Data Needs to Support the Development of Fuel and Materials Performance Modeling and Simulation

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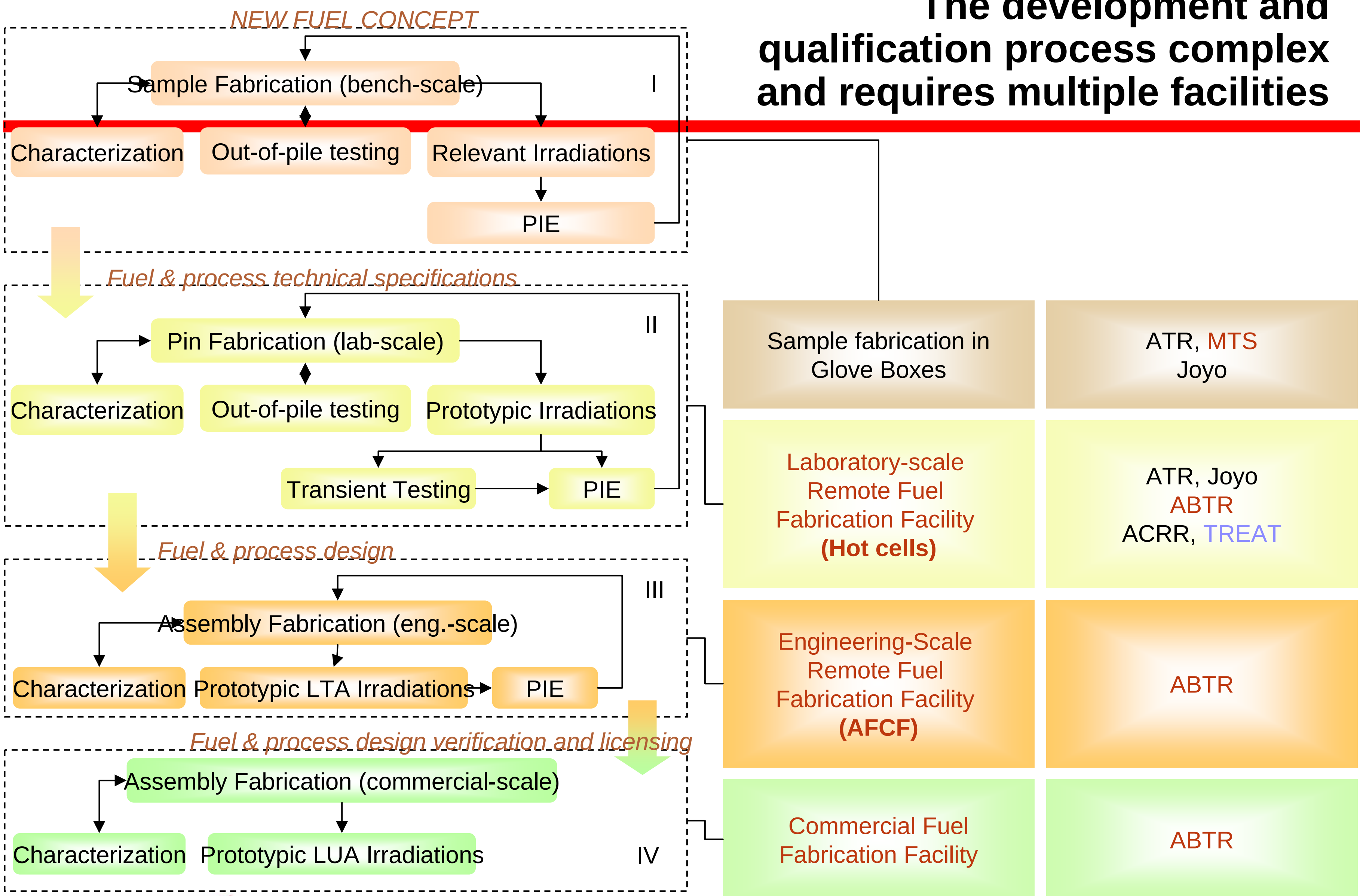
Background

