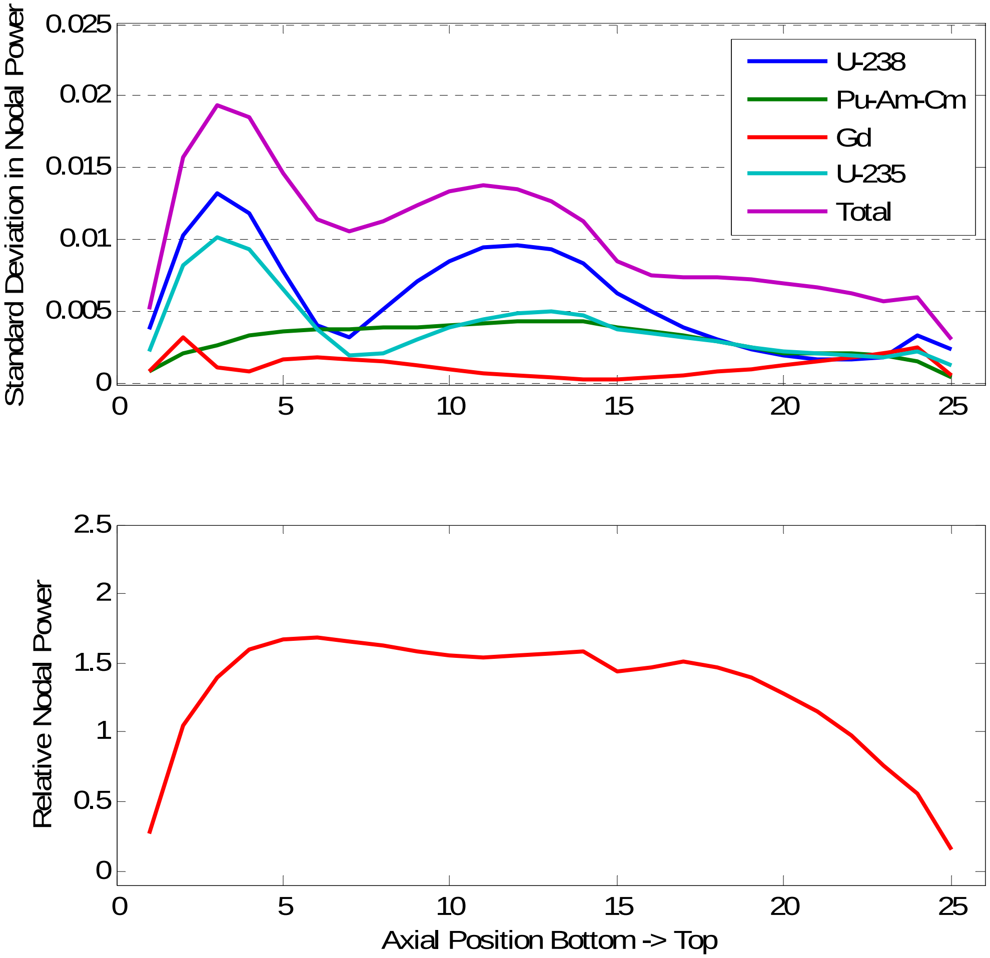




GE14 10x10 lattice design

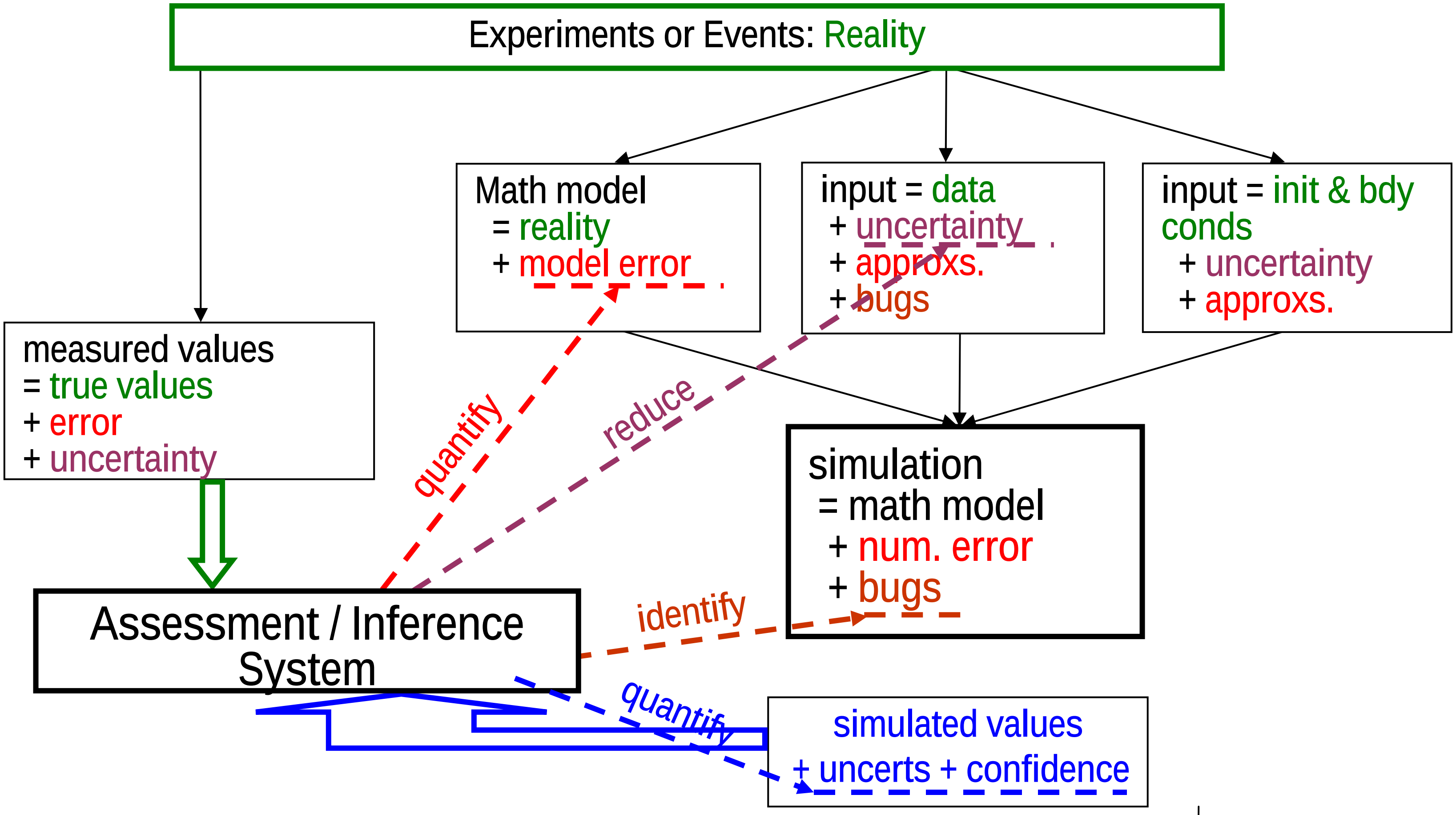


FG Cross-section UP



BOL Uncertainty Profile

We must go beyond traditional V&V and UQ.



Experiments or Events: Reality

measured values
= true values
+ error
+ uncertainty

Math model
= reality
+ model error

input = data
+ uncertainty
