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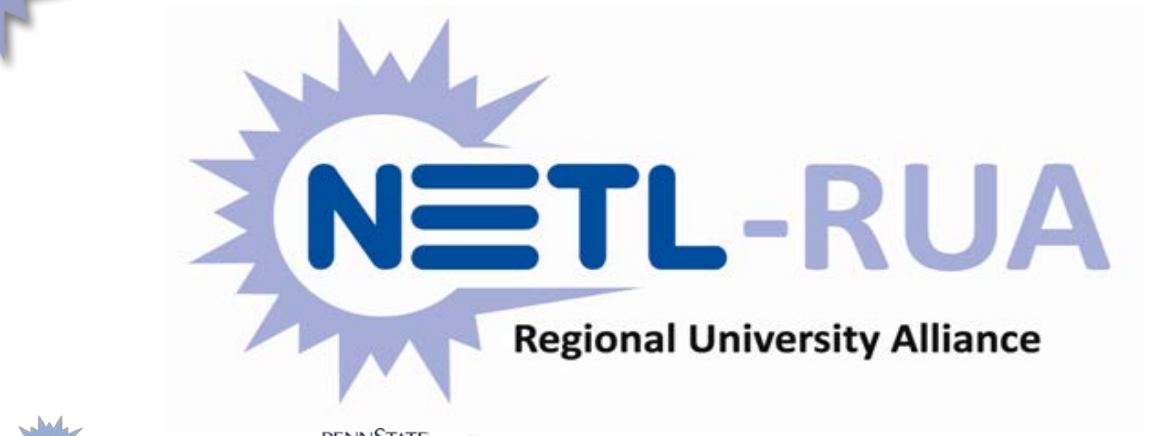

NETL Carnegie Mellon PENNSTATE University of Pittsburgh VirginiaTech WestVirginiaUniversity URS

A Global Approach to Operational Modeling with Degradation

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DOE-NETL, Technical Coordinator – Fuel Cells

U.S. DEPARTMENT OF ENERGY

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- **NETL RUA Fuel Cell Team**
  - Researchers at NETL, CMU, PSU, WVU, and URS
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- **NETL and URS Collaborators**
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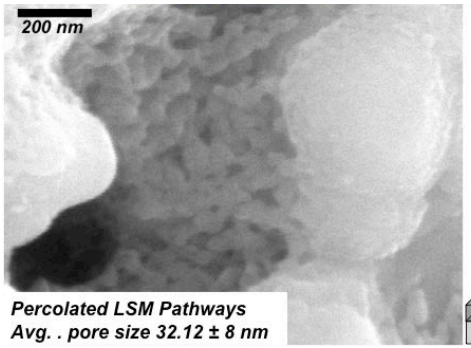
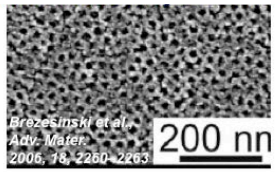
NETL RUA - Solid Oxide Fuel Cells

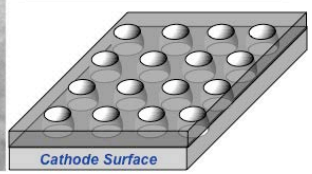
Support Industrial Development

Operation of NETL Solid Oxide Fuel Cell Multi-Cell Array on direct, coal-derived synthesis gas at the National Carbon Capture Center at Wilsonville, AL in August/Sept 2009.

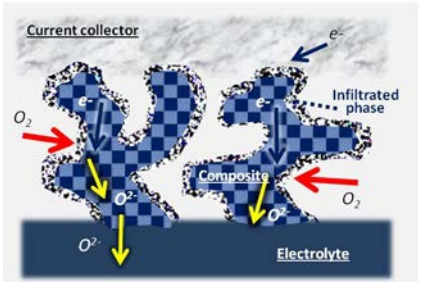
Collected 4,000 + cell-hours of data to support development of gas cleanup systems sufficient for gasifier / fuel cell integration.





