High Speed Computing Conference
Salishan Lodge, Gleneden Beach, OR, April 27-30, 2009

Computer Simulations for Nuclear Energy Applications

Marius Stan[1]

Contributors: C. R. Stanek[1], B. P. Uberuaga[1], B. Mihaila[1], S. M. Valone[1], A. D. Andersson[1], P. Cristea[2] , S. Y. Hu[3], J. C. Ramirez[4], V. Tikare[5], P. Turchi[6], and M. Samaras[7]

[1]Los Alamos National Laboratory, U. S. A.
[2]Univ. of Bucharest, Romania
[3]Pacific Northwest National Laboratory, U. S. A.
[4]Exponent, Inc., U. S. A.
[5]Sandia National Laboratory
[6] Lawrence Livermore National Laboratory
[7]Paul Scherer Institute, Switzerland

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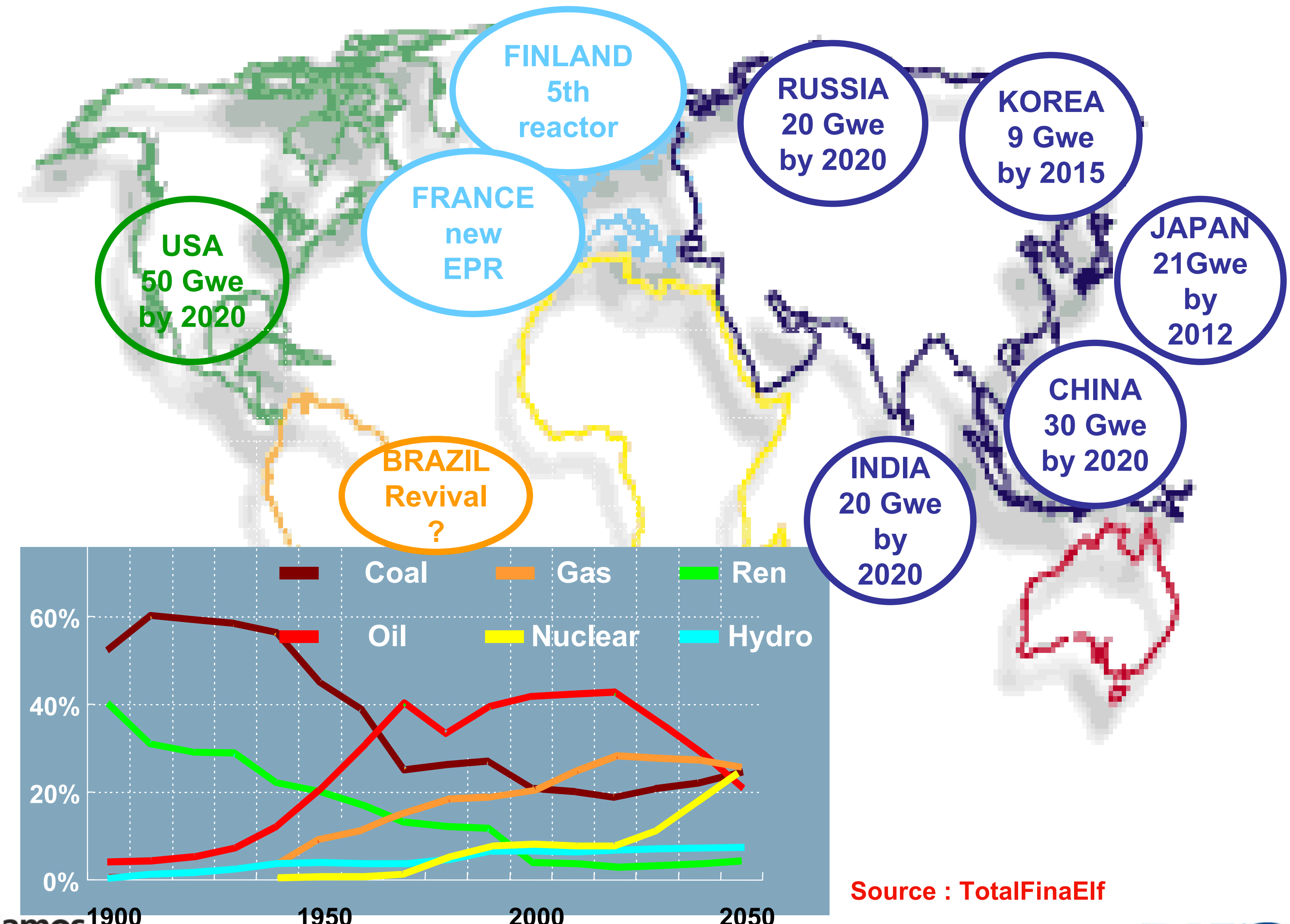
Outline

- Nuclear energy prospects
- Study case: Models of radiation effects
- Study case: Fuel performance simulations
- Uncertainty analysis
- The case for science-based models and high-speed simulations
- International Collaborations
- Summary

Significant prospects for nuclear energy in the world



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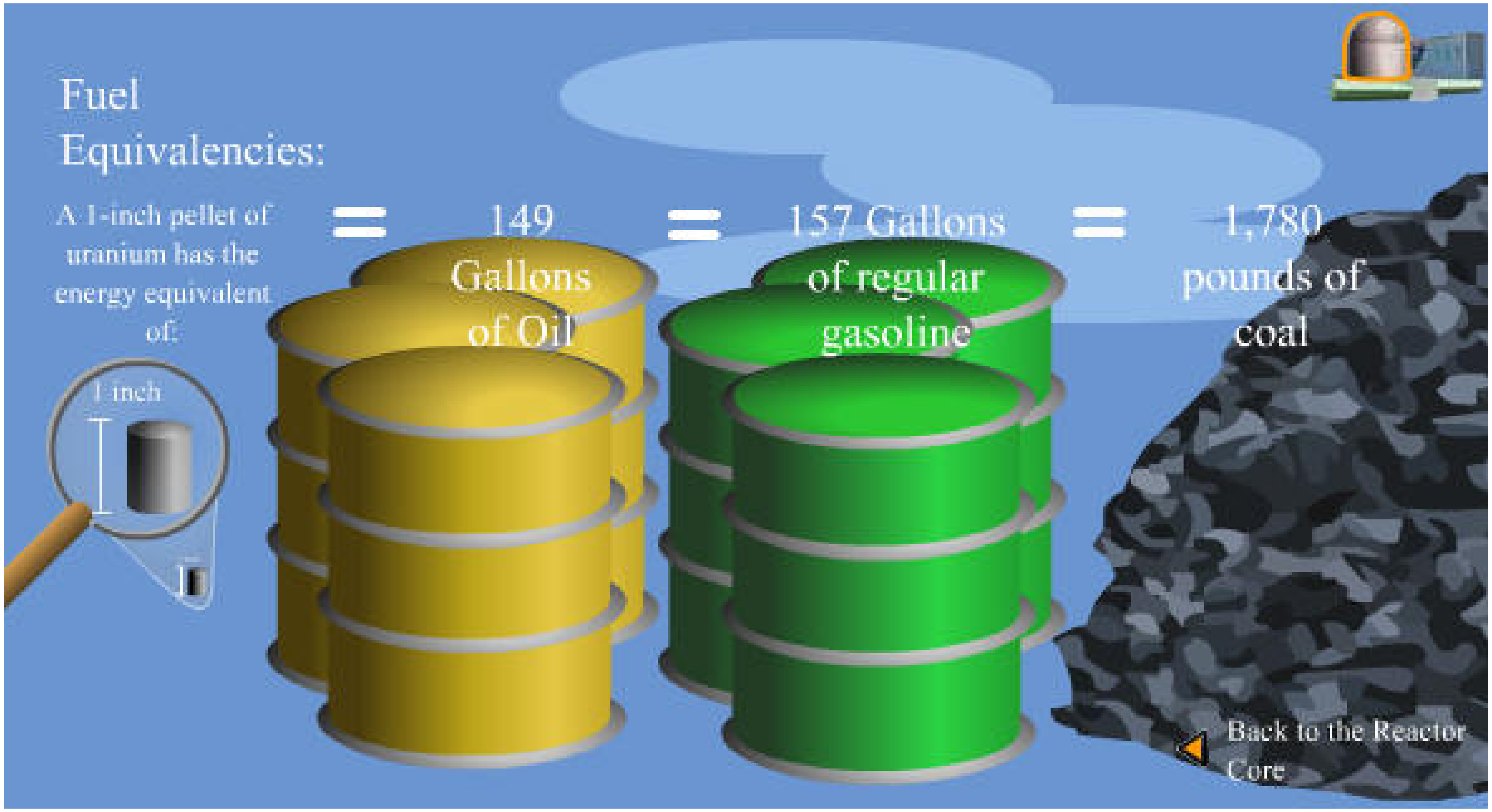
Energy Density