+ approxs.
+ bugs

input = init & bdy conds
+ uncertainty
+ approxs.

simulation
= math model
+ num. error
+ bugs

Assessment / Inference System

simulated values
+ uncerts + confidence

After this, must assess *predictive* capability for *next* event.

Slide complement of Marv Adams.

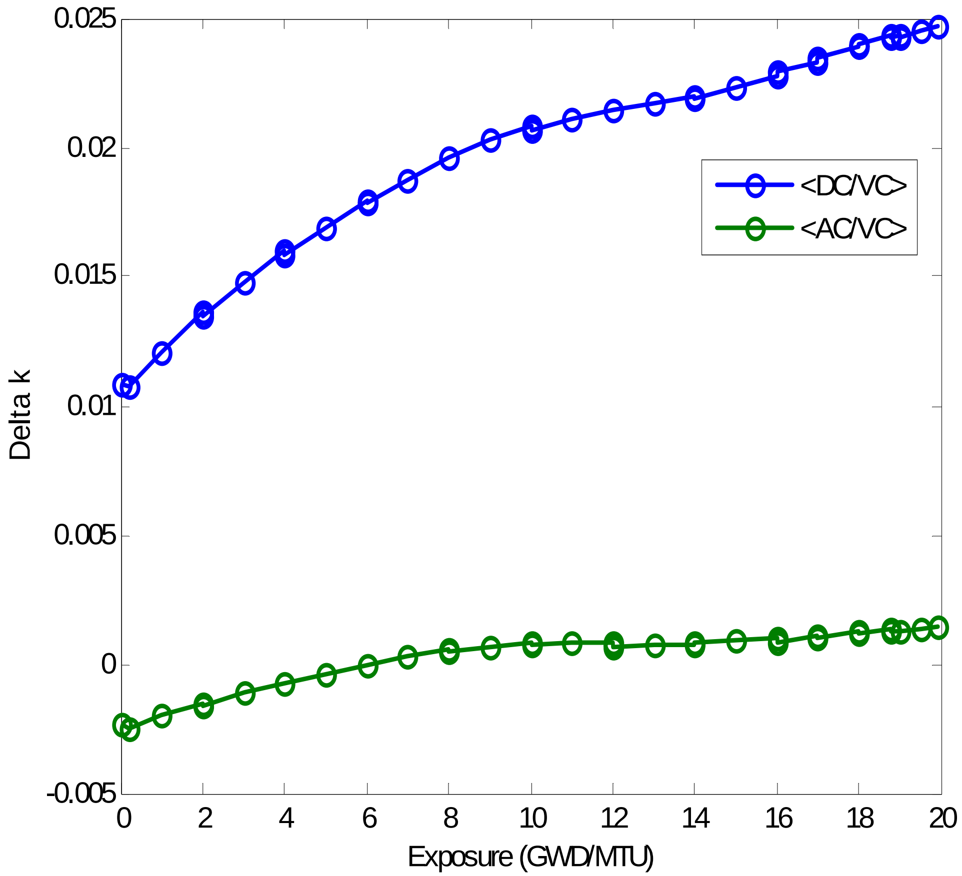
Where Are We At?

