NEAC meeting
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Advanced Modeling and Simulation for Nuclear Energy

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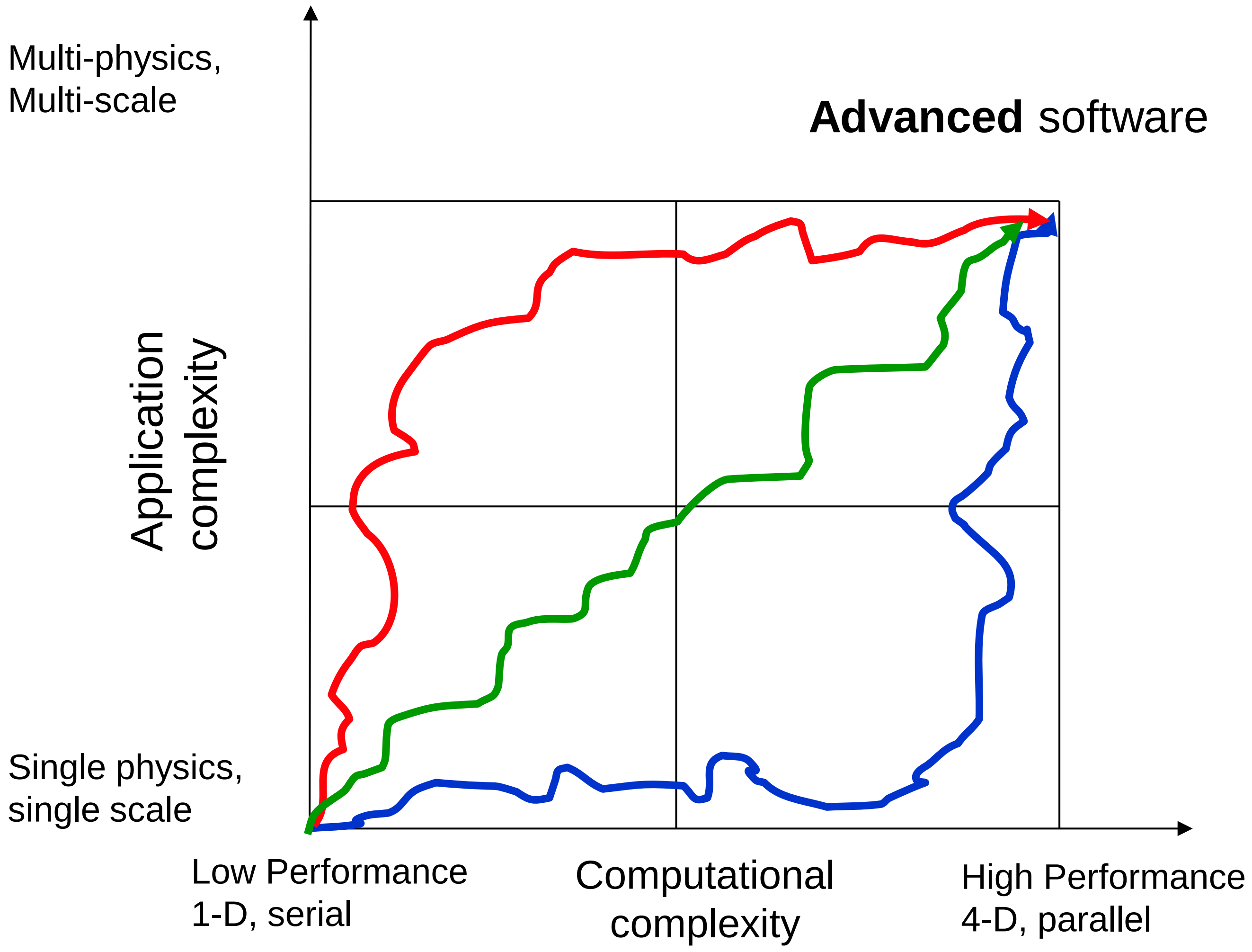
Models and Simulations

Model: A logical description of how a system performs.
- empirical (interpolation based on observation)
- theory-based (interpolation based on theory)