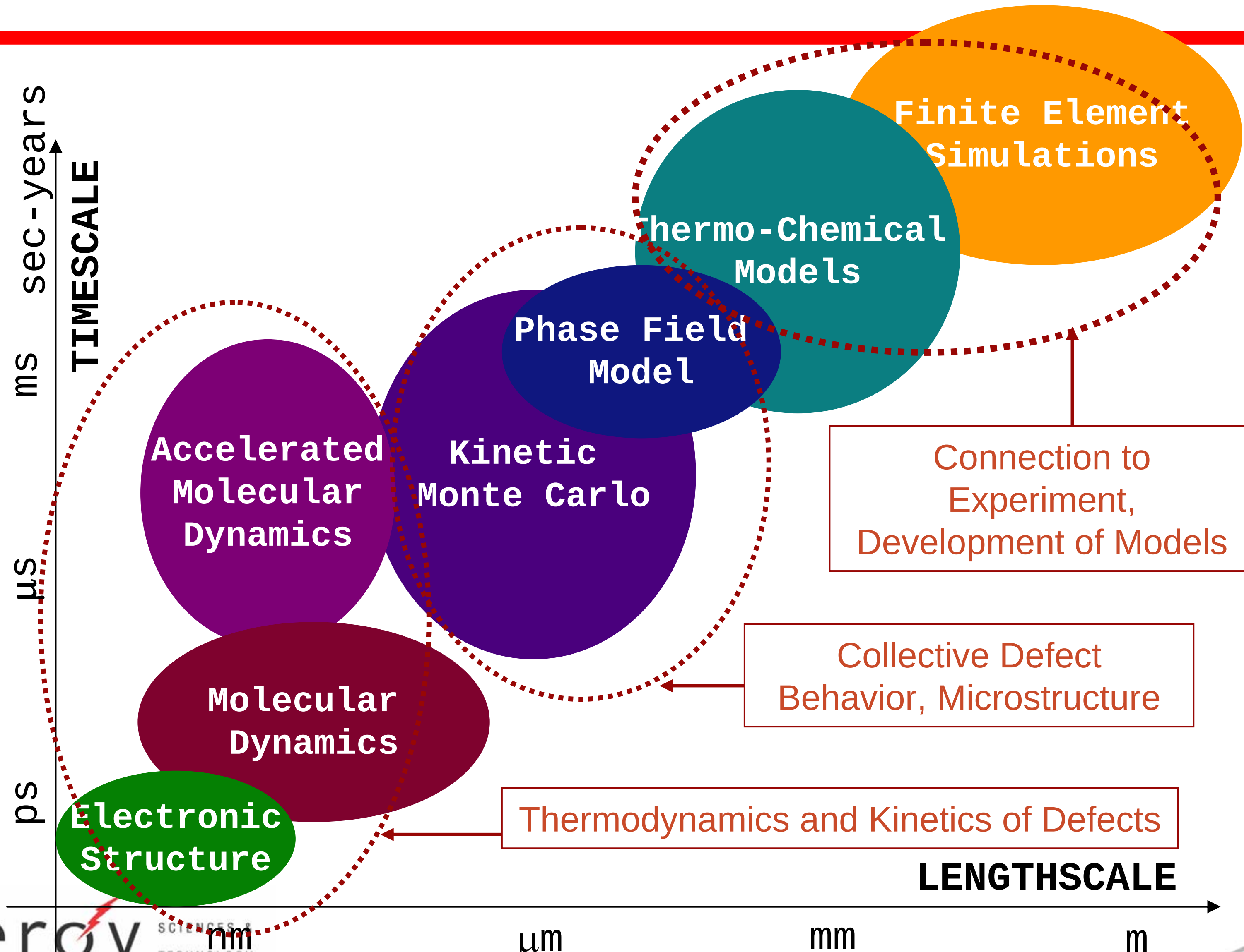
- Development and qualification of new fuels and materials for Advanced Fuel Cycles has many challenges:
  - Must perform in severe operating environment (e.g., temperature, radiation)
  - Properties vary with "life" (e.g., thermal conductivity, strength, composition)
  - Time consuming and costly
  - Strict requirements imposed by NRC licensing
  - ………
- Current codes used for fuels and materials performance are empirical and only semi-predictive
- The ability to model fuel and material performance from "first principles" is critical component of AFC:
  - Can be used to optimize candidate materials and fuels
  - Can be used to prioritize R&D on promising candidates $\rightarrow$ can reduce time and cost
  - Critical element of NRC licensing
  - …….