- Verification & Validation
- Coarser scale models and numerical errors can be addressed via adjoint based method to 1st order accuracy, but not commonly done.
- Little work done on B.C. & I.C. introduced uncertainties, though amendable to adjoint based method when linear responses.

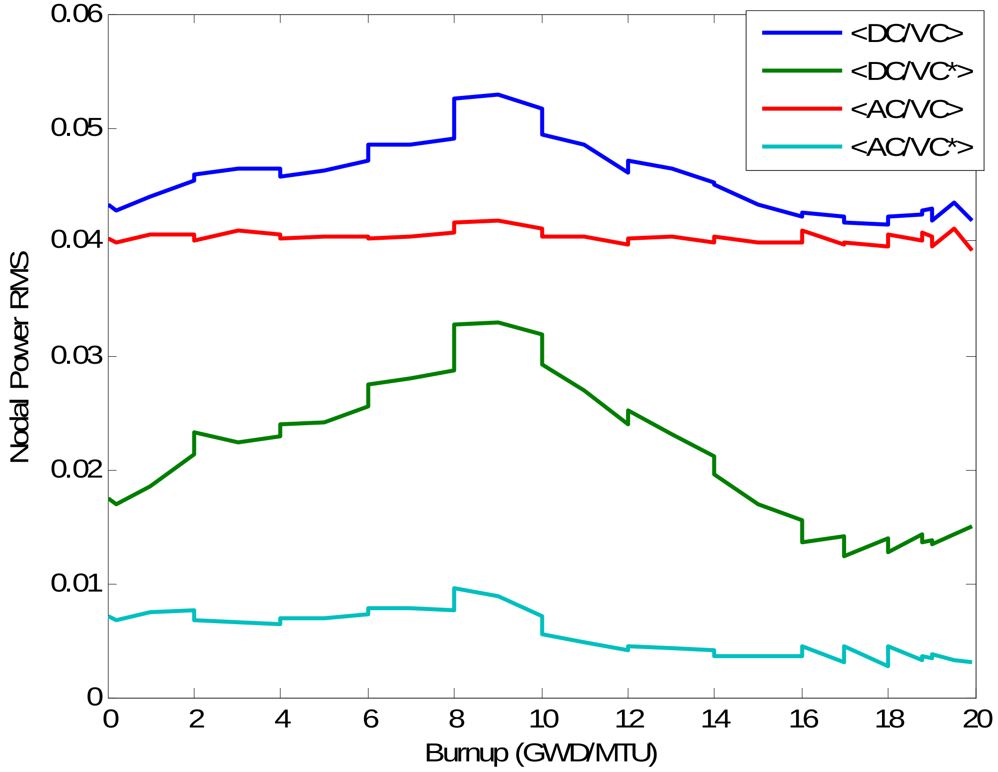
Where Are We At?

- Automated Data Assimilation
- Needs to be part of code development effort, not an after thought.
- Nuclear enterprise lags far behind other application areas, e.g. weather forecasting, so no systematic mining of data sources, e.g. plant data.
- Capabilities well known for linear observables with normal distributions
- For nonlinear observables and non-normal distributions, some capabilities exist but less well known and hence less utilized by nuclear energy related codes.