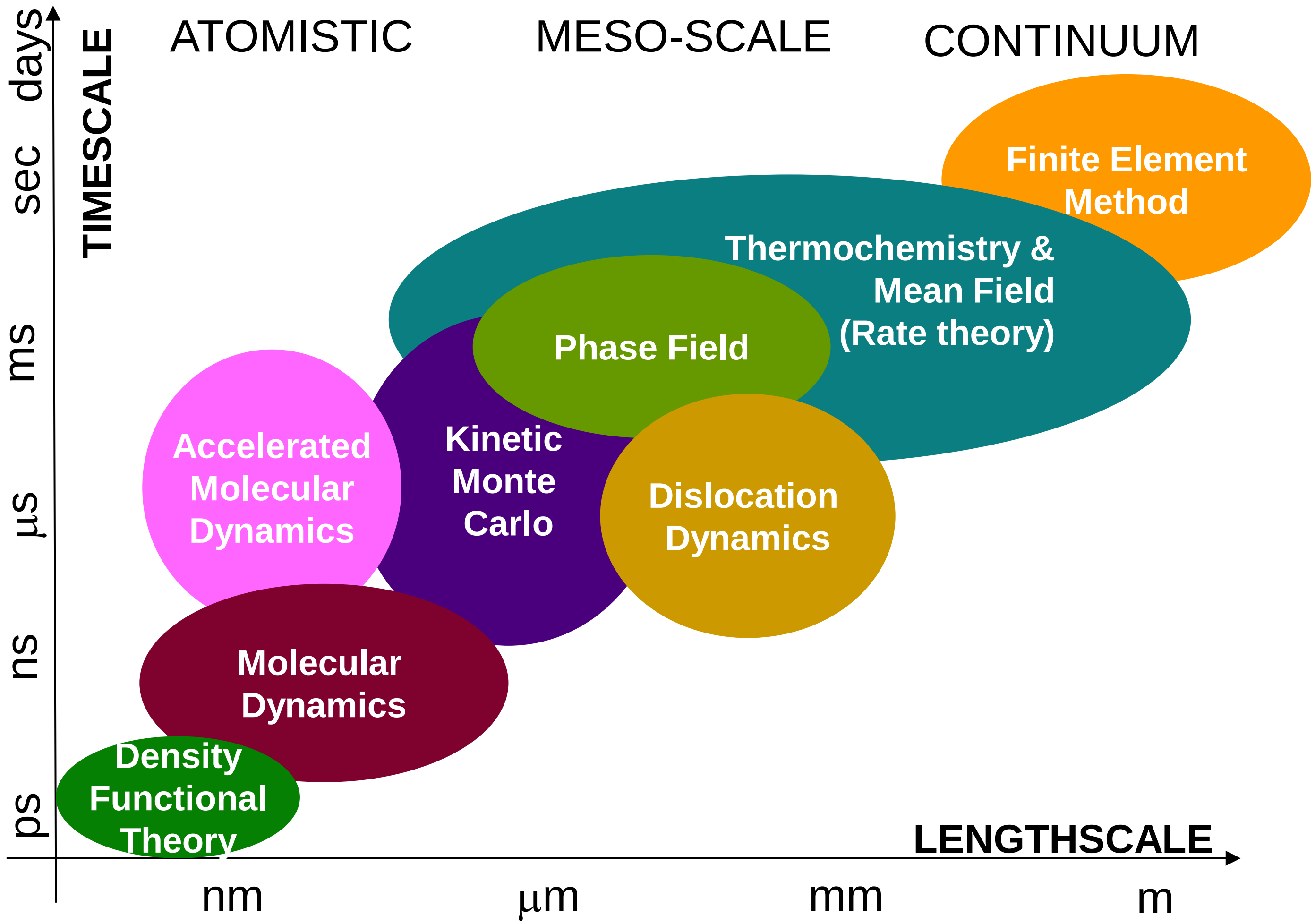
and: bringing together the two communities

Simulation: The process of running computer programs to reproduce, in a simplified way, the behavior of a system.
- low performance (workstation)
- high performance (Petascale, Exascale,)

Advanced software: development paths



Multi-Physics and Multi-Scale Methods



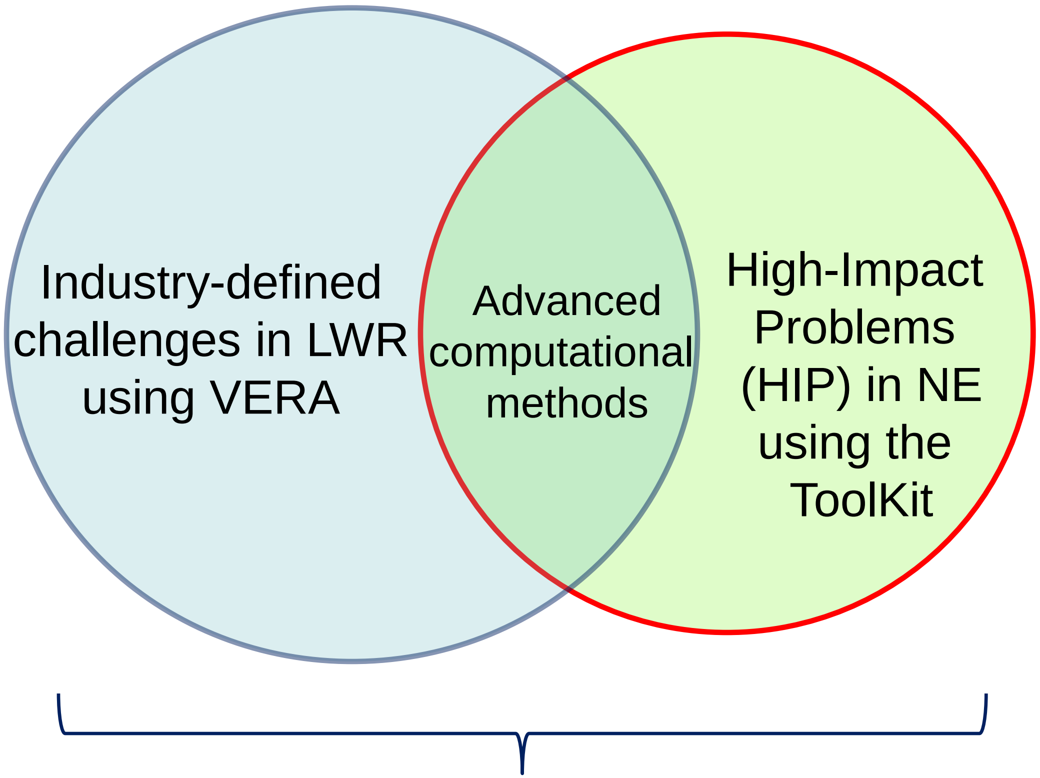
CASL and NEAMS – Complementarity and Coordination

- **Complementarity - differences**
  - CASL
    - Delivers solutions to industry-defined challenges in LWR technology
    - Develops "virtual reactor" software, VERA
    - Provides strength to the program
  - NEAMS
    - Delivers solutions to high-impact problems (HIP) in various NE technologies
    - Develops a ToolKit of computational tools
    - Provides flexibility to the program

- **Coordination – common goals**
  - Improve advanced, multi-physics computational methods
  - Accelerate Innovation in NE technology
  - CASL and NEAMS coordinate activities to avoid duplication of efforts