The development and qualification process complex and requires multiple facilities



FUEL QUALIFICATION

Multi-scale modeling approach is being used to develop fuel performance suite of codes



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Advanced Models, Simulations, and Fuel Performance Code

Advanced Fuel Performance Code

- **Fission products kinetics and concentration**
- **Heat transfer simulations**
- **Diffusion of species (gas and fission products) simulations**
- **Chemical reactions simulations**

Incorporation of the Advanced Models

- **Continuum-scale: Thermo-mechanical properties**
- **Meso-scale: Microstructural evolution, Species mobility**
- **Atomic-scale: Defect formation free energy, Irradiation effects,**
- **Electronic Structure: Structural stability, elastic constants**

Advanced First-Principles Models and Simulations

Fuel Performance Prediction Requires Integral Understanding of Multiple Phenomena

- Thermal conductivity
- Fission gas formation, behavior and release
- Materials dimensional stability
  - Restructuring, densification, growth, creep and swelling
- Defect formation & migrations
- Diffusion of species
- Radial power distribution
- Fuel-clad gap conductance
- Fuel-clad chemical interactions
- Mechanical properties
- Thermal expansion
- Specific heat
- Phase diagrams

Dynamic properties:
Changes with radiation effects, temperature, and time

Nonlinear effects
Initial condition dependence (fabrication route)

Examples of Nuclear Physics Related Needs

- Radiation Damage:
  - Dpa cross section
  - ………
- Gas production
- Activation products:
  - Species
  - Evolution with time
  - Diffusion/migration
  - ………
- Fission products:
  - Species
  - Evolution with time
  - Diffusion/migration
  - ………

Back-up

Linking Modeling & Experimental Efforts

AFC
Advanced Fuel Cycle Initiative

Defect Energies
First Principles Calculations

Cascade Dynamics
Molecular Dynamics

Bubble Evolution
Kinetic Monte Carlo

1 — 10 — 100

Bubble Size (nm)

Irradiated samples of iron/steel

Diffraction
Defect Geometry
NMR Spectroscopy
Defect Energies

Positron Annihilation
Helium/Hydrogen content
TEM
Defect Distribution

Microstructural evolution
SEM
TEM

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Requests from Fuels Community

General agreement for:

• Strongly coupled experiments and computational studies

• Ultrafast experiments

• Real time experiments under realistic conditions

• New experimental approaches for handling radioactive materials

• Need for “new,” “novel,” “innovative,” and “revolutionary” experiments

• New sensors, detectors, and methods for in situ experiments and on-line monitoring:
  - Fuel manufacturing and processing
  - Reactor and fuel performance

Phenomenological focused experiments considered crucial to developing and verifying new modeling capability

Examples of Specific Needs for Fuel Development

- Basic material properties of actinide-bearing materials
- Thermal conductivity of highly defective materials
- Phase diagrams and kinetics for multi-component systems
- Understand microstructural evolution
- Techniques to study behavior of "f" electrons
  - localized or delocalized ?
  - Critical to accurate atomistic models
- Design and control of nanostructures and complex defect structures
  - New evidence that some nano-structured materials may be structurally stable under irradiation (low swelling and growth)
- Possibility of using small (nano-sized) irradiation specimens to verify models because the entire specimen could be modeled with Molecular Dynamics