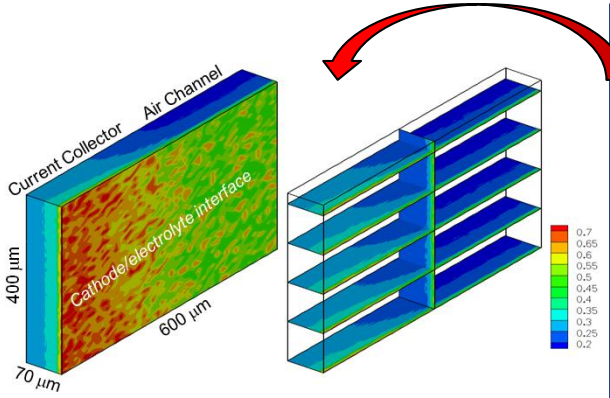


Innovate Technology



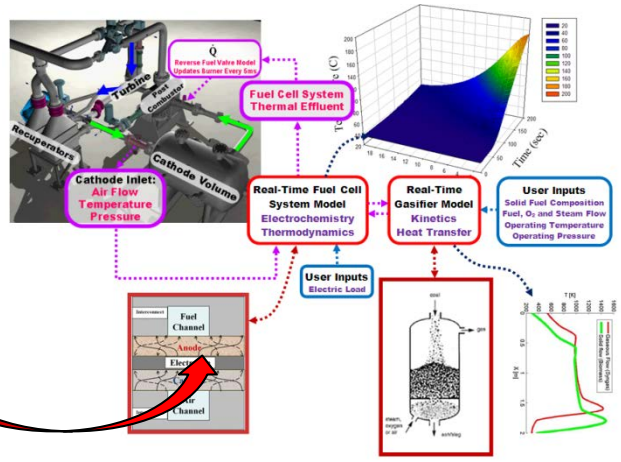
Cathode infiltration technology is being developed to enhance the SOFC operating performance. Initial results have demonstrated > 40% performance improvement and acceptable material stability.

Evaluate Advanced Concepts



Fundamental computations (3D multi-physics model, at left) inform modeling of advanced degradation, performance, and microstructural evolution at the cell and stack level.

Integrated gasifier / fuel cell / turbine systems (IGFT, at right) support advanced fuel cell demonstrations efforts (2013+). NETL operates a system hardware evaluation and controls development platform.



Topic of Presentation

Global Consideration of the Role of Degradation on Performance

- **Degradation persistently affects cell operation**
- **Instantaneous operation depends on the cumulative history of degradation (path dependent)**
- **Degradation could be sourced in any component or structure, but here consider only the cell**
  - Cell is most complex among all SOFC system components
  - Function is tightly coupled with structure

Topic of Presentation

Proposal for Global Framework

- **Degradation occurs (or doesn't!) within a vast operational parameter space**
- **Predictive models fail absent complete accounting of degradative processes**
  - Empirical models: Statistical, costly in time
  - Phenomenological/descriptive models: Inflexible
  - Predictive models: Computationally large
- **Common approach engenders more rapid consensus**

Operational Modeling

Outline

- Modeling Concept
- Definitions
- Degradation Framework
- Operating State + Transitions
- Global Framework

Modeling Concept

- **Create a flexible modeling system that can**
  - Describe instantaneous degradation
  - Predict the operational impact of degradation
- **At each time step, the model requires:**
  - Structural description
  - Operating state
- **Realistic time scale of state transitions**

Analogous to Hurricane Forecasting

http://www.katrina.noaa.gov/forecast

Definitions

Designed State

- A composition, structure, morphology (or combination thereof) existing in an initial state, and possessing predictable characteristic properties and demonstrating known behaviors

Degradation

- The departure of any functional SOFC composition, structure, morphology (or combination thereof) from its designed state in response to perturbing forces

Operating State

- A “complete” description of the thermodynamic and structural state of a cell at a given point in time

Degradation Framework

General

Specific

Source/Order

- Intrinsic v. Extrinsic
- Direct v. Indirect

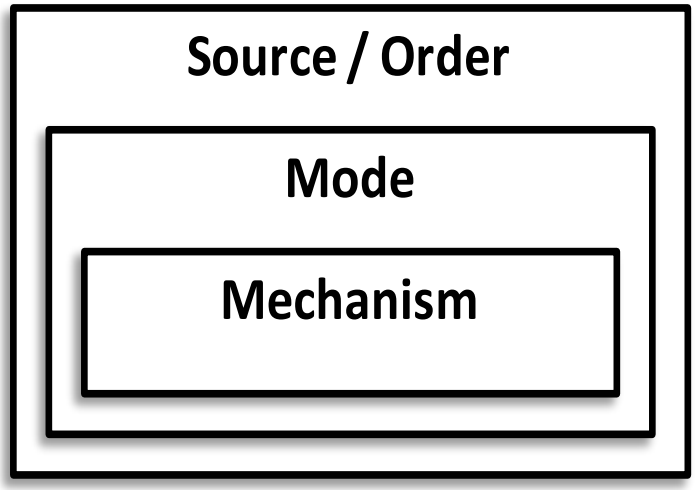
Mode

- The physical nature of the forces applied to a fuel cell describing the perturbation