CASL Consortium for Advanced Simulation of LWRs

NEAMS NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM



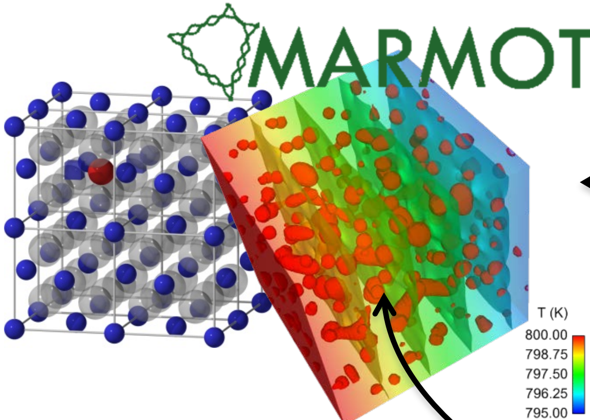
Accelerate innovation in NE technology

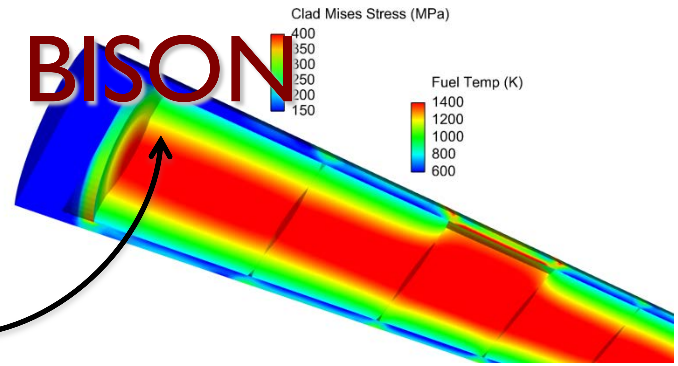
Modeling and Simulation Budgets

	FY-08	FY-09	FY-10	FY-11	FY -12	FY-13	FY-14	FY-15
NEAMS	7,792	20,000	26,574	40,495	15,299	17,242	9,536	21,536
HUB			22,000	22,000	23,517	24,588	24,300	24,300

The “Fuels Product Line” from microstructure to the fuel elements

MOOSE-BISON-MARMOT toolset provides an advanced, multiscale fuel performance capability





Mesoscale Material Model Development Tool

- Simulates microstructure evolution in fuels under irradiation
- Used with atomistic methods to develop multiscale materials models

Engineering-scale Fuel Performance Tool

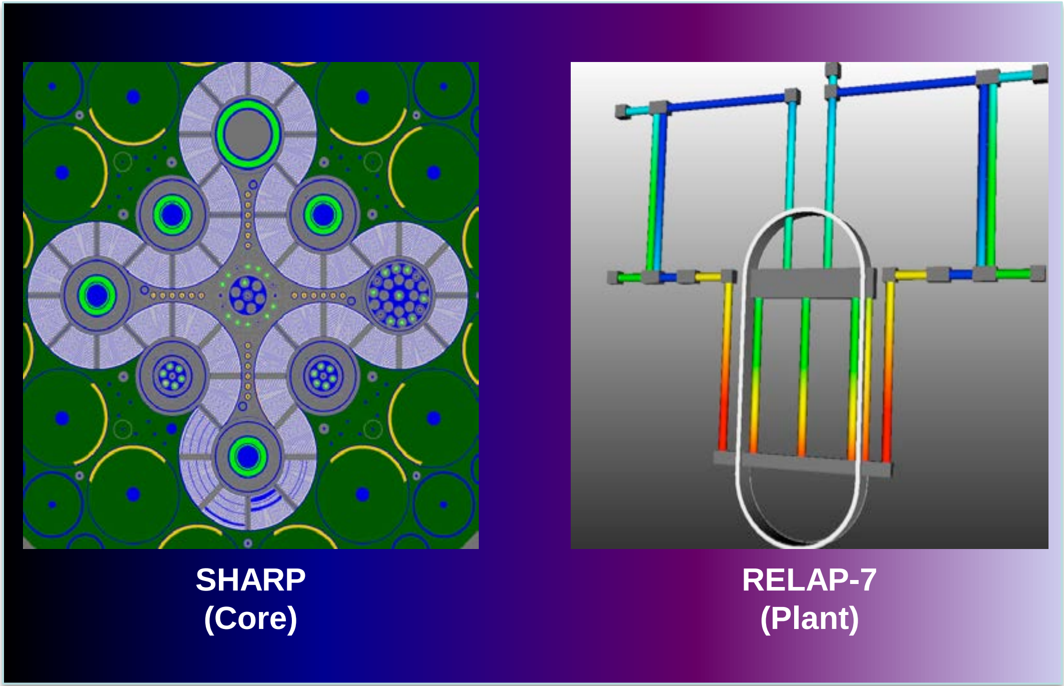
- Models LWR, TRISO and metallic fuels in 2D, 3D
- Steady-state and transient reactor operations

MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework enabling rapid development of FEM-based applications

The “Reactors Product Line” from the reactor core to the full plant



- Seamless interoperability
- Robust, useful stand-alone products
- Enables traditional workflow but positions the toolkit for future approaches and superior predictability where needed

The survery

Jan-March, 2014, 32 participants from NEAMS, CASL, Nat. Labs, and DOE-NE

Q1: What is good/bad with the NEAMS R&D plan?

1. The quality of the NEAMS software is very good
2. Being technology versatile is good
3. NEAMS must solve a problem

Q2: What CASL successful experience can be used in NEAMS?

1. The focus - concentrated effort to solve a problem
2. The synergy – industry is a partner
3. The stability – funding, personal, work scope

Hubification: Using the positive experience of a hub (CASL) to improve a program (NEAMS)

High-Impact Problems (HIP)

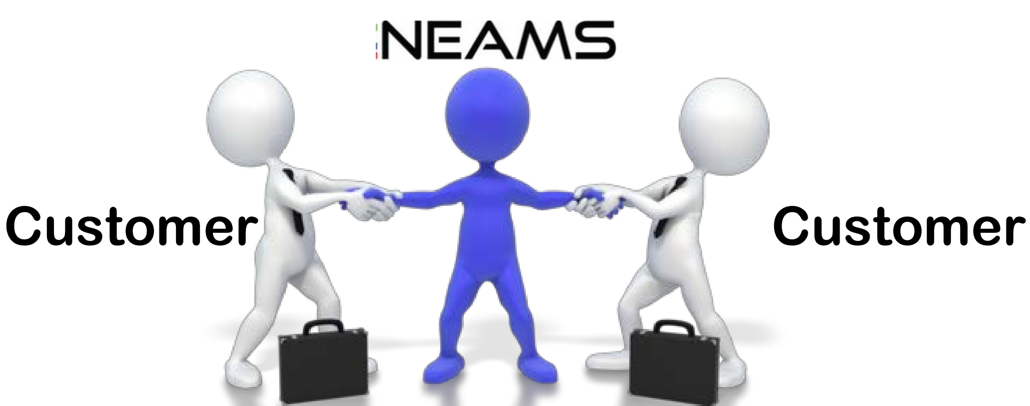
High-Impact Problem: a problem that has a solution which significantly improves, in a short period of time, an application of exceptional importance for the customer.

NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

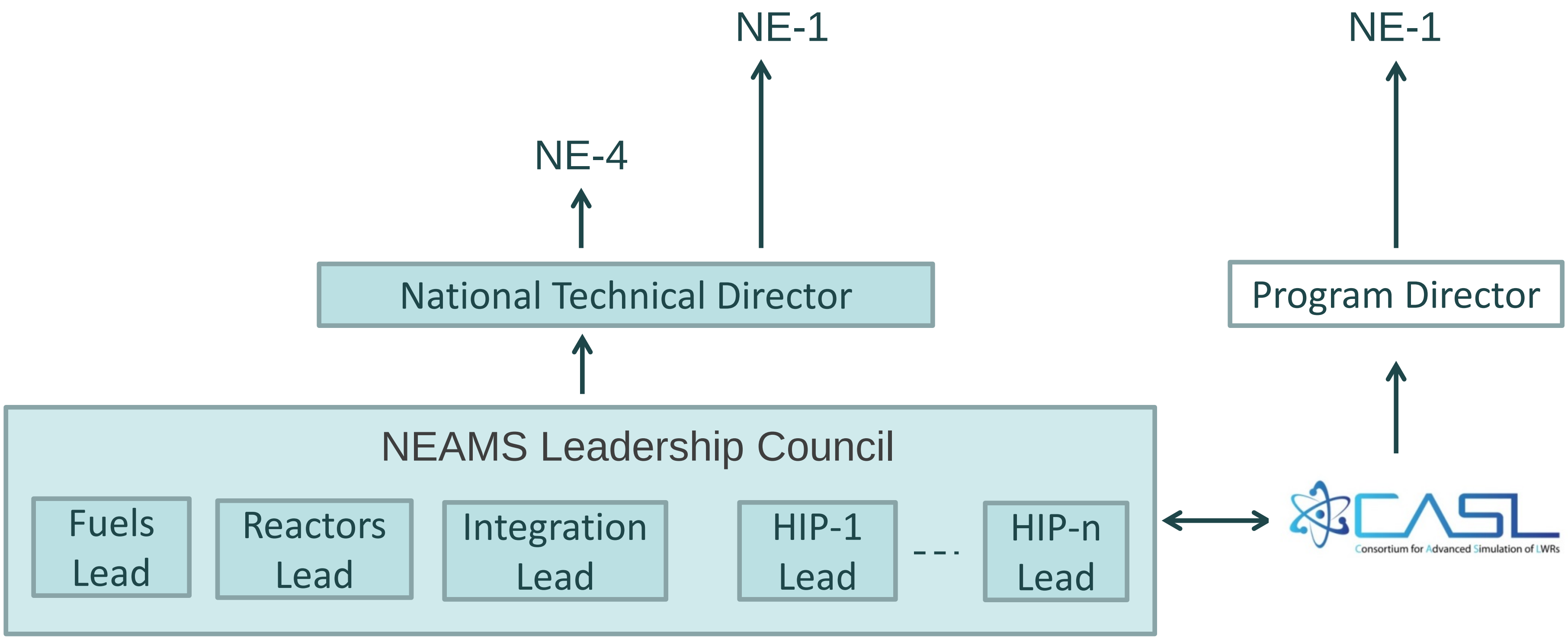
- Participates in problem definition
- Leads the scientific and engineering approach ($5 mil/year for 3 years)
- Demonstrates the high-impact

Customer

- States the high-impact level of the problem
- Provides technical support, validation data, experiments, etc. (> 20% NEAMS funding, in-kind)
- Certifies the high-impact



Leadership and Management



Management philosophy:

- Build upon what works well
- Encourage innovation, take risks
- Build and maintain a community of passionate people

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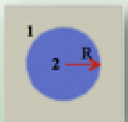
NEAMS
NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

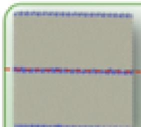
Highlight: New model for the average grain size in UO_2 fuel using atomistic and mesoscale simulations

- The GB mobility was calculated using two molecular dynamics methods for three GB types as a function of temperature.
- Ongoing work is determining the impact of impurity drag.



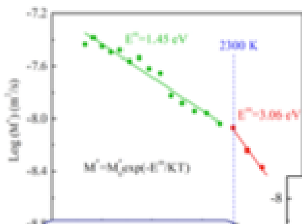
Curvature method
- Rate of shrinkage of a circular grain is used to determine the reduced mobility

$$v = M\frac{\sigma_{GB}}{R} = \frac{M*}{R}$$



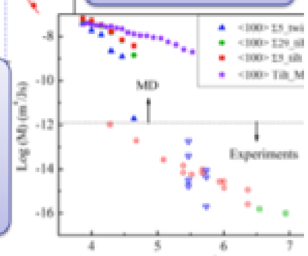
Random fluctuation method
- No driving force
- Random fluctuations determine mobility

$$\langle \bar{h}^2 \rangle = 2Dt \qquad M = \frac{DA}{K_b T}$$

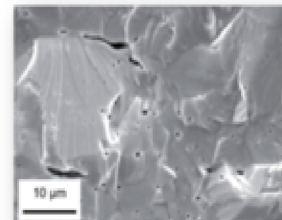


MD results indicate there is a transition to a different diffusion mechanism at 2300 K (driven by interstitial instability)

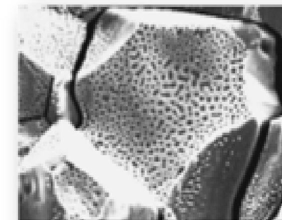
MD Calculated values are 4 orders of magnitude too high. Difference is due to impurity drag and is being investigated.