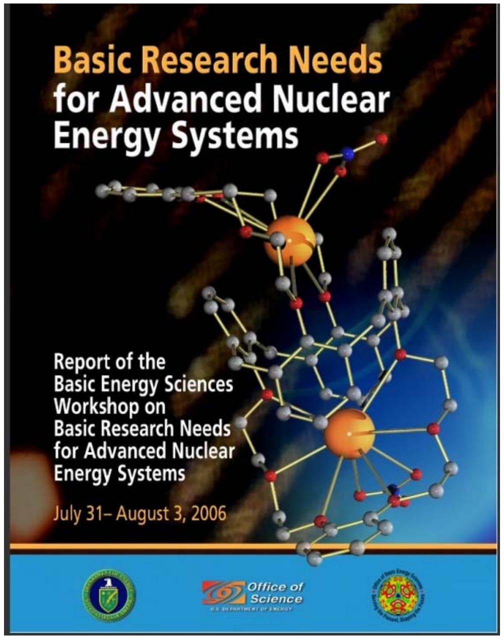


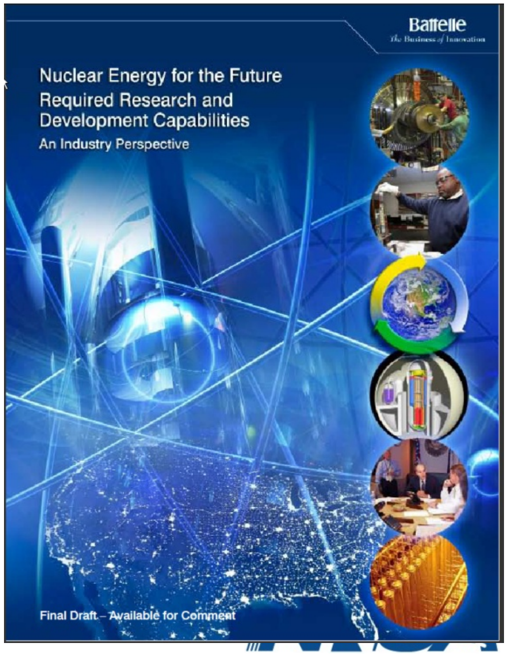
from http://www.dom.com/about/stations/nuclear/nuctour.html

Nuclear fuels have the highest energy density and are ideal for applications that require small volume but long term energy sources such as space travel and the military.

Basic and Engineering Research Needs

- Fundamental Issue (s)
  - **Develop new tools for NRC licensing & material qualification**
  - **Closing the nuclear fuel cycle in a proliferation resistant and environmentally sensitive manner.**
  - Timely fuel development ; Timely irradiation insights
  - If world goes nuclear then fuel availability requires breeder reactors.
- Needs
  - **Agile design and engineering application for nuclear materials;**
  - Trusted standards and principles based on predictive capability;
  - Faster and cheaper design cycle to materials discovery
  - Production and certification of new fuels (oxide, metal, nitride, carbides, hydrides) and geometries; durability to large burn up ; Range of fuels and geometries;
  - Full scale system analyses; alternative fuel cycles; fast reactor studies; small scale fast reactors; bench size Urex; long term waste storage
  - Increase operating margins & reduced licensing conservatism
  - LWR - lifetime extension
  - Train next generation of work force base
  - In situ measurements (including defects and temperature)
  - **Fuel codes (e.g. Frapcon) to evolve from empirical to deterministic**
- Performance Gaps
  - Certified transmutation fuels with high minor actinide content for fast reactors that can take high burnup (>100 GWD/MTM)
  - Structural materials that remain in service beyond 200 dpa.





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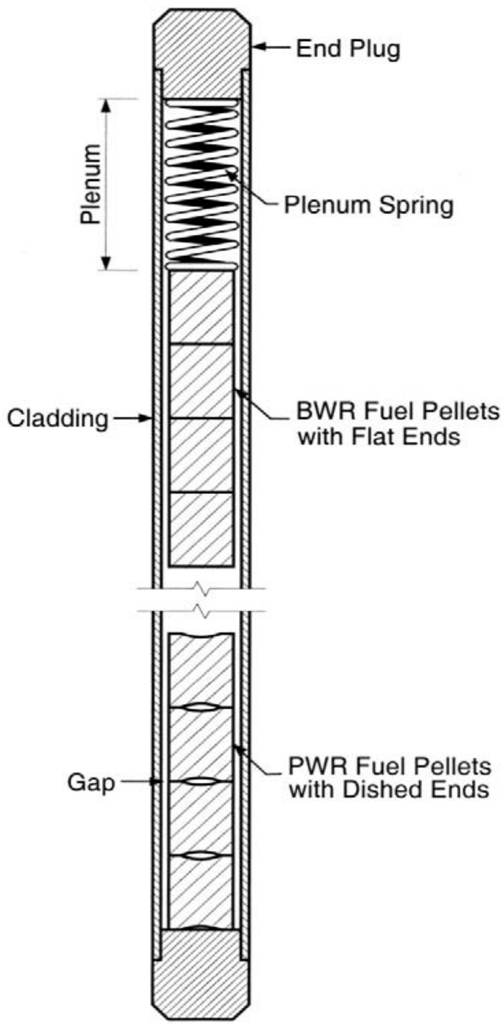
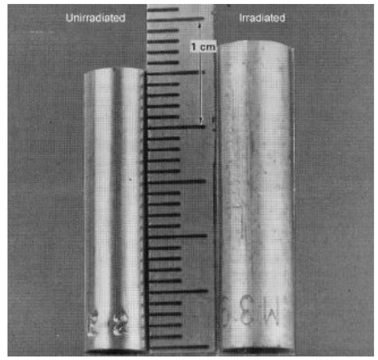
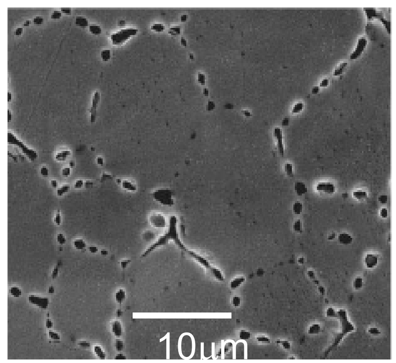
Irradiation Effects on Fission Reactor Materials