Mechanism

- The specific process by which degradation occurs in a cell

Hierarchy

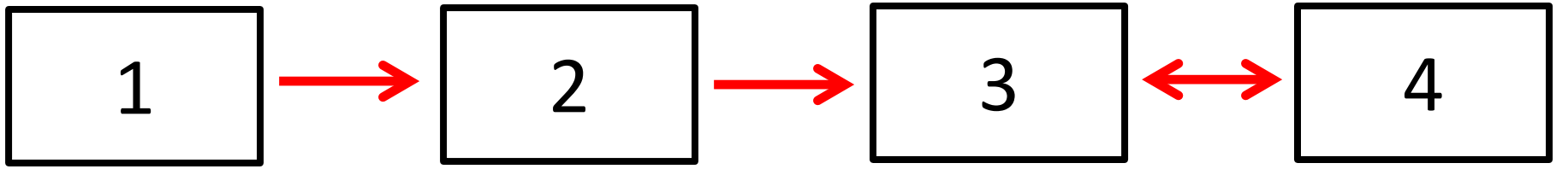


Operating State

4 common operating states

1	2	3	4
As fabricated	Pre-treated	Designed Operation	Off-Design Operation

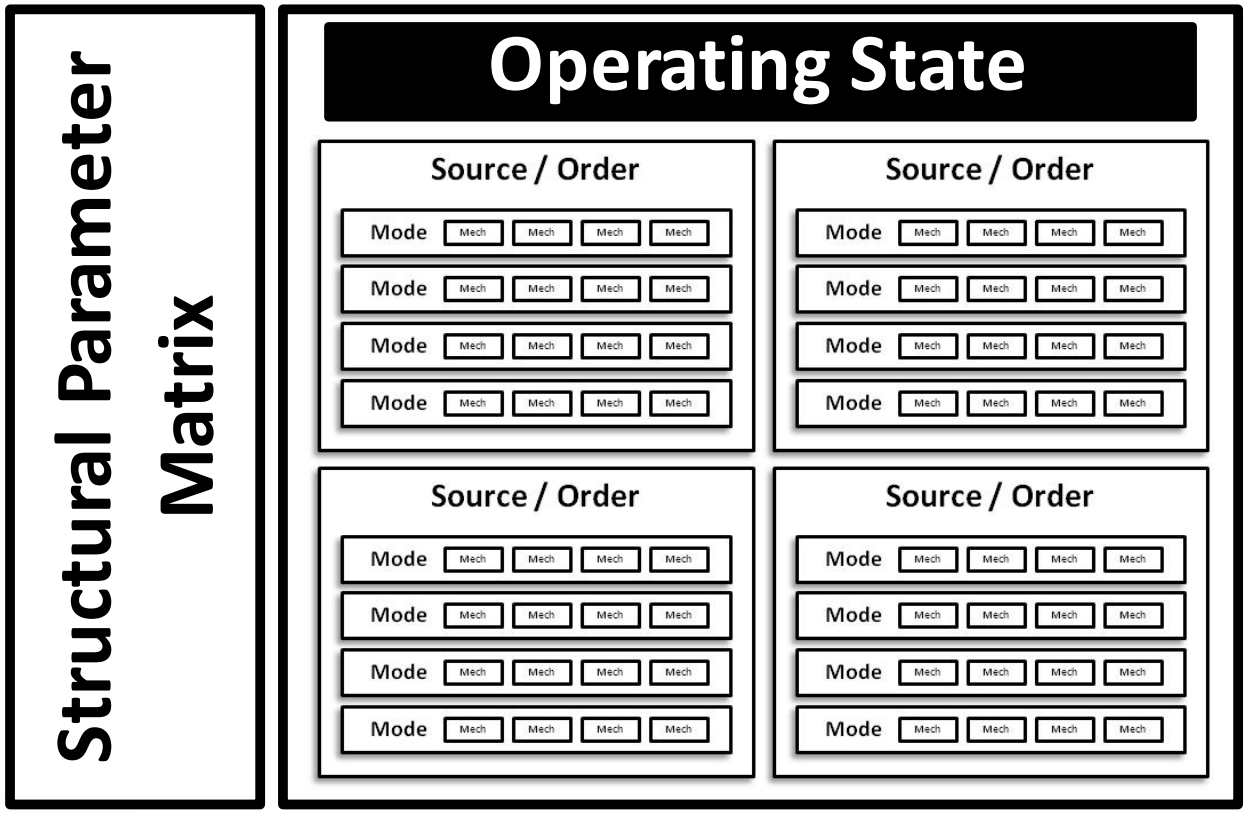
Conventional state transitions



Absolute operational time scale

Framework plus Operating State

A complete description of instantaneous performance at all physical locations



Global Framework

- **Global framework is used to step in time**
  - Steady state operation
  - Operating state changes (instant or gradual)
  - Relaxation/response processes