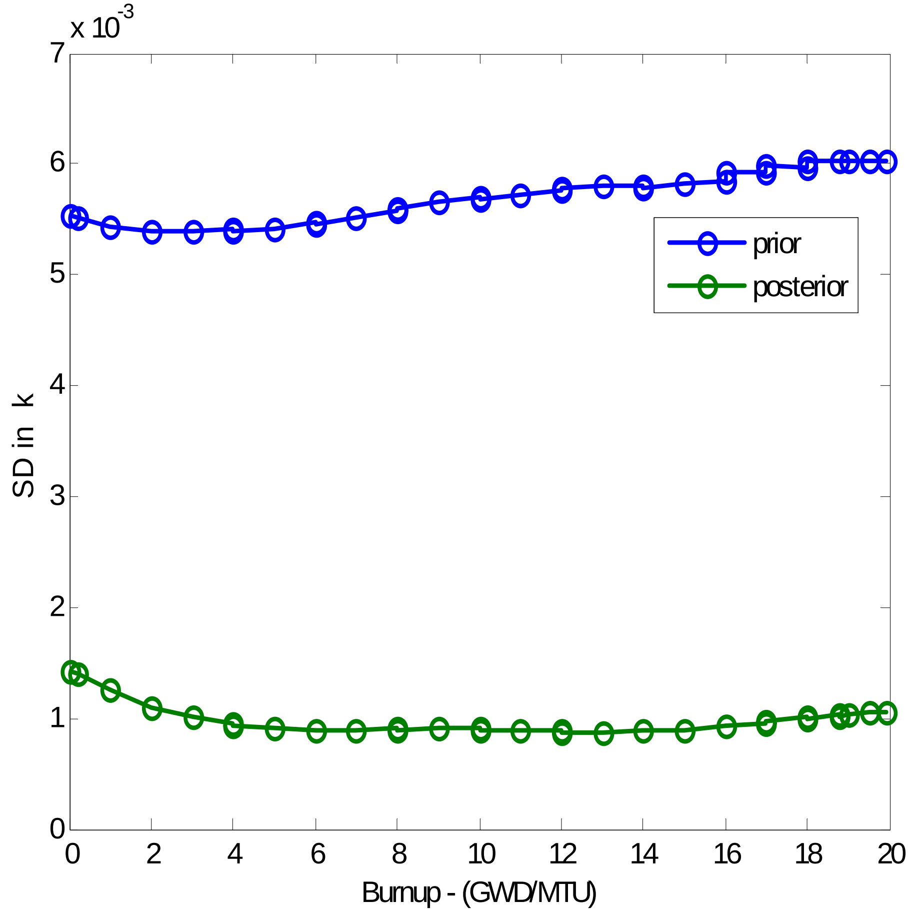
Adaptive Core Simulation



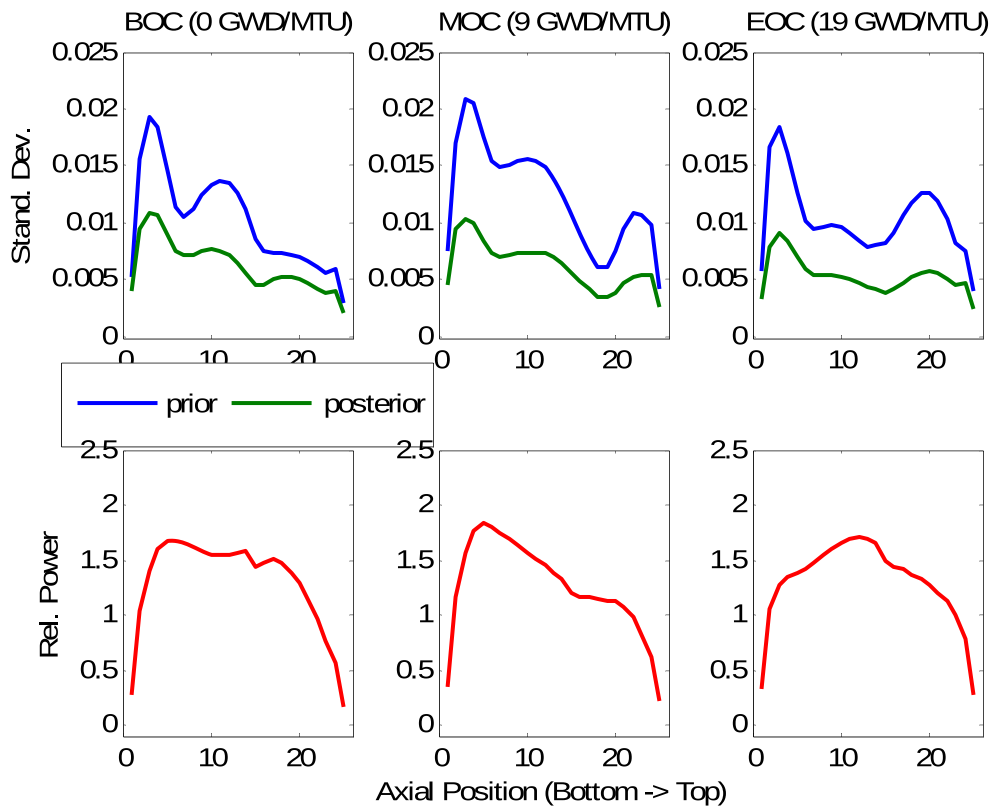
Adaptive Core Simulation



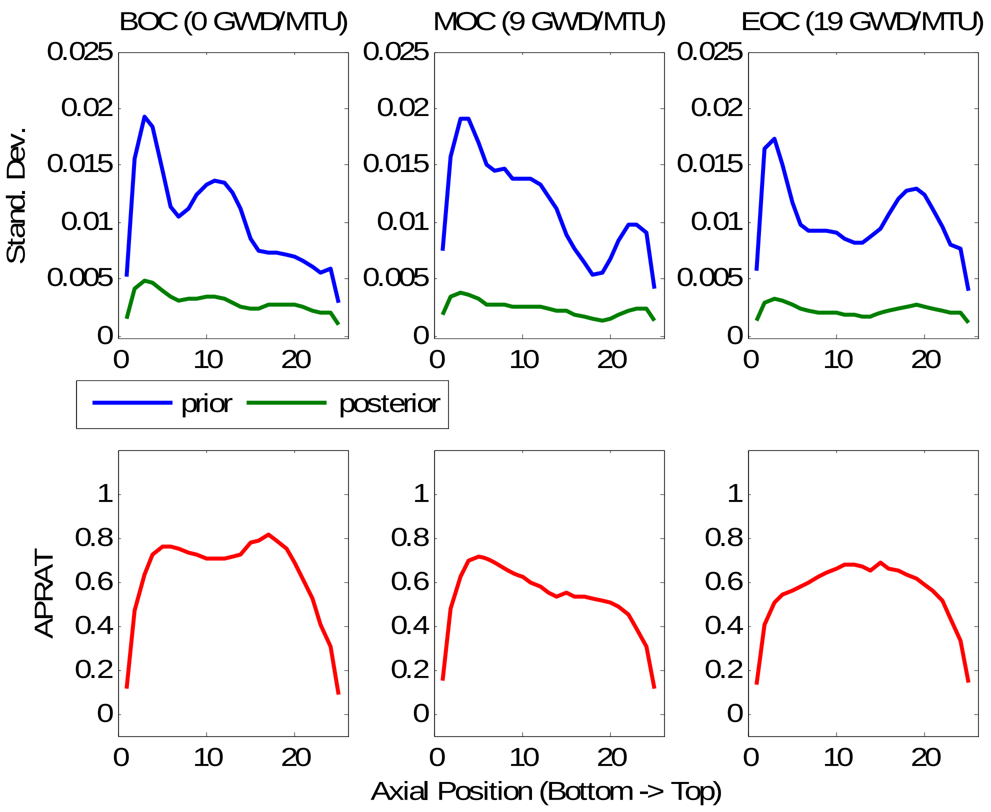
Adaptive Core Simulation