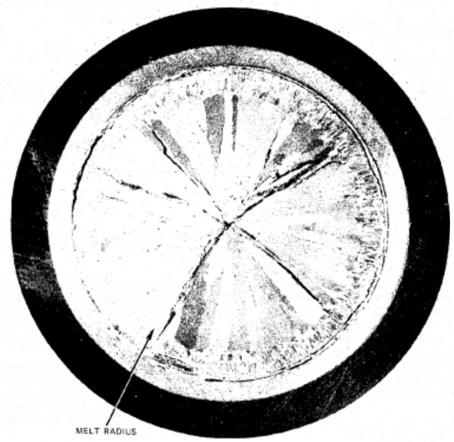
Schematic representation of a fuel element



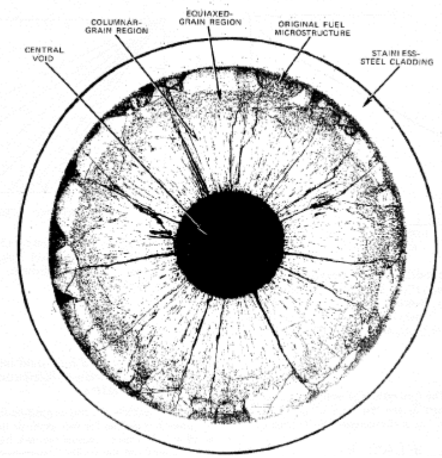
Cladding swelling, deformation



Fission products accumulation, changes in heat release

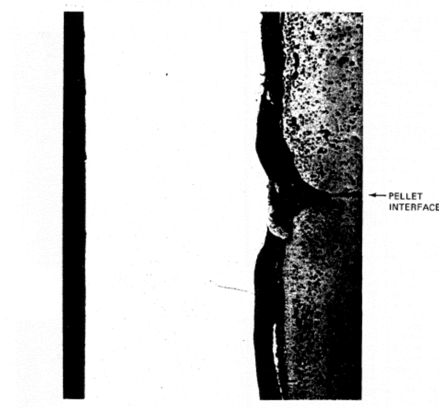


Localized melting, phase stability issues



Fuel restructuring, changes in chemistry

Fission Product Oxide Formation, Corrosion



Fuel/Cladding Chemical Interactions

*From Donald R. Olander, "Fundamental Aspects of Nuclear Reactor Fuel Elements," TID-26711-P1, Technical Information Service, U.S. Department of Commerce, Springfield, Virginia.
*With contributions from G. Hansen (INL) and T. Totev (ANL)

Materials Discovery and Design

Materials discovery: Scientific exploration of existing or new materials toward identifying useful properties and functionality.

Note: “Chance favors the prepared mind” (Louis Pasteur)

Methodology:

- Conduct sound scientific research in areas that are likely to lead to discovery of new materials with desirable properties
- Identify promising materials and develop models of properties as functions of parameters
- Perform simulations to predict the properties and functionality outside the initial parametric intervals.
- Validate using experimental data

Materials design: Scientific development of new materials toward obtaining predefined properties and functionality.

Methodology:

- Define target properties, functionality and the acceptable uncertainty
- Identify promising materials and develop models of properties as functions of parameters
- Perform simulations to predict the properties and functionality outside the initial parametric intervals.
- Validate using experimental data

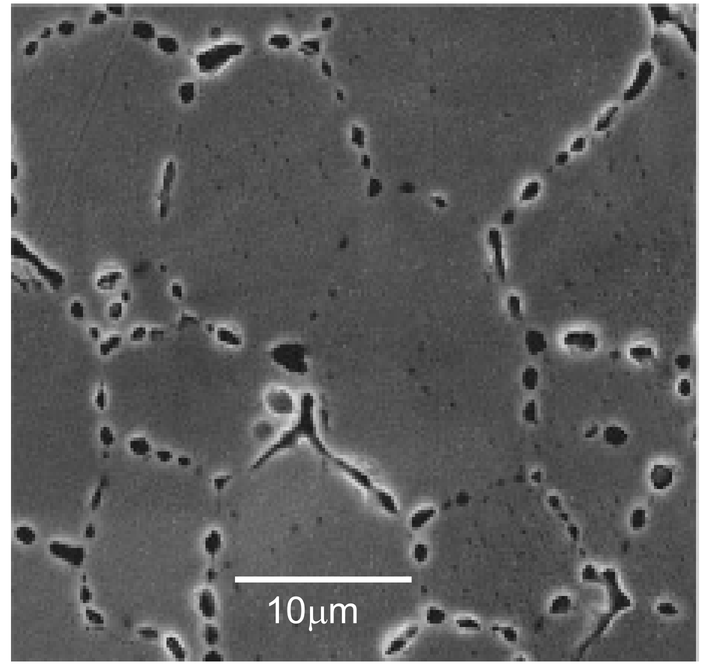
Note: Rarely a material is developed entirely “by design”; discovery is often a hidden ingredient.

Challenge: Fission Gas Bubbles

Importance: Gas bubbles form in the fuel due to irradiation and the nucleation, growth, and coalescence of fission products (FP). The bubbles form in the grain or at the grain boundaries. The PF gas bubbles decrease thermal transfer and can lead to the formation of “tunnels” (channels) that release the gas into the gap (fuel-clad) region.

Irradiation effects:

• Gas bubbles favor the creep deformation of the fuel.
• Radiation induced changes in microstructure modify the effective thermal conductivity.
• Due to gas bubbles formation , species diffusivities become highly anisotropic with burnup.
• Gas release limits burn-up levels.
• Nucleation times are of the order of picoseconds. Coalescence times go all the way to micro-seconds.
• Typical size distributions of gas bubbles range from nano-meters to tens of µm.



Fission gas bubbles in UO_2 irradiated in a Pressurized Water Reactor at burnup level 25GWd/t. The sample was annealed at 1275 ºC for 5 hours[1].

[1] I. Zacharie, S. Lansiart, P. Combette, M. Trotabas, M. Coster, and M. Groos J. Nucl. Mater. 255 (1998) 92-104.

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Atomistic Simulations of Irradiation Effects on Clad

Results:

•Molecular Dynamics (MD) methods can predict defect configurations in irradiated materials.

• The size of the defects and clusters is in the range of angstroms to tens of nanometers.

• The defects form, interact, recombine in pico-seconds.