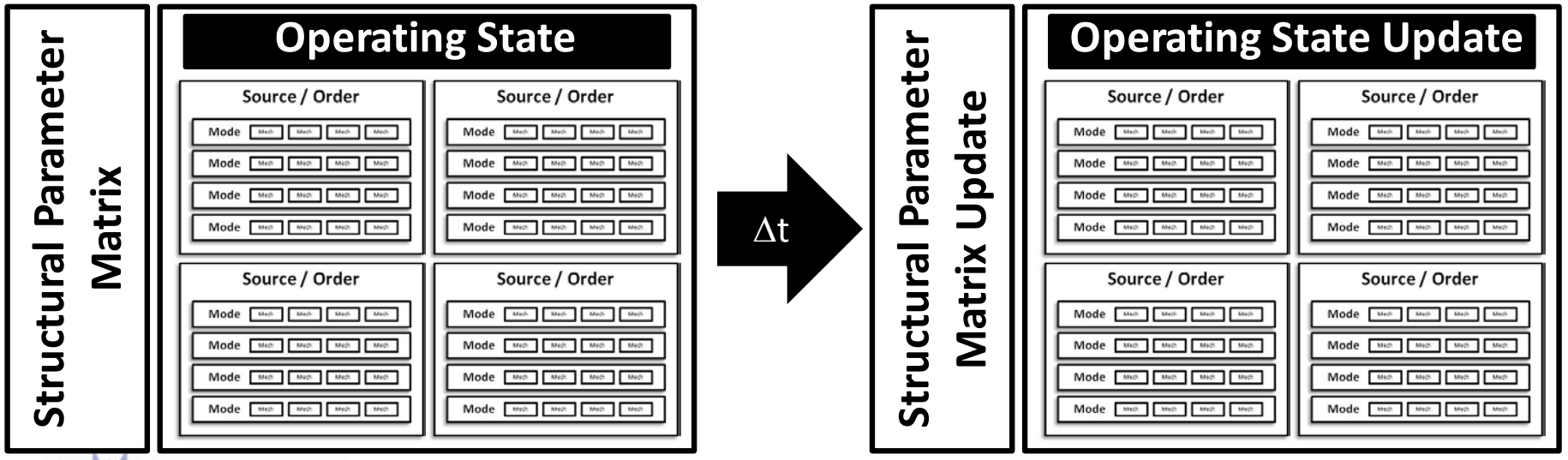


Illustration 1: Path Dependence