Adaptive Core Simulation

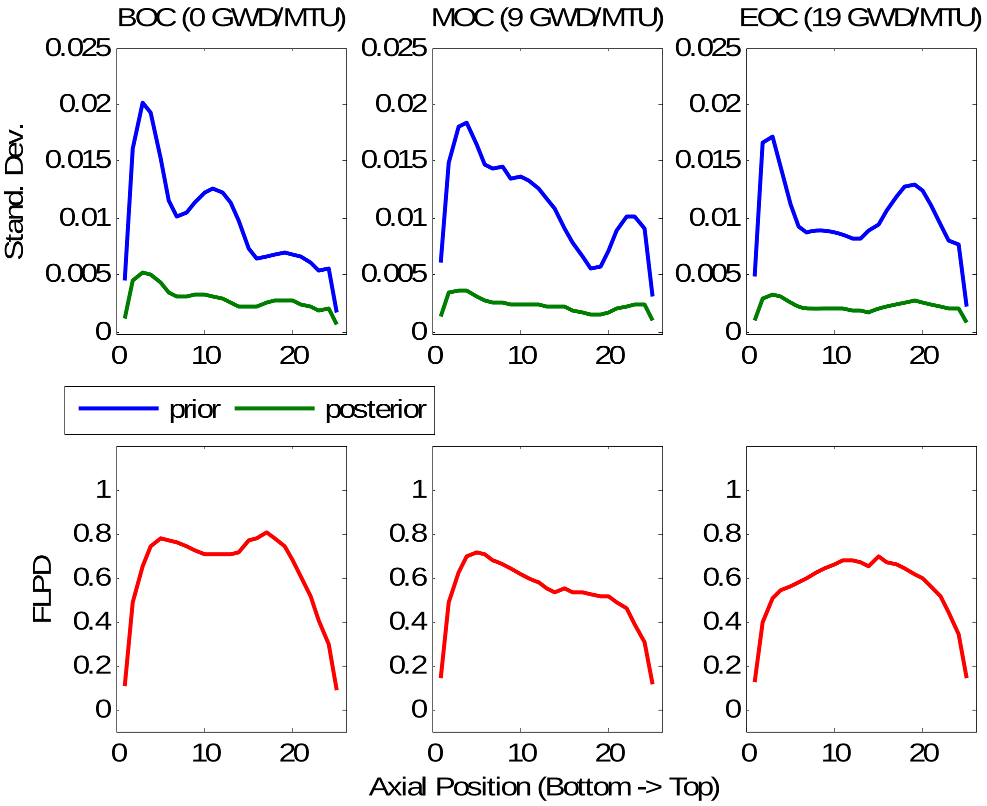


Adaptive Core Simulation



APRAT: Average Linear Power Density Ratio

Adaptive Core Simulation



FLPD: Fraction to Limiting Power Density

Where Are We At?

