Multidisciplinary multi-physics simulation and analysis tool to support “Fusion Materials Science” research – Charge 3

Y-K.M. Peng

USBPO Webinar Input to FESAC Panel on MFE Research Priorities

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Multidisciplinary multi-physics (MDMP) simulation & analysis tool

• The need, in support fusion materials science research
  • Clarify benefit-cost-risk among options of internals, configuration, mission, performance
  • Inform research choices based on leverage
  • Can become tool needed to integrate research, FNSF designs, and eventually operation scenarios
• Help introduce a “fighting chance” for this research in ITER era
Fusion internals interact strongly and form option sets due to compatibility and safety

Examples:

A) Hot divertor surface with $\text{H}_2\text{O}$-cooled steel wall components (ITER)
   1. W surface divertors
   2. Be first wall
   3. Water-cooled steel shield-blocks
   4. Several TBM’s each of $\sim 1\text{m}^2$ area

B) All-W PFC’s (EU)
   1. Surface $T = 750\text{C} - 1000\text{C}$
   2. High pressure He cooling
   3. Solid or Li-Pb liquid breeder blankets
   4. High power conversion efficiency

C) Large flowing liquid Li PFC’s (US)
   1. Surface $T = 450\text{C}$+, inlet $T \sim 200\text{C}$
   2. He cooled internals
   3. Avoid solid surface material damages
   4. Need to remove Li-LiT on solid surfaces

D) Water-cooled solid breeder blankets (JN)
   1. Super critical steam $\sim 300\text{C}$, He-cooled solid breeder
   2. Extend LWR materials and technologies
   3. Standard power conversion efficiency

ITER, 500 MW

These options drive differing requisite research and FNSF
Fusion Materials Science underpins fusion nuclear science research and FNSF

Integrated-Effects Fusion Materials Science Research
Using A Normal or Small Aspect Ratio Plasma

Toroidal & Burning Plasma
Plasma Enabler & Control
Plasma Material Interaction
Material Irradiation & Damage
Tritium Cycle
Power Extraction
Measurement Science
Modeling, Computation & Validation

In Asia
SST-1
C-Mod
EAST
KSTAR
DIII-D
NSTX
JT-60SA
New High Gain Device
ITER R&D

Elements in which Fusion Materials Science research determines outcome
Fusion internals option further determines the support systems of the entire facility – ITER example

ITER Organization Configuration Management Model
Revision April 2010

3D site layout with Tokamak Complex, Auxiliary Buildings and PF Coils construction building

Need to estimate relative benefit-cost-risk of different internals options and the associated requisite research
MDMP simulation & analysis methodology has been successfully applied in aerospace & started for LWR’s.
This methodology applies to fusion systems and the associated R&D

**MIT esd**

**Exploration and Optimization**

**MSDO Framework**

- **Strongly interacting internals:**
  - Plasma core & edge, PFC’s,
  - actuators & controls, blankets,
  - shields, neutron & T transport,
  - materials responses

- **Figures of merit:**
  - Performance vs. cost, risk from uncertainties (data base, TRL’s), R&D leverage, B-C-R ratios

- **Other systems:**
  - Fusion externals, remote handling, site power, waste management, safety, environment, infrastructure, etc.

- **Mission space, non-technical constraints, etc.**

- **Interfaces, constraints**

- **Numerical Techniques** (direct and penalty methods)
  - (SA, GA)

- **Heuristic Techniques**

**Simulation Model**

- **Design Vector**
  - \[ \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \]

- **Objective Vector**
  - \[ \begin{bmatrix} J_1 \\ J_2 \\ \vdots \\ J_z \end{bmatrix} \]

**Coupling**

**Optimization**
How does this tool support fusion materials science research?

- Goal: help quantify uncertain benefit-cost-risk for differing internals option sets and the associated research
  - Cover options of mission, configuration, performance, cost, research choices, impact due to uncertainties (risks)
  - Inform critical decisions
  - A vehicle to develop in-kind collaboration with SC, NE, NNSA
- Start soon to benefit early, from simple to complex, point model to detailed modeling, and link to available advanced simulation codes
- Work with practitioners of plasma dynamics & control and materials science research, and also other interested within DOE

How could this possibly be realized within the constraints of Charge 3?
To introduce a “fighting chance” while addressing Charge 3