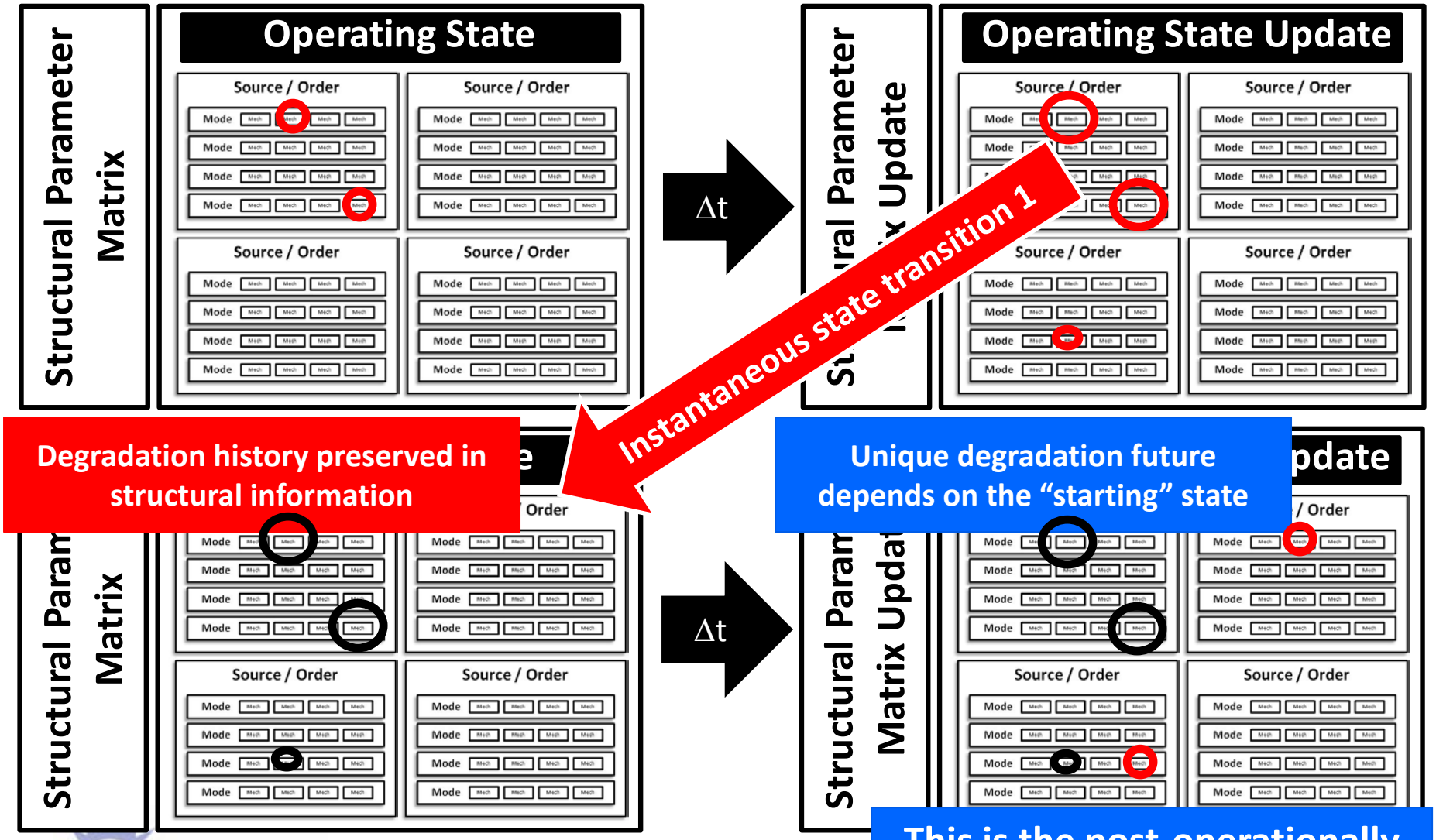


Illustration 2: Path Dependence