- User Friendly
- Visualization is being addressed by commercial software in discipline specific framework.
- Robustness via numerical algorithms is being addressed in V&V activities.
- Automation: Optimization of complex phenomena will require mathematical optimization. Already being used routinely in incore fuel management optimization (10^{50} decision space) and fuel cycle optimization, but needs extension to other areas of application.

Where Are We Going Now?

- By DOE laboratory structure => Diverse nuclear energy program.

  EXAMPLES

- ❖ ANL: Focus on core analysis via multiphysics code, i.e. Numerical Simulator.

  Have developed advanced neutronics capabilities, i.e. UNIC (Ultimate Neutronic Investigation Code)

- ❖ INL: Learning experiences on fuel and core multiphysics/multiscale with AMoR and UQ.

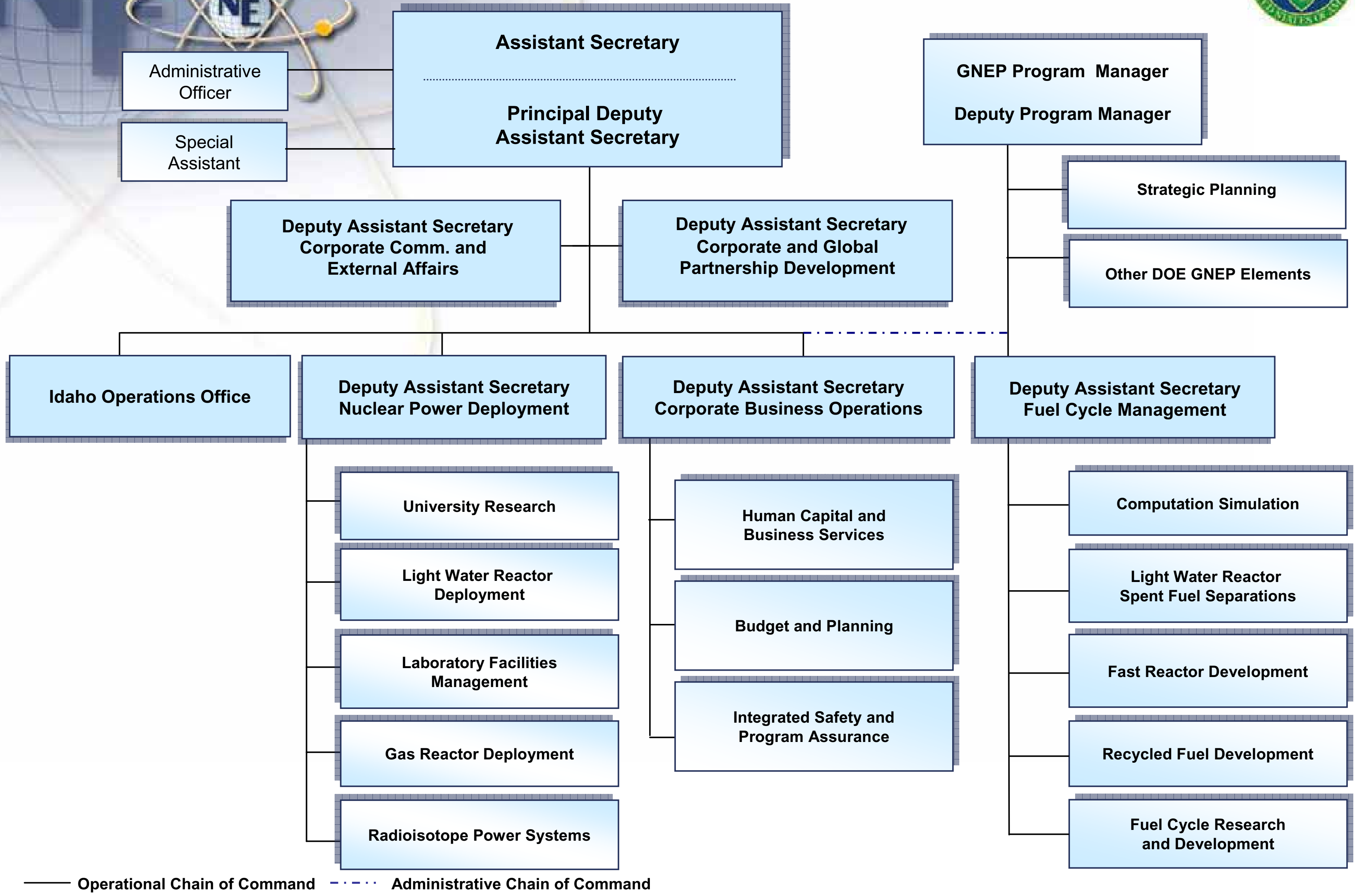
  RELAP7 development about to be implemented.