- Two distinct distributions of porosity exist within the fuel



Initial Porosity (from sintering)



Fission Gas Bubbles

- Neither can be accurately represented with Zener's model
- Existing models from the literature exist for the sintered porosity
- Mesoscale modeling will be used to develop a model for the fission gas bubbles

- GBs migrate to reduce the total free energy of the system
- Driving forces include
  - Reduction in GB energy (curvature driving force)
  - ~~Reduction in elastic energy~~
  - ~~Reduction in defect energy~~
  - (Temperature gradient)

$$\dot{D} = 2M\,(P_{DF} - P_p)$$

Curvature driving force:
- Results in an increase in the average grain size.
- Is well understood:

$$P_{DF} = \frac{\sigma_{GB}}{R}$$

- GB energy has been calculated using MD.
- An existing phase field model has been verified by

Temperature gradient driving force:
- Causes GBs to migrate to higher temperatures
- Is defined by (*Gottstein and Shvindlerman, 1999*):

$$P_{DF} = \frac{\Delta S\, w_{GB}}{\Omega_a}\nabla T$$

- This equation is unreferenced and so was investigated using MD.
- Relative importance was determined using phase field modeling.

Highlight: MAX – Validation of CFD simulations

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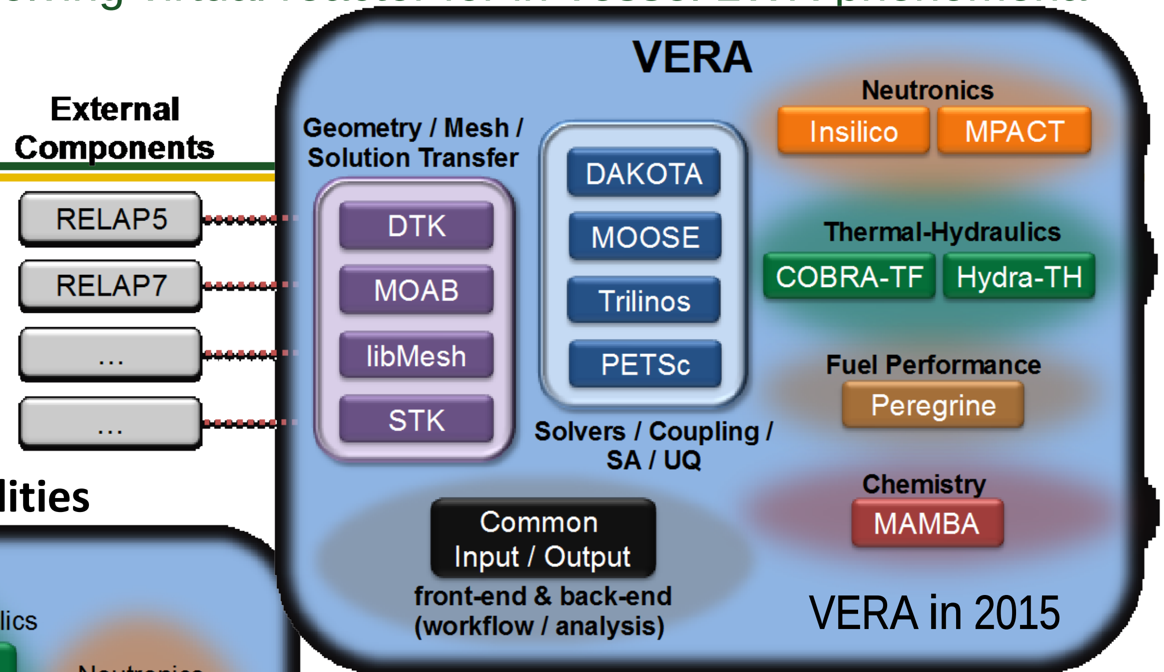
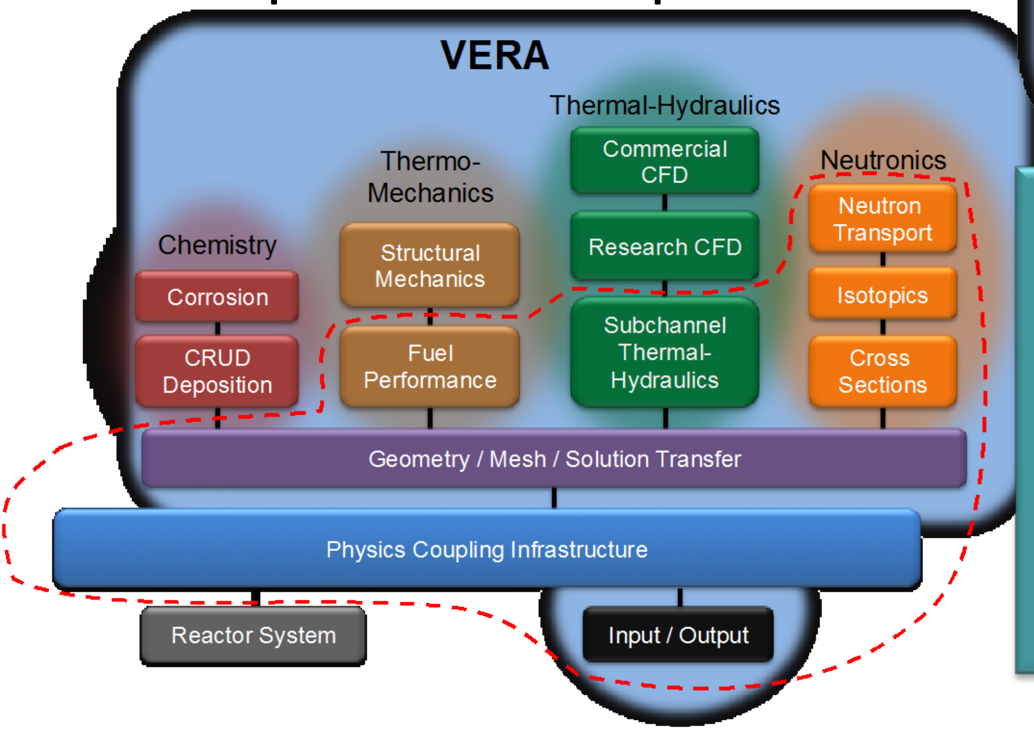
VERA: Virtual Environment for Reactor Applications
CASL's evolving virtual reactor for in-vessel LWR phenomena