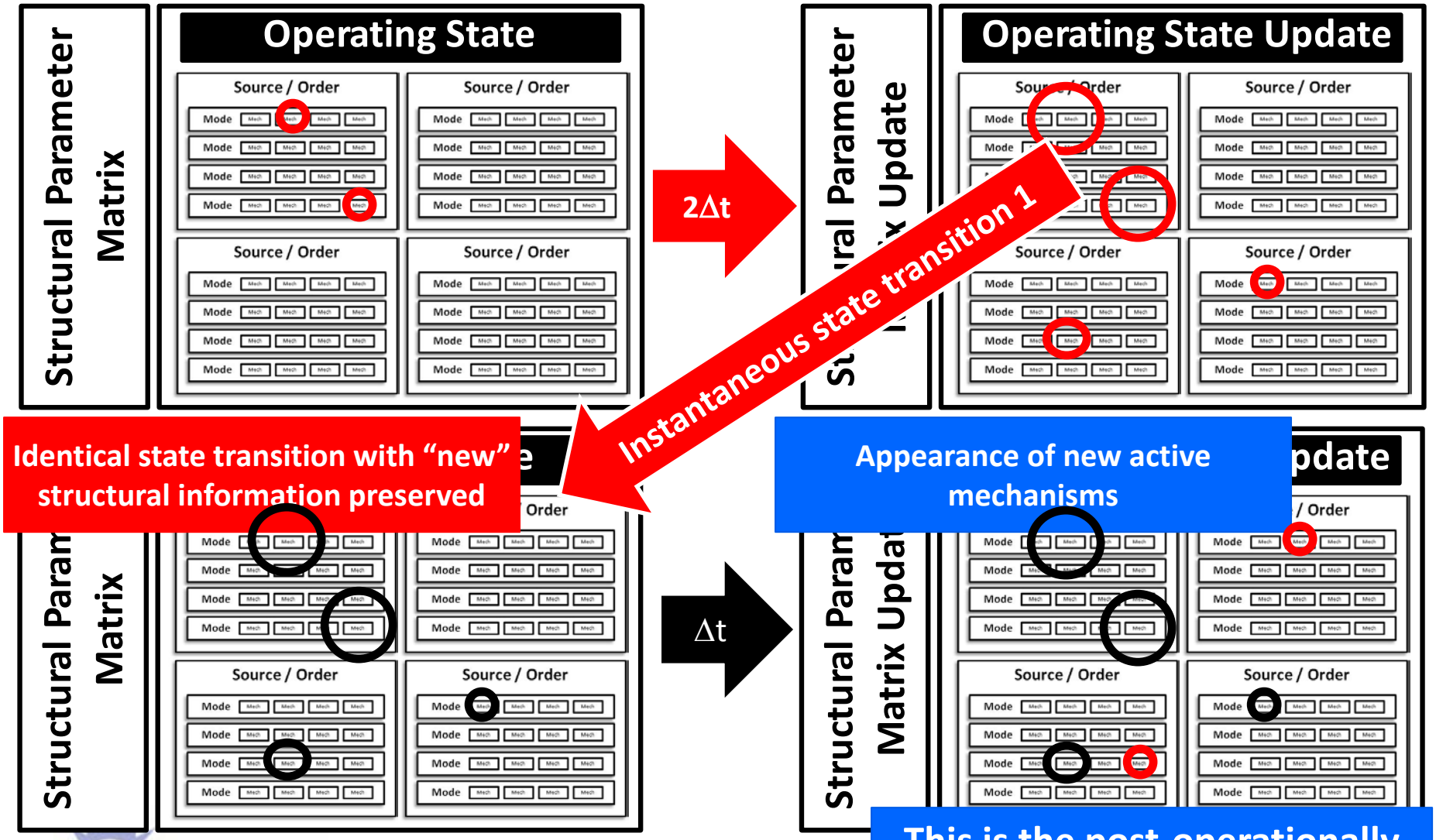
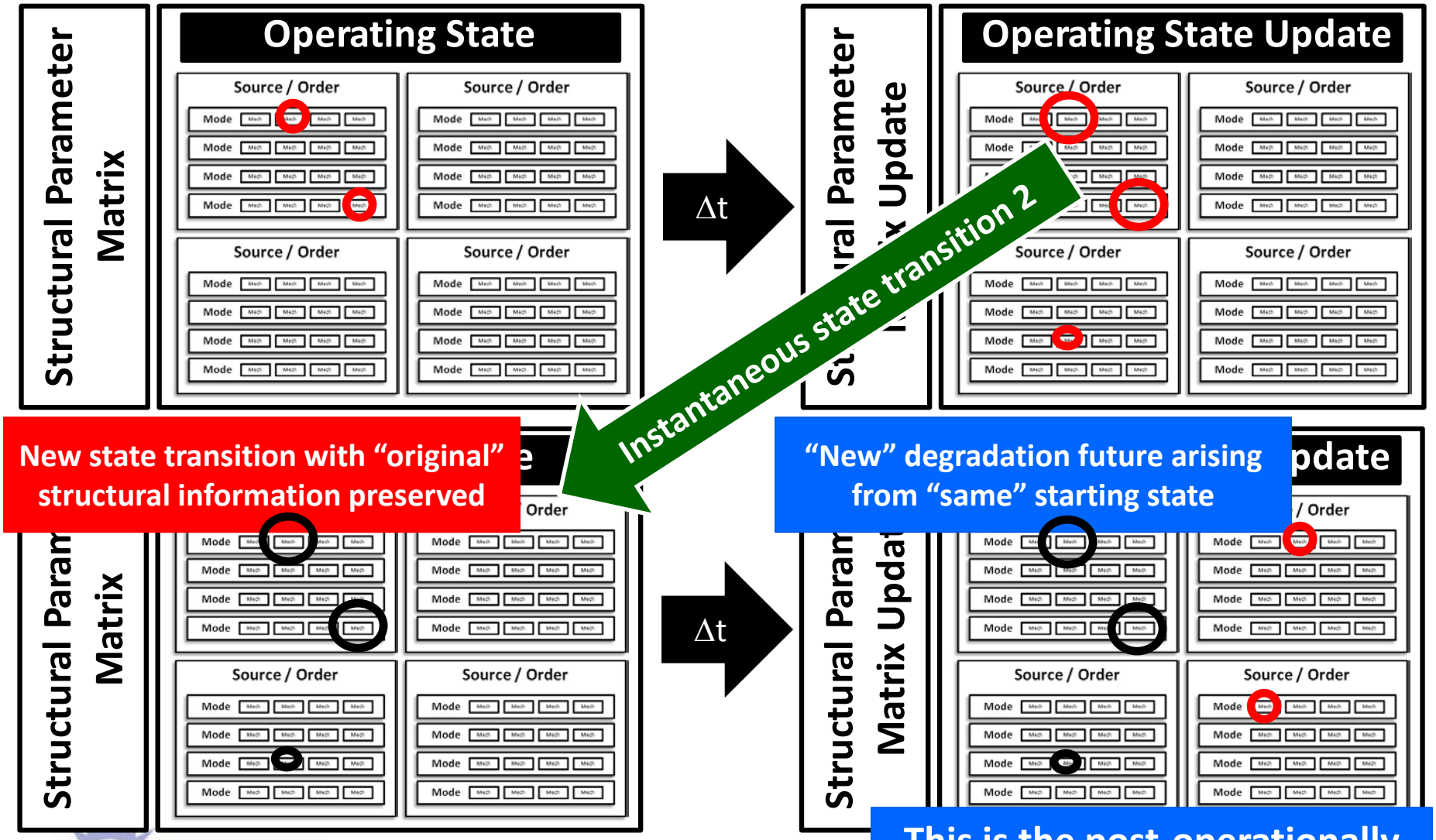