- ❖ ORNL: Extending SUNAMI capabilities beyond criticality.

Where Are We Going In The Future?

- Nuclear Energy Advanced Modeling and Simulation (NEAMS) cross-cut activity within the GNEP program.

Office of Nuclear Energy



Assistant Secretary

Principal Deputy Assistant Secretary

Administrative Officer

Special Assistant

Deputy Assistant Secretary Corporate Comm. and External Affairs

Deputy Assistant Secretary Corporate and Global Partnership Development

GNEP Program Manager

Deputy Program Manager

- Strategic Planning
- Other DOE GNEP Elements

Idaho Operations Office

Deputy Assistant Secretary Nuclear Power Deployment

- University Research
- Light Water Reactor Deployment
- Laboratory Facilities Management
- Gas Reactor Deployment
- Radioisotope Power Systems

Deputy Assistant Secretary Corporate Business Operations

- Human Capital and Business Services
- Budget and Planning
- Integrated Safety and Program Assurance

Deputy Assistant Secretary Fuel Cycle Management

- Computation Simulation
- Light Water Reactor Spent Fuel Separations
- Fast Reactor Development
- Recycled Fuel Development
- Fuel Cycle Research and Development

—— Operational Chain of Command

-·-·- Administrative Chain of Command

Nuclear Energy Advanced Modeling & Simulation
NEAMS

- ***Vision***

  To rapidly create, and deploy “science-based” verified and validated modeling and simulation capabilities essential for the design, implementation, and operation of future nuclear energy systems with the goal of improving future U.S. energy security.

- ***Approach***
  - Produce the new modeling and simulation capabilities with appropriate flexibility to allow them to be applicable to a variety of nuclear energy system options and fuel cycles
  - Continuously deliver improved modeling and simulation capabilities relevant to existing and future nuclear systems (in the near, mid, and long term)
  - Apply the best ideas through open, competitive processes to the challenges of achieving the NEAMS vision

NEAMS Foundation

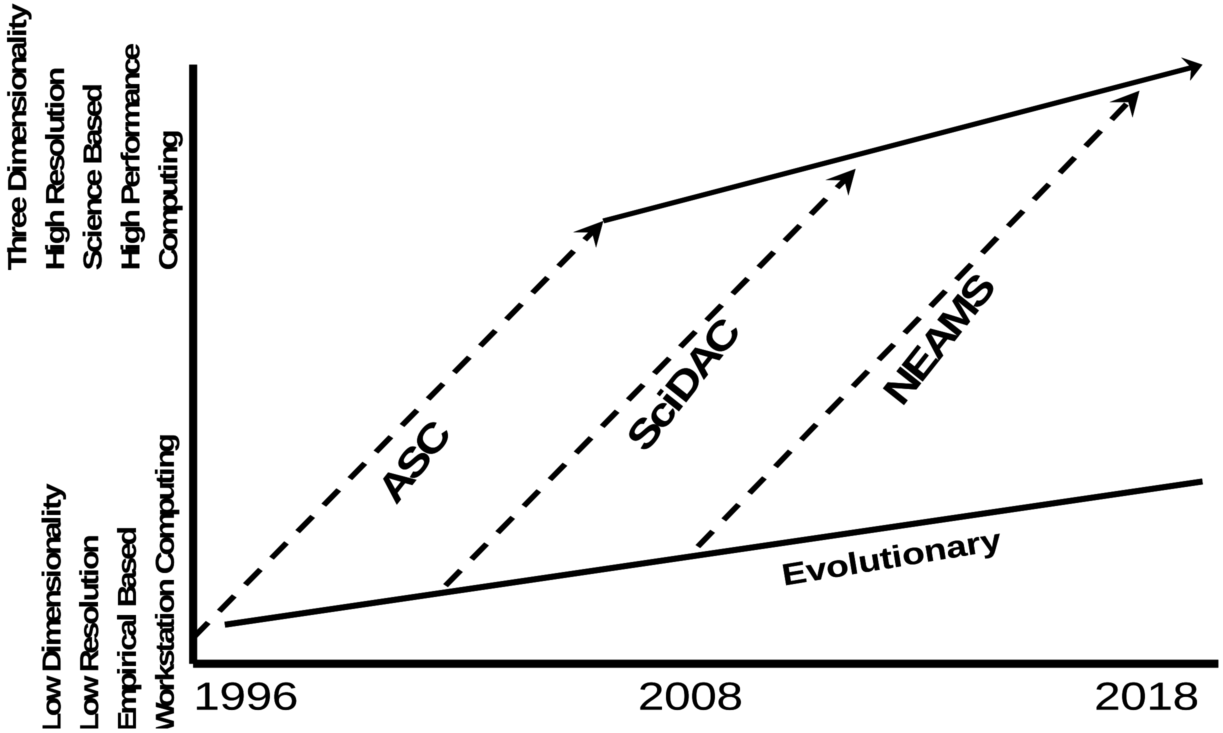
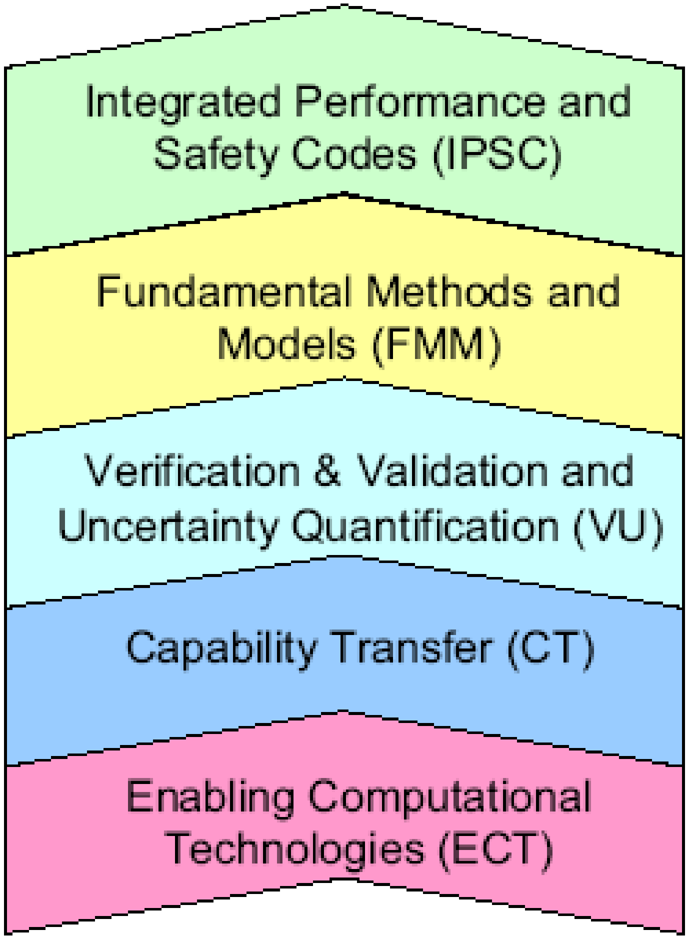