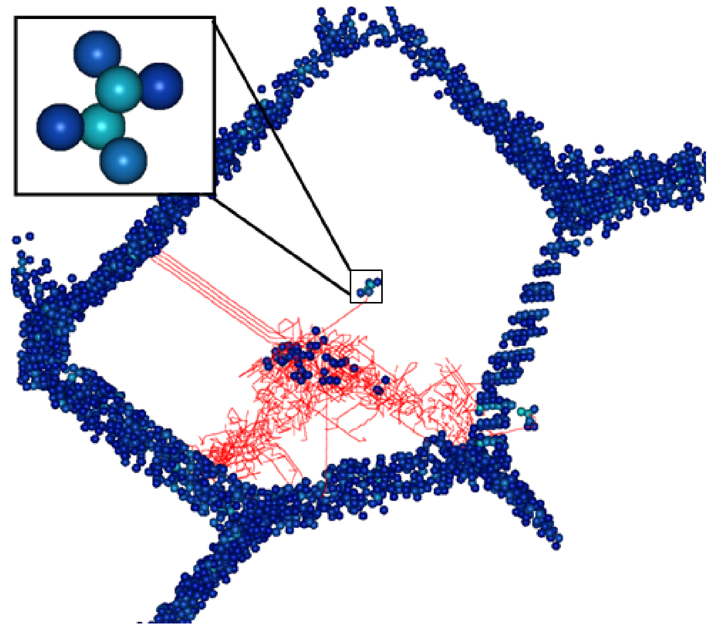
• Current confirmation of defect types is indirect, via continuum properties.

Needed:

• Experimental confirmation of point defects and defect clusters formation.

• Validation of short range order predictions. Ex: EXAFS for Fe-Cr alloys.

• Experimental input into inter-atomic potential optimization. Ex: synchrotron experiments, EXAFS to determine the charge environment.



Molecular Dynamics Simulations of irradiation effects on Fe, showing the grain boundary structure and damage (spheres inside the grain) produced at the end of a 20keV cascade.[1]

[1]T. Allen, H. Burlet, R. K. Nanstad, M. Samaras, and S. Ukai, MRS Bulletin, 34 (2009) 20-27.

Meso-Scale Models and Simulations of Gas Bubbles Evolution

Results:

• The microstructure was created using a Voronoy scheme.

•The free energy model was created using both experimental information and atomistic calculations.

• Although He is not a major fission product, its mobility is known in the bulk and at grain boundary.

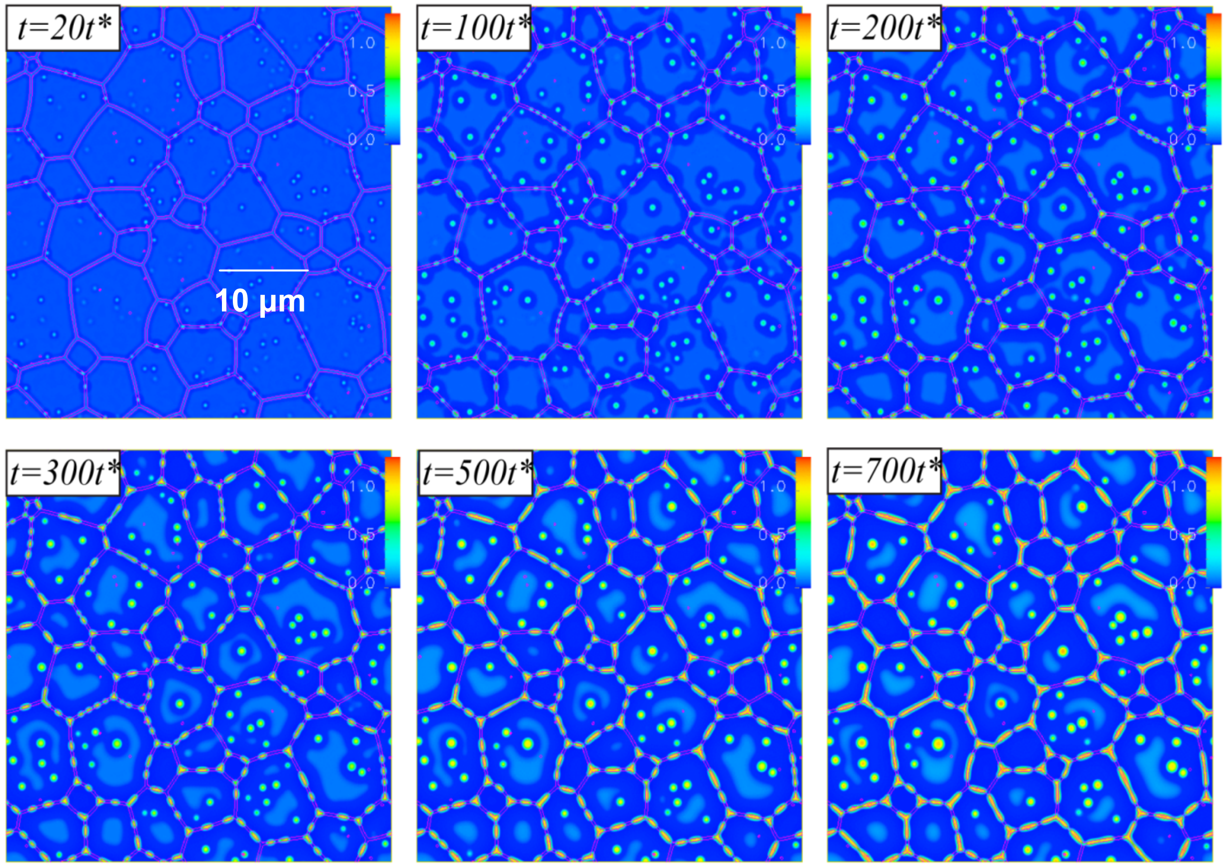
• The simulation can predict thermal conductivity as function of time (irradiation)

Needed:

• Mobility of FPs in the bulk and at the grain boundary

• Validation of microstructure evolutions: at least average grain size with time and burnup (dose).

• Validation of the thermal conductivity model.