Illustration 3: Path Dependence



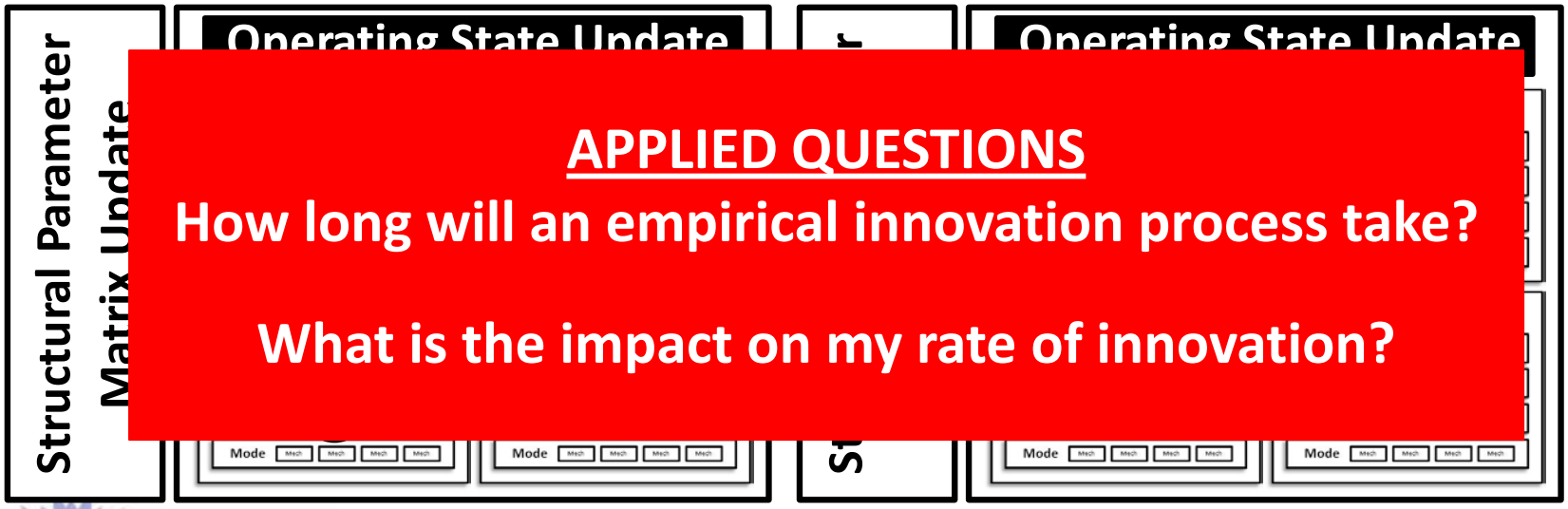
Final State Comparison

FUNDAMENTAL QUESTIONS

To what mechanism is degradation attributable?

How do I engineer performance improvement?

How do I control degradation operationally



APPLIED QUESTIONS

How long will an empirical innovation process take?

What is the impact on my rate of innovation?

Framework Utility

- Computational approach enables low-cost comparison of path-dependent degradation outcomes
- Track relative contributions from degradation processes in real time
- Establishes correlation between operating conditions and manifestation of degradation
- Improves predictive accuracy of performance models applied to commercially relevant time scales
- Accelerates innovation

NETL RUA Research

- **NETL RUA Present Task:**
  - Populate the framework and identify contributing models

- **NETL is developing 3 core models that align to the framework to describe spatio-temporal operations while considering degradation**

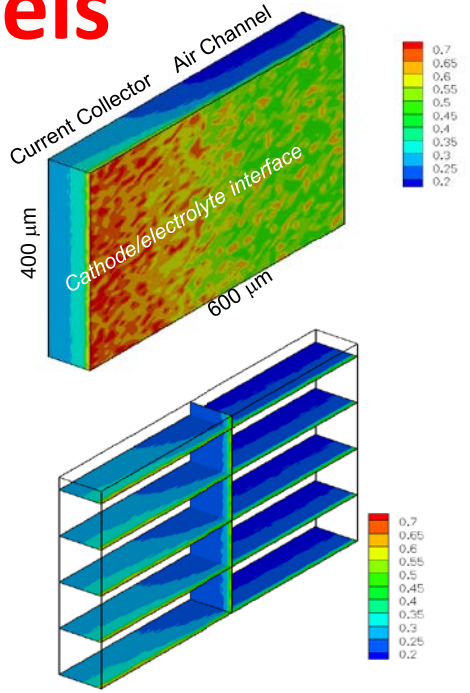
- **The 3 core models operate at the sub-grain (<20 nm) level to the single stack level, and through the entire operational service time domain (100 khr)**

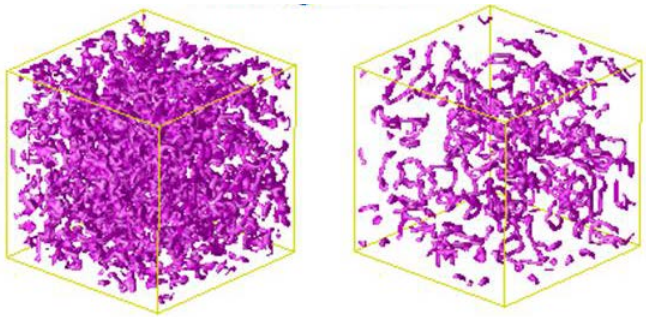
NETL RUA Research

3 Domain Scale Models

- **3D multi-physics**
  - Describes complete physics with high fidelity ORR
  - Robust in the spatial domain
- **3D microstructural evolution**
  - Describes temporal changes in microstructure
  - Robust in the time domain
- **Uncertainty Quantification (UQ)**
  - Establishes the magnitude of uncertainty associated with predictive or extrapolative computations