<table>
<thead>
<tr>
<th>Fusion materials science research in ITER era ($M/yr)</th>
<th>2015-2019 (preparation)</th>
<th>2020-2029 (research program &amp; project)</th>
<th>2030-2039 (integrated research)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. MDMP tool</td>
<td>1-2 (part of III)</td>
<td>5 (part of IV)</td>
<td>3 (part of IV)</td>
</tr>
<tr>
<td>II. Other DOE in-kind, equivalent</td>
<td>1</td>
<td>~10% of III + IV</td>
<td>~10% of III + IV</td>
</tr>
<tr>
<td>III. Fusion materials science research</td>
<td>10 (requisite)</td>
<td>50 (internals)</td>
<td>50 (integrated testing)</td>
</tr>
<tr>
<td>IV. FNSF</td>
<td>1-2 (metrics, mission and options)</td>
<td>50 (facilities)</td>
<td>50 (operations)</td>
</tr>
<tr>
<td>V. Fusion plasma dynamics and control in-kind</td>
<td>Guidance to MDMP tool development</td>
<td>5 (plasma dynamics and control design)</td>
<td>10 (plasma dynamics and control operation)</td>
</tr>
<tr>
<td>VI. International in-kind, equivalent</td>
<td>Possibly, 1</td>
<td>80 (45% of VIII)</td>
<td>83 (45% of VIII)</td>
</tr>
<tr>
<td>VII. Total DOE (II + III + IV + V)</td>
<td>12-13</td>
<td>115</td>
<td>120</td>
</tr>
<tr>
<td>VIII. Total level of effort equivalent (VI + VII)</td>
<td>13-14</td>
<td>195</td>
<td>203</td>
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</table>

- Assume readiness to start FNSF (integrated research) in mid-2020’s
- Multiple internals options drive FNSF modularization and research flexibility (measure, discover, understand, improve, re-measure).
- Constrained fund likely leads to “adjacent possible” FNSF options
Multidisciplinary multi-physics (MDMP) simulation & analysis tool has high leverage

- Supports fusion materials science research
  - Clarifies benefit-cost-risk among options of internals, configuration, mission, performance
  - Informs research choices based leverage
  - Can become tool needed to integrate research, FNSF designs, and eventually operation scenarios
- Helps introduce a “fighting chance” for this research in ITER era
- Has broader potential applications
  - Can retool for other fusion energy systems / facilities
  - With early progress, can inform ITER operation and upgrade choices
Backup
CASL vision: Create a virtual reactor (VR) for predictive simulation of LWRs

<table>
<thead>
<tr>
<th>Leverage</th>
<th>Develop</th>
<th>Deliver</th>
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<tbody>
<tr>
<td>• Current state-of-the-art neutronics, thermal-fluid, structural, and fuel performance applications</td>
<td>• New requirements-driven physical models</td>
<td>• Toolkit for predictive simulation of physical nuclear reactors</td>
</tr>
<tr>
<td>• Existing systems and safety analysis simulation tools</td>
<td>• Efficient, tightly coupled multiscale/multiphysics algorithms and software with quantifiable accuracy</td>
<td>• Architected for platform portability ranging from desktops to DOE’s leadership-class and advanced architecture systems (large user base)</td>
</tr>
<tr>
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<td>• Improved systems and safety analysis tools</td>
<td>• Validation basis against 60% of existing U.S. reactor fleet (PWRs), using data from TVA reactors</td>
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<td>• UQ framework</td>
<td>• Base M&amp;S LWR capability</td>
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[Diagram showing a virtual reactor model with primary and secondary systems, and a nuclear power plant background.]
CASL mission: Develop and apply the VR to address 3 critical performance goals for nuclear power

1. Reduce capital and operating costs per unit energy by:
   - Power uprates
   - Lifetime extension

2. Reduce nuclear waste volume generated by enabling higher fuel burnups

3. Enhance nuclear safety by enabling high-fidelity predictive capability for component and system performance from beginning of life through failure
"Multiphysics Integrator" simulates reactor core

Virtual Environment for Reactor Analysis (VERA)
A code system for scalable simulation of nuclear reactor core behavior

- Flexible coupling of physics components
- Toolkit of components
  - Not a single executable
  - Both legacy and new capability
  - Both proprietary and distributable
- Attention to usability
- Rigorous software processes
- Fundamental focus on V&V and UQ
- Development guided by relevant challenge problems
- Broad applicability
- Scalable from high-end workstation to existing and future HPC platforms
  - Diversity of models, approximations, algorithms
  - Architecture-aware implementations

Multiphysics Integrator

- Neutronics (diffusion, transport)
- Thermal Hydraulics (thermal fluids)
- Structural Mechanics
- Reactor System
- Multi-resolution Geometry
- Mesh Motion/Quality Improvement
- Multi-mesh Management
- Chemistry (crud formation, corrosion)
- Fuel Performance (thermo-mechanics, materials models)
Nuclear materials science underpins LWR performance

MPO science innovation is micro-meso coupling in both complexity of physical phenomena and modeling and simulation capability

- Multiphysics complexity
- Integral phenomena
- Unit processes

**Project**
1. CMPM
2. Microstructure evolution: Fuel
3. Microstructure evolution: Clad
4. Corrosion of clad/internals
5. CRUD deposition
6. Failure modes
Example of FNSF internals modularity & flexibility to address options, with low support-structure lifetime-dpa