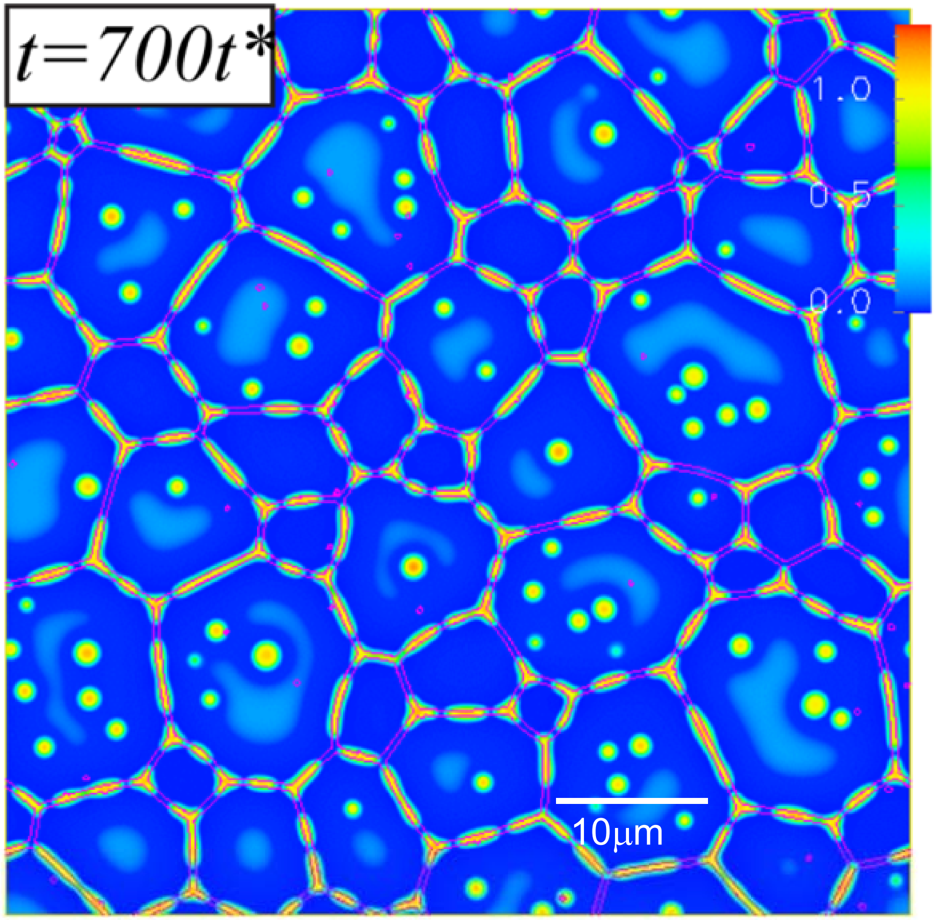


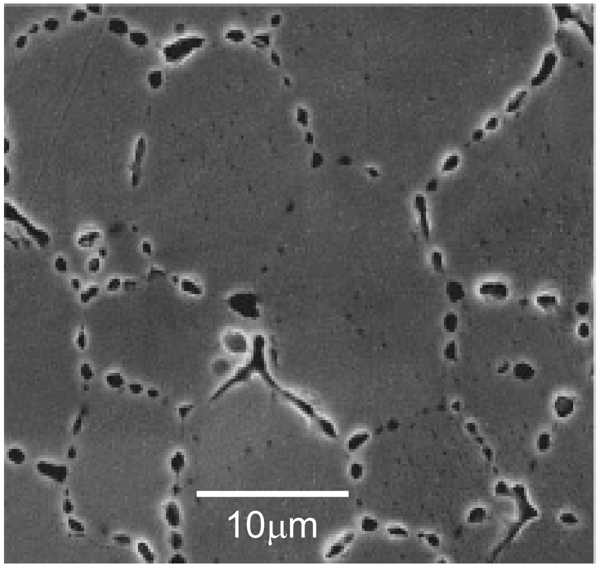
Time evolution of gas bubbles in a polycrystalline material[1]. The colors correspond to He concentration: red = high, blue= low. The characteristic nucleation time, t*, is retrieved from experiment (pico-seconds).

We need 3-D simulations of millions of grains.

[1]S. Y. Hu, C. H. Jr. Henager, M. Stan, M. I. Baskes, S. M. Valone, C. E. Beyer, and K. J. Geelhood, Acta Mater., (2009) in press.

Validation of Meso-Scale Simulations of Gas Bubbles[1]





Fission gas bubbles in UO_2 irradiated in a Pressurized Water Reactor at burnup level 25GWd/t. The sample was annealed at 1275 ºC for 5 hours[1].

Time evolution of gas bubbles in a polycrystalline material. The color scheme represents the He concentration. The purple lines show the grain boundaries. Here t* is the characteristic nucleation time (ns).

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[1]S.Y. Hu, C. H. Jr. Henager, M. Stan, M. I. Baskes, S. M. Valone, C. E. Beyer, and K. J. Geelhood, Acta Mater., (2009) in press.
[1]I. Zacharie, S. Lansiart, *et. al.,* J. nucl. Mater. 255 (1998), 92-104.

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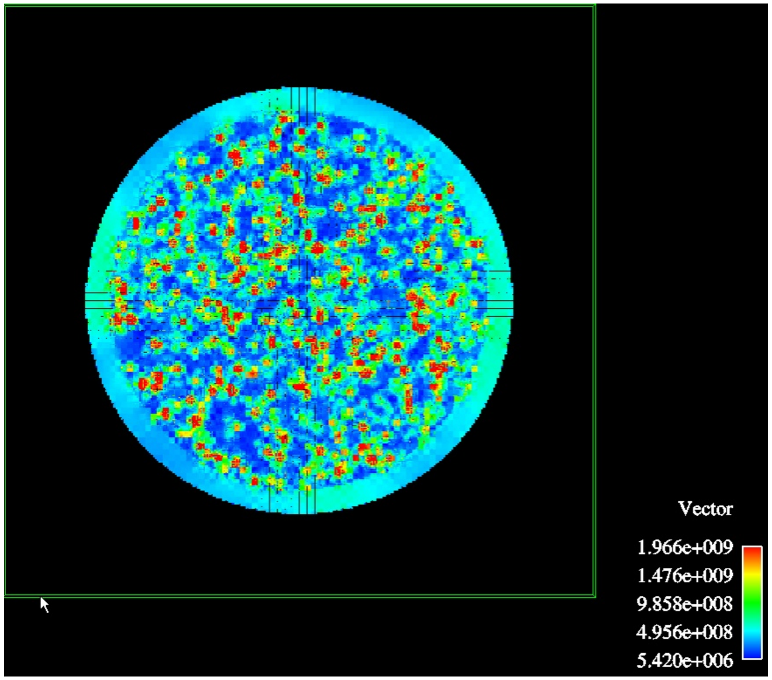
Continuum Simulations of Gas Bubbles Evolution

Results:
- Materials Point Method (MPM)
- Gas bubbles formed by fission products
- Intra-grain transport via Potts Model
- Coupling via stress field
- No microstructure (homogeneous materials)
- Two phases: solid and gas MPM particles
- Pressurized gas "bubbles" (MPM particles) lead to swelling of the fuel.

Needed:
- Information about microstructure
- Information about 3-D distribution of pores in the fuel pellet, for both input to the MPM simulation and the validation of results



Gas "bubbles" distribution (MPM particles) in a fuel element (cross section)[1].

More models and simulations of metallic fuels from Tom Arsenlis and Patrice Turchi (Livermore National Laboratory)

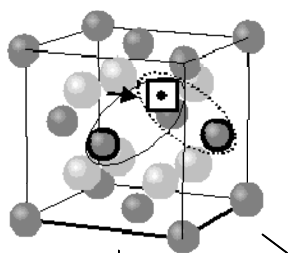
[1]Courtesy of Veena Tikare (Sandia National Laboratory), article in preparation (2009).