Required functional capabilities



CASL has 3 M&S technology products

1. VERA-CS as the fast running core simulator, which has value both standalone and for providing power histories for more detailed codes
2. Engineering suite of standalone codes with ability to couple 2 or more within VERA or in other environments
3. Leadership suite of high fidelity codes used to drive improvements in 1 and 2

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Highlight: VERA Analysis of Watts Bar Unit 1 Hot Full Power

Purpose

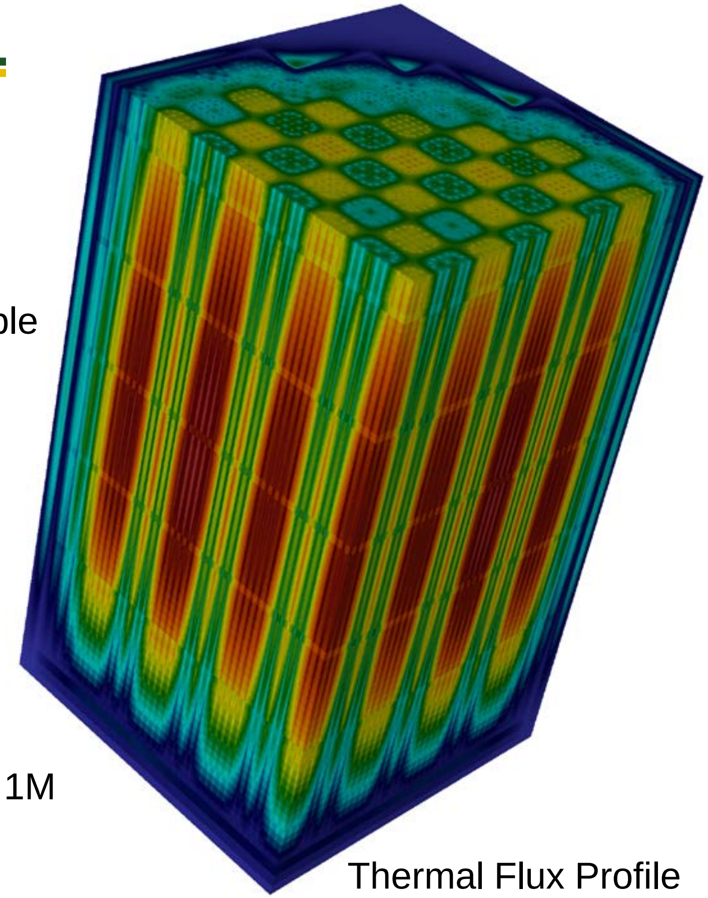
- First large-scale coupled multi-physics model of operating PWR reactor using Components of CASL's Virtual Environment for Reactor Applications (VERA)
- Features resolved are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1: geometry for fuel, burnable absorbers, spacer grids, nozzles, and core baffle

Execution

- Common input used to drive all physics codes
- Multigroup neutron cross sections calculated as function of temperature and density (SCALE/XSPROC)
- SPN neutron transport used to calculate power distribution (DENOVO)
- Subchannel thermal-hydraulics in coolant (COBRA-TF)
- Rod-by-Rod heat conduction in fuel rods (COBRA-TF)
- Simulation ran in 14.5 hours on Titan using 18,769 cores – over 1M unique material (fuel/coolant/internals) regions resolved

Next Steps

- Add fuel depletion and core shuffling
- **Compare results to plant measured data**



Thermal Flux Profile in Reactor Core

Remarkable resolution of physics and geometry

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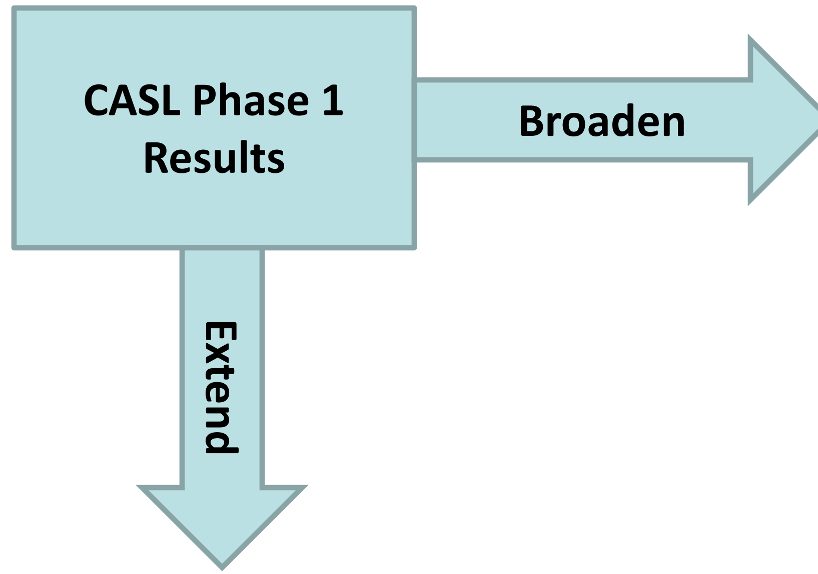
NE Hub Phase 2 Considerations
(Renewal Application Due by July 1, 2014)

Phase One Performance

- Technical Performance
  - Successful completion of planned milestones
- Annual Reviews
  - Meeting criteria of the NE Hub Oversight Plan
- Impact on Science and Engineering
  - Significant number of publications and invited presentations
- Technology Deployment
  - Substantial evidence of technology transfer.