Figure 4: History of Leaping to New Levels of Modeling and Simulation Capability

NEAMS Program Elements



Integrated Performance and Safety Codes (IPSC)

Fundamental Methods and Models (FMM)

Verification & Validation and Uncertainty Quantification (VU)

Capability Transfer (CT)

Enabling Computational Technologies (ECT)

NEAMS Program Elements

- **Integrated Performance and Safety Codes (IPSC)**
  - Reactor Performance and Safety Simulations that include:
    - Transmutation Fuels Performance
    - Nuclear core performance
    - Balance of plant operations and safety
  - Separations and Safeguards
  - Waste Forms and Repositories

NEAMS Program Elements

- **Fundamental Methods and Models (FMM)**

  Smaller length scale material modeling work, and Atomistic-to-Continuum (AtC) multi-scale simulation supported by experiments

NEAMS Program Elements

- **Verification &Validation and Uncertainty Quantification (VU)**

- Provide confidence that results are a prediction of the “real world.”
- Develop & implement methodologies to understand margins & uncertainties associated with simulation results.

NEAMS Program Elements

- **Capability Transition (CT)**

  Provide necessary pathways to get capabilities out of R&D world & into hands of the end users.

NEAMS Program Elements

- **Enabling Computational Technologies (ECT)**

  Ensure that enabling technologies are available to make the first four program elements possible.

  - advanced algorithms and solvers
  - programming debuggers
  - code performance analyzers
  - model setup
  - results analysis (e.g. visualization)

  Also includes platforms that will be required to support the code development and the application work.

Program Element	**FY-09**	**FY-10**	**FY-11**	**FY-12**	**FY-13**
Integrated Performance and Safety Codes (IPSC)	$40M	$70M	$90M	$100M	$120M
Fundamental Methods & Models (FMM)	$8M	$10M	$15M	$20M	$25M
V&V and UQ (VU)	$5M	$10M	$15M	$25M	$30M
Capability Transfer (CT)	$1M	$5M	$10M	$12M	$15M
Enabling Computational Technologies (ECT)	$1M	$5M	$40M	$50M	$60M
Totals	$55M	$100M	$170M	$207M	$250M

LWR Sustainability Program

Program Elements

1. ***Nuclear Materials Aging and Degradation*.**
2. ***Advanced LWR Fuel Development*.**
3. ***Risk-Informed Safety Margin Characterization.***
4. ***Advanced Instrumentation and Control Technologies***