Models and Simulations of Nuclear Fuel Materials[1]

Electronic Structure Calculations (DFT)[1]

Inter-atomic potential parameters

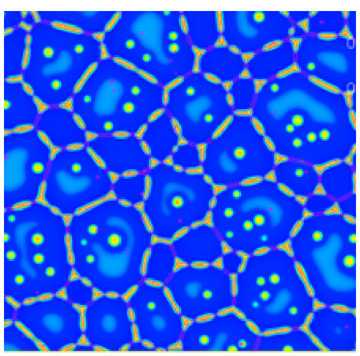
Molecular dynamics calculations of point defect energy[1]



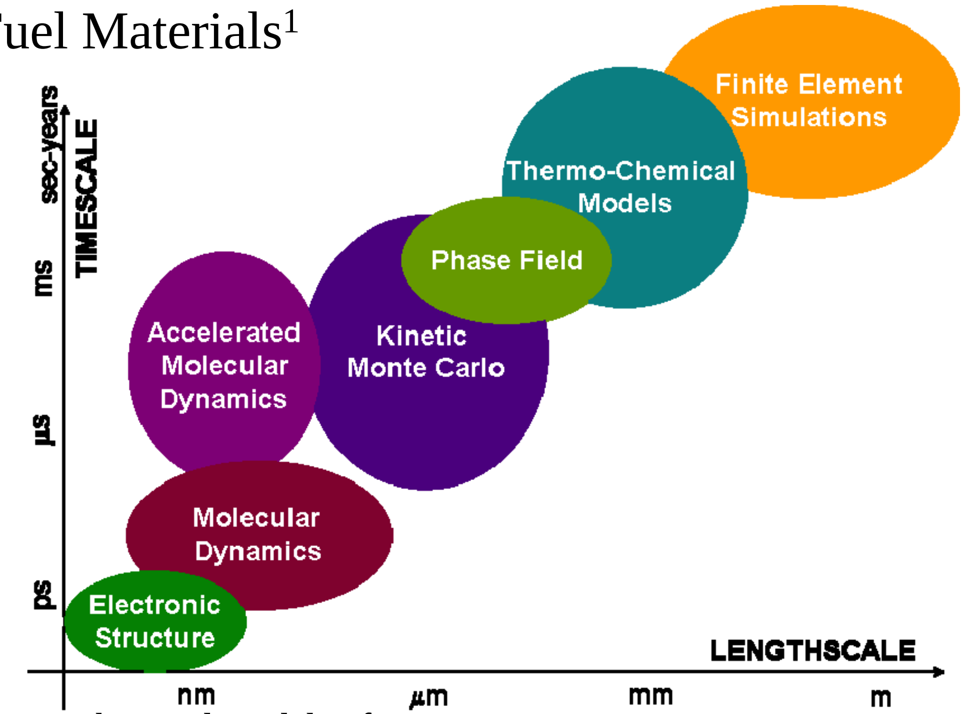
Point Defects

Nucleation sites

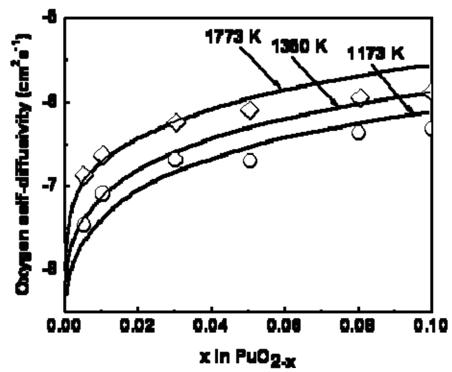
Phase Field simulations of gas bubbles formation and evolution[2]



Porosity



Thermo-chemical models of oxygen diffusivity[1]

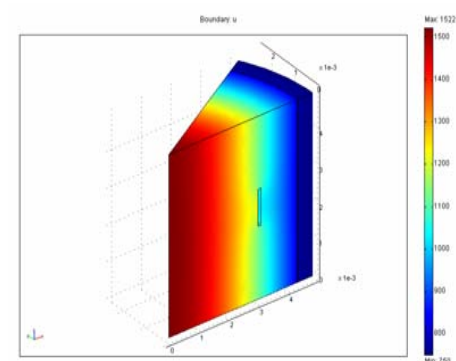


thermal conductivity

D(T,x,p)

k(T,x,p)

Simulations of heat transfer and diffusion in nuclear fuels[3]



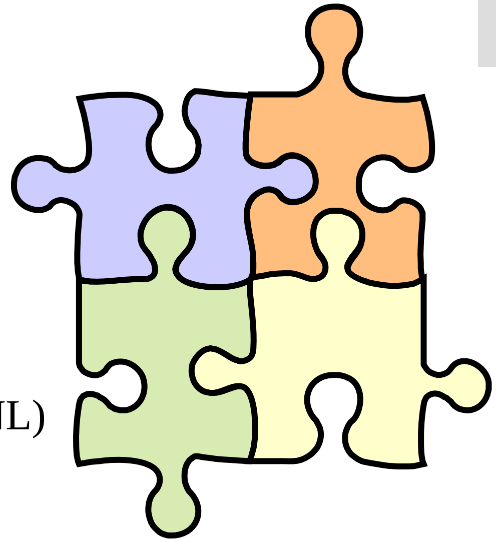
*mastan@lanl.gov

[1]M. Stan, J. C. Ramirez, P. Cristea, et al., J. Alloys Comp., **444–445** (2007) 415–423.
[2]S.Y. Hu, M. I. Baskes, and M. Stan, Appl. Phys. Let., **90** (2007) 081921.
[3]J. C. Ramirez, M. Stan, and P. Cristea, J. Nucl. Mater., **359** (2006) 174-184.

Integration of People, Experiment, Theory, and Computation

People

B. Mihaila, S. Valone,
B. Uberuaga, C. Stanek, D. Anderssen,
K. McClellan, D&D Korzekwa (MST)
S. Rudin, J. Wills, A. Zubelewicz (T)
M. Stan, N. Carlson, B. Lally (CCS)
R. Kennedy, R. Hansen (INL)
T. Besmann, S. Zinkle, D. Kothe (ORNL)
T. Arsenlis, P. Turchi (LLNL)
S. Hu (PNNL), M. Baskes (California)
V. Tikare, J. Aidun (SNL)
J. Tulenko, S. Phillpot, S. Sinnot (UFL)
J. Ramirez (Exponent)
P. Cristea (Univ. Bucharest)
R. Grimes (Imp. Col., UK)
R. Konings, P. V. Uffelen (ITU)
C. Gueneau, C. Valot (CEA)
M. Kissane (IRSN)
T. Ogawa, K. Minato, Y. Kaji (JAEA)



Computation

Finite Element Simulations
Calculations of Phase Stability
Phase Field
Molecular Dynamics
Electronic Structure Calculations

THEORY

Density Functional Theory
Solid State Physics
Thermodynamics & Stat. Phys.
Transport Theory

EXPERIMENT

X-Ray Diffraction
Neutron Diffraction
Calorimetry
Dilatometry
Microscopy

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Philosophy

Science is a rigorous, systematic use of observations and logic to attempt to support or falsify possible explanations of natural phenomena.

Theory: A formal statement of ideas which are suggested to explain a fact or event.
Experiment: A procedure undertaken to make a discovery, test a hypothesis, or demonstrate a known fact.
Computation: A procedure used to determine the solution of a mathematical problem by means of a computer.