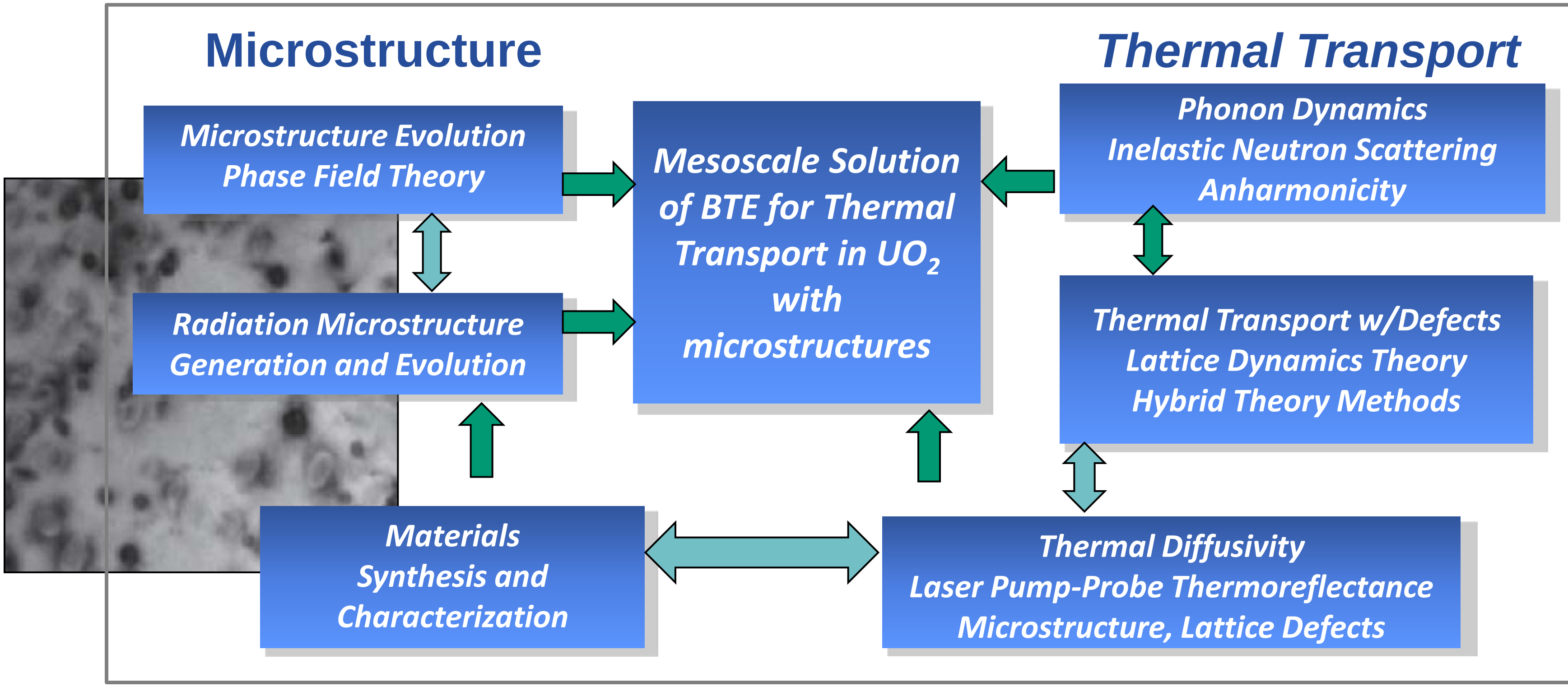
Plans for Phase Two



- CASL to Propose
  - Exact Technical Balance, Specific Focus & Expected impact
  - Proposed Approach
  - Composition of the Team to Execute

Center for Materials Science of Nuclear Fuels (CMSNF)

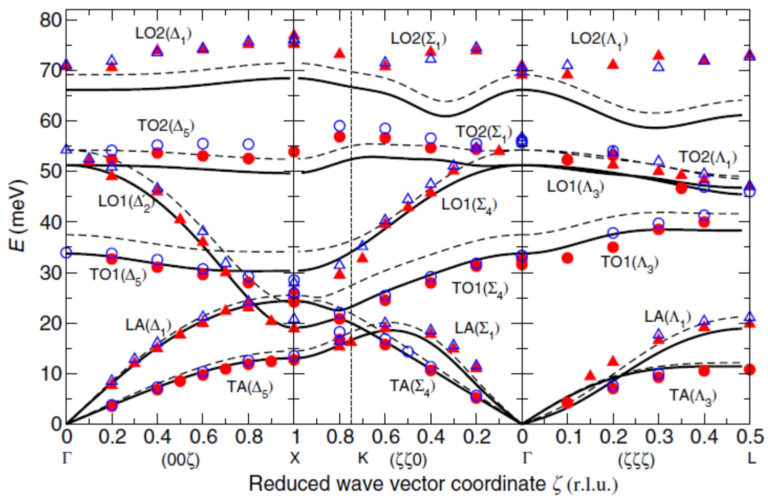
EFRC focused on understanding the effects of microstructure on thermal transport in irradiated nuclear fuels (UO_2 as a model)

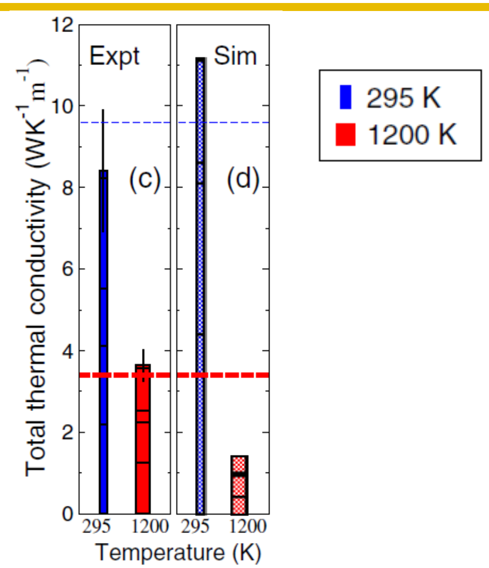


CMSNF – Center for Materials Science of Nuclear Fuel

Idaho National Laboratory · Purdue University · University of Florida · Colorado School of Mines · University of Wisconsin–Madison · Oak Ridge National Laboratory

Highlight: Thermal Transport at Different Phonon branches





Phonon branches: inelastic neutron scattering (symbols) vs DFT modeling (lines)

DFT overestimates k at low T, underestimates at high T.