** Initiated in April 2013

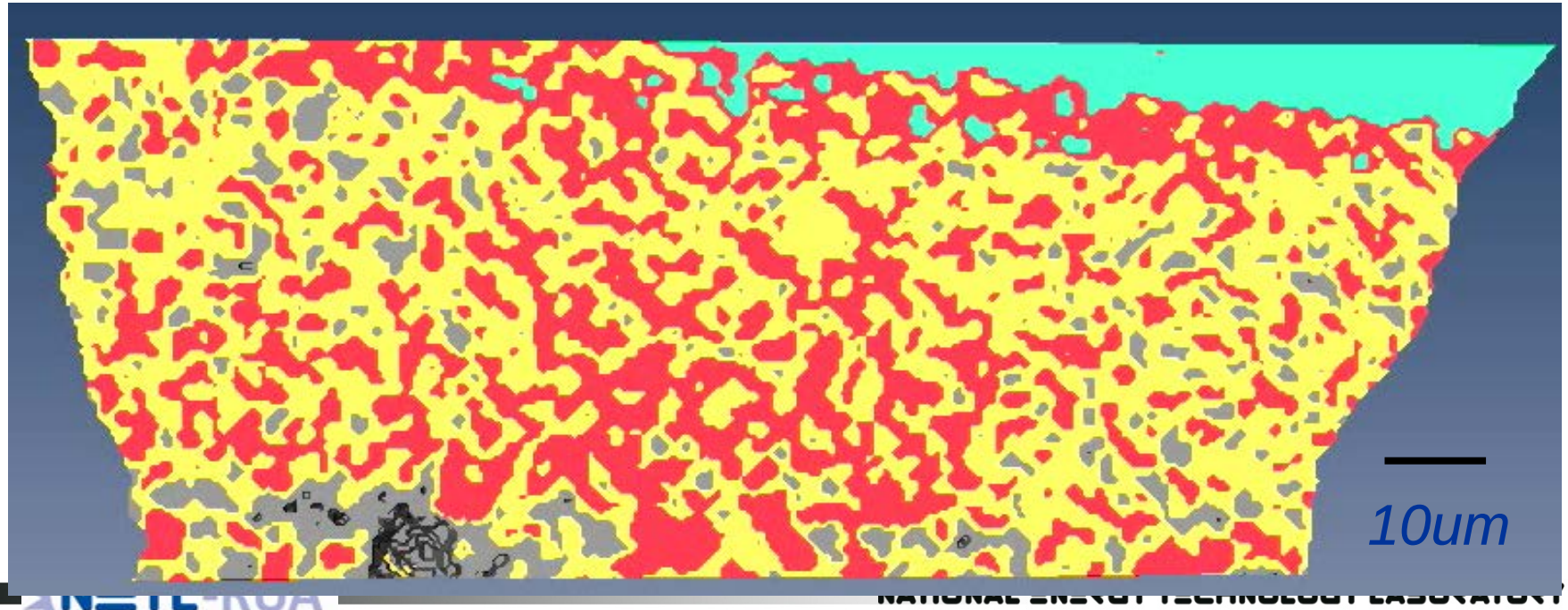




NETL RUA Research

Additive Models

- **Domain scale models are complimented by fundamental models including**
  - High fidelity ORR model for LSM/LSCF
  - Complete digitized 3D cell reconstructions in $(65\mu m)^3$ volume resolved to 150 nm

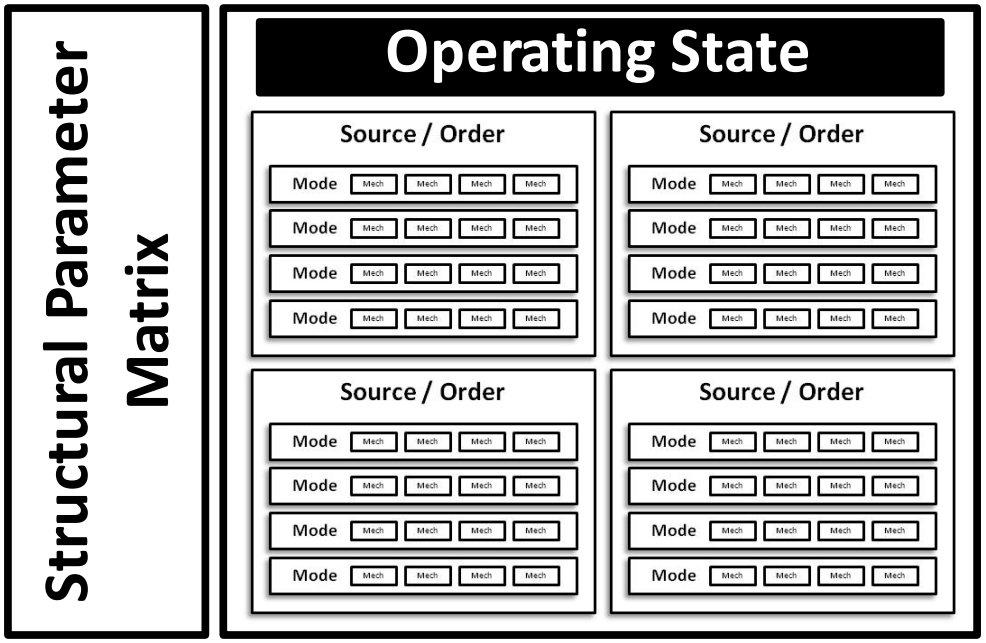


NETL RUA Research

Efforts in FY14

- The proposed modeling effort will require substantial computing resources
- Beginning to transfer all codes to a super-computing environment at NETL (SBEUC)
- SBEUC also contains an advanced visualization center that will allow detailed examination of computational results
- A series of tools will also be produced that support performance analysis – tools will be commonly accessible

Opportunities



- Identification of specific modes and mechanisms within the framework is a community-wide project
- Discussion required to identify prevalent (critical) mechanisms
- Integration of global framework with system models

Summary

- A global framework is described to facilitate a complete description of degradation in an operating SOFC stack
- NETL is using existing models and developing new models to describe degradation in accord with the framework
- The NETL RUA Fuel Cell Team would strongly welcome the opportunity to collaborate with all teams (including SECA external) in developing the comprehensive degradation models described