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

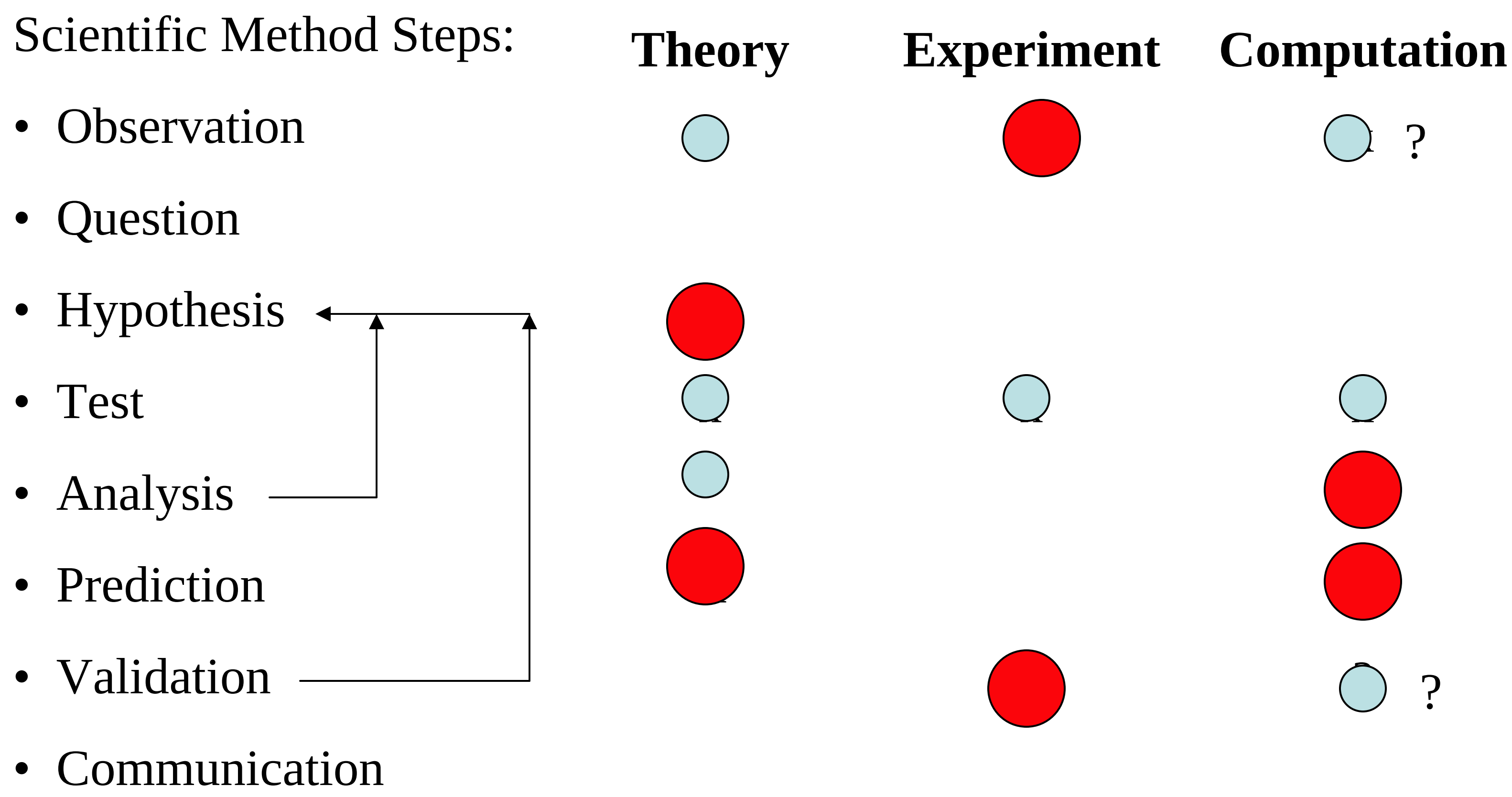
Simulation: The process of carrying out experiments and/or running computer programs to reproduce, in a simplified way, the behavior of a system.
- low performance (workstation)
- high performance (Petascale, Exascale,)

The goal is to engage theorists, experimentalists, and computer scientists in developing theory-based models, conducting innovative experiments, and running high performance simulations for energy applications.

The Scientific Method

Theory, Experiment, and Computation play various roles in the Scientific Method

Leading role Important contribution



Theory enhances our understanding
Experiments provide confirmation, reality check
Computation expands the investigation space

Forget Theory and Experiment
Focus on Computation

Roadrunner: Still the Fastest Computer in the World

• New LANL Supercomputer
• 7,000 dual-core "Opterons" (IBM), approx 50 teraflops.
• 14,000 cells (Sony-Toshiba-IBM), 100 GF-DP/cell, approx 1.4 petaflops.
• These are PlayStation-3-like chips!!!!

Simulation: The process of carrying out experiments and/or running computer programs to reproduce, in a simplified way, the behavior of a system.

Computational methods:

- Rare contribution to discovery
- Critical components of design
- Important contribution to analysis
- Good predictive character, **expand the investigation space**
- Do the results describe reality?
- Expensive, time consuming, but we love them.

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Review of Commercial Fuel Performance Codes[1]

COMETHE (Belgonucleaire, Belgium)

COPERNIC (FRAMATOME, Germany)

ENIGMA (British Energy, BNFL, UK)

FALCON (EPRI, USA)

FRAPCON (PNNL, USA)

FRAPTRAN (PNNL, USA)

LIFE (ANL, USA)

MACROS (SCK-CEN, Belgium)

ORIGEN (ORNL, USA)

PARFUME (INEEL, USA)

PLEIADES (CEA, France)

SPHERE (PSI, Switzerland)

TRANSURANUS (ITU, Germany)

Benefits

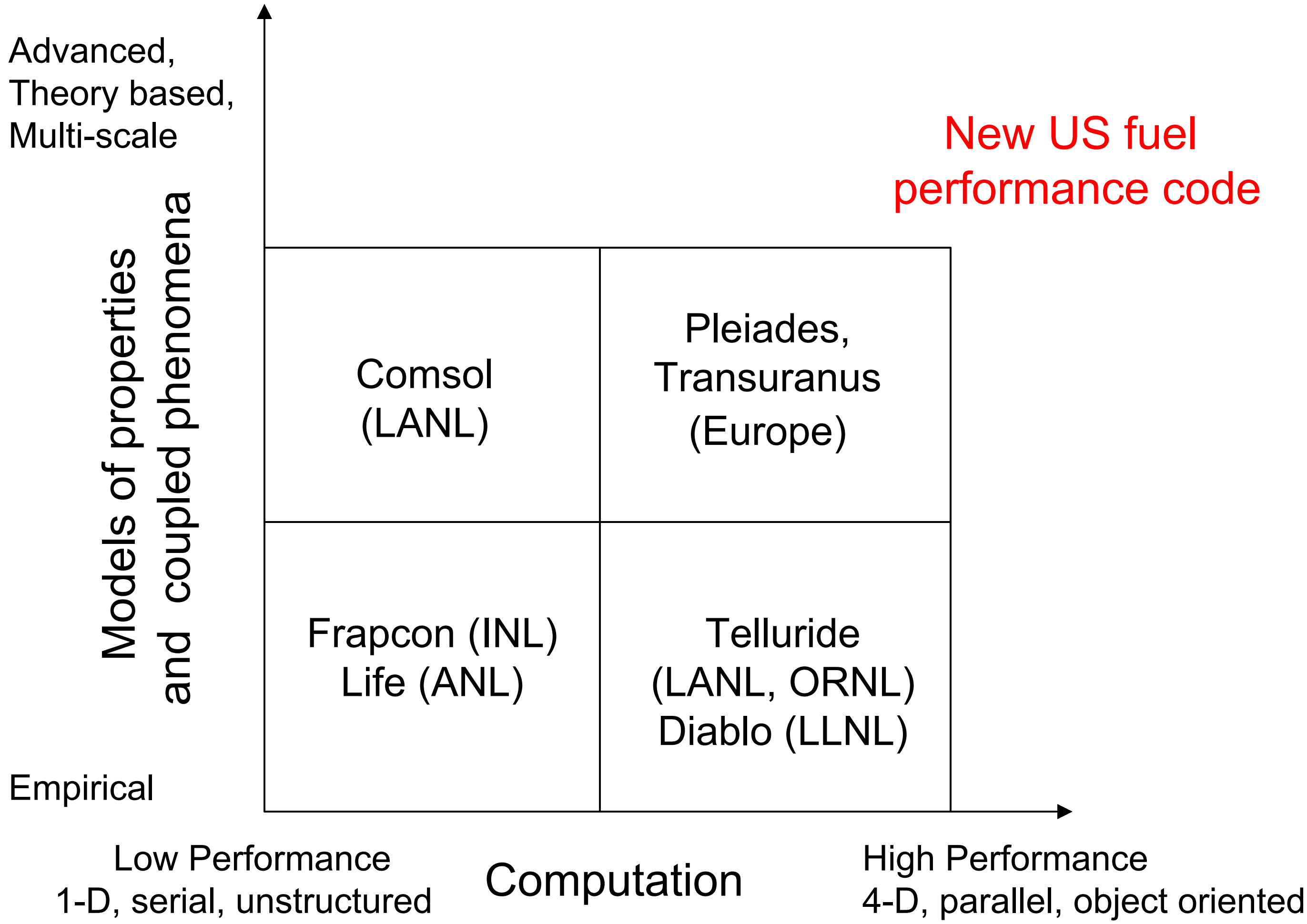
- Most important models are included
- Sanctioned by licensing org. (NRC)
- Experienced user groups
- Good, fuel specific databases

Status:

- Design
  - Not object oriented
  - Do not run parallel
- Models
  - Empirical correlations, unreliable extrapolations
  - Too material specific
  - No uncertainty evaluation
- Input/Output
  - No user friendly interface
  - Rudimentary post processing
  - Difficult to interconnect

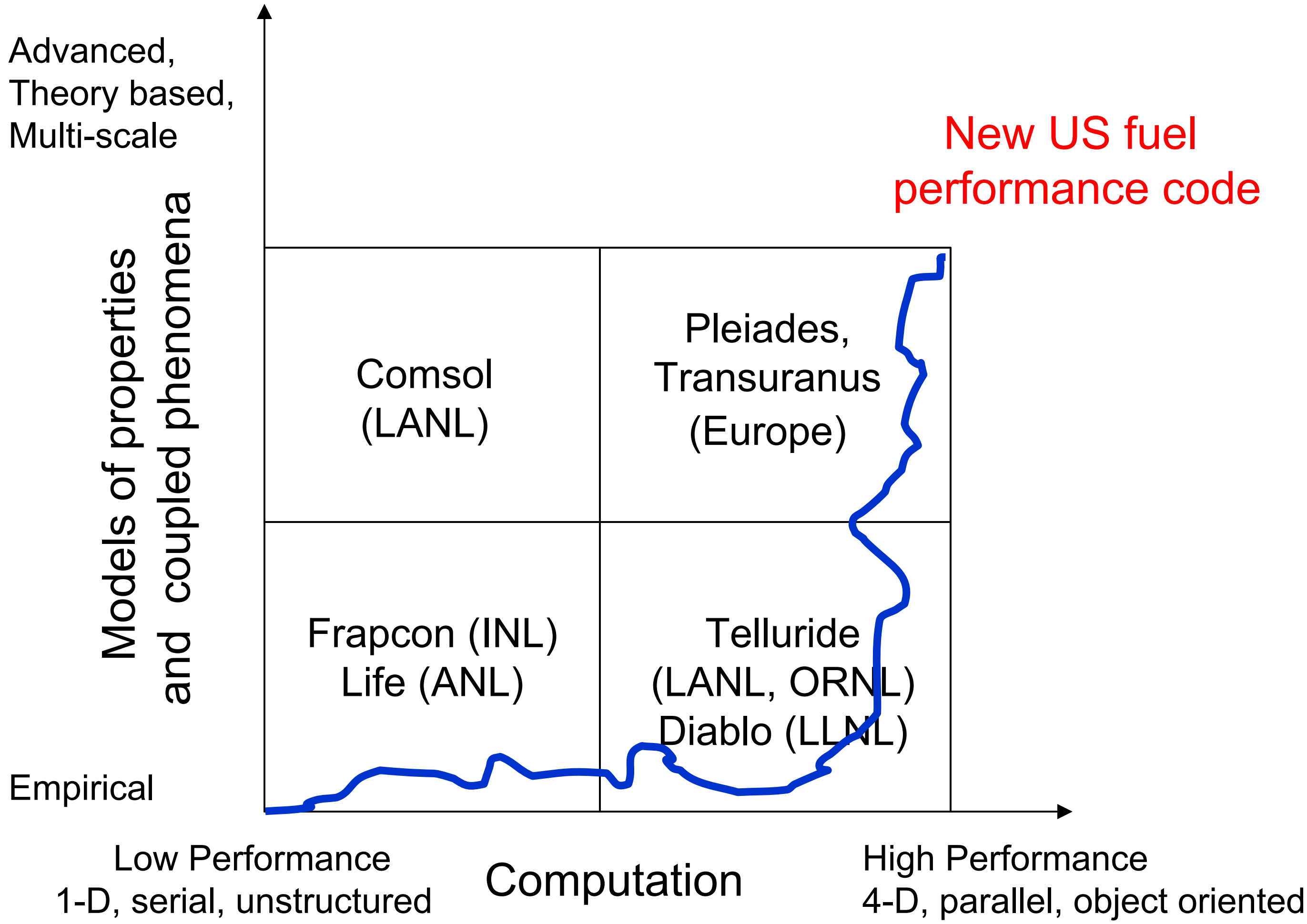
[1]M. Stan, J. Nucl. Eng. Techn., **41** (2009) 39-52.

Fuel Performance Models and Simulations: A Vision*



*M. Stan "Models and Simulations of Nuclear Fuels", in preparation for Taylor and Francis.
Figure based on "The Pasteur's Quadrant" by Donald E. Stokes

Fuel Performance Models and Simulations: A Vision*



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