- Understand thermal transport at the level of phonon
- “5f electron” problem in DFT causes the discrepancy – Scope in renewal proposal
- A good example of using experiments to validate modeling

Pang et al., Physical Review Letters 110, 157401 (2013).

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Center for Exascale Simulation of Advanced Reactors (CESAR)

Exascale co-design center

Mission: Work with industry and DOE research partners to influence the design of future hardware architecture, system software, and applications based on the key algorithms underlying computational nuclear engineering.

Software: CFD + neutron transport optimized in parameter regime relevant to nuclear reactor simulation

Objective: Develop a new generation of underlying algorithms that enable the solution of significant outstanding nuclear engineering problems by leveraging exascale resources.

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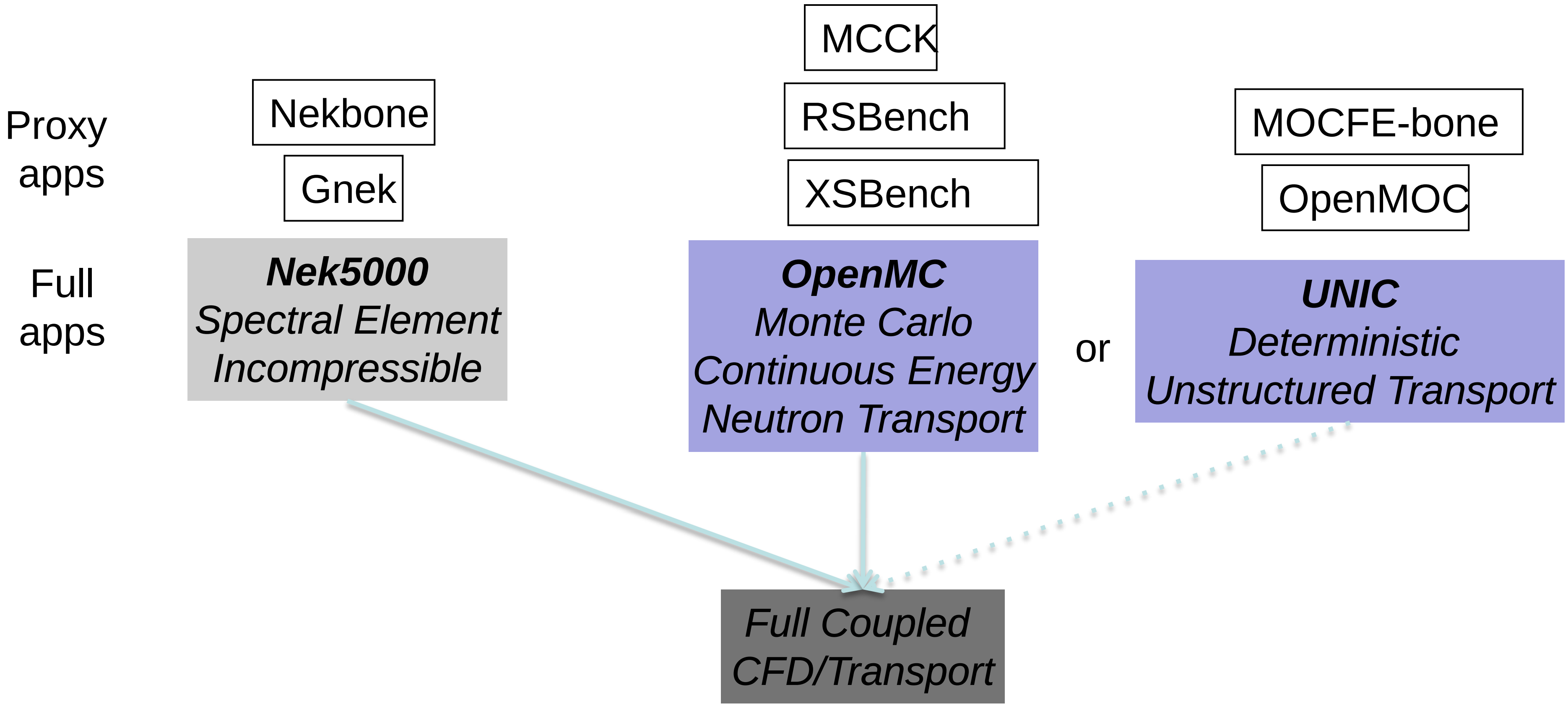
CESAR Highlight: Proxy Apps



- In CESAR, ***proxy applications*** (PAs) are the main vehicle of collaboration with vendor
- PAs abstract key performance characteristics of full applications
- Suitable for testing with architectural simulators, new programming models/algorithms

Conclusions

- CASL and NEAMS complement each other and coordinate their activities. CASL provides strength while NEAMS provides flexibility.
- NEAMS is undergoing a transformation that builds upon successful fuel and reactor simulation software and adds solutions to high impact problems.
- Validation is integrated in software development.
- CASL is preparing for the renewal process
- The Office of Nuclear Energy and the Office of Science fund a spectrum of NE-relevant programs that go from fundamental science to advanced computation.
- In addition to engineering solutions, the programs deliver exciting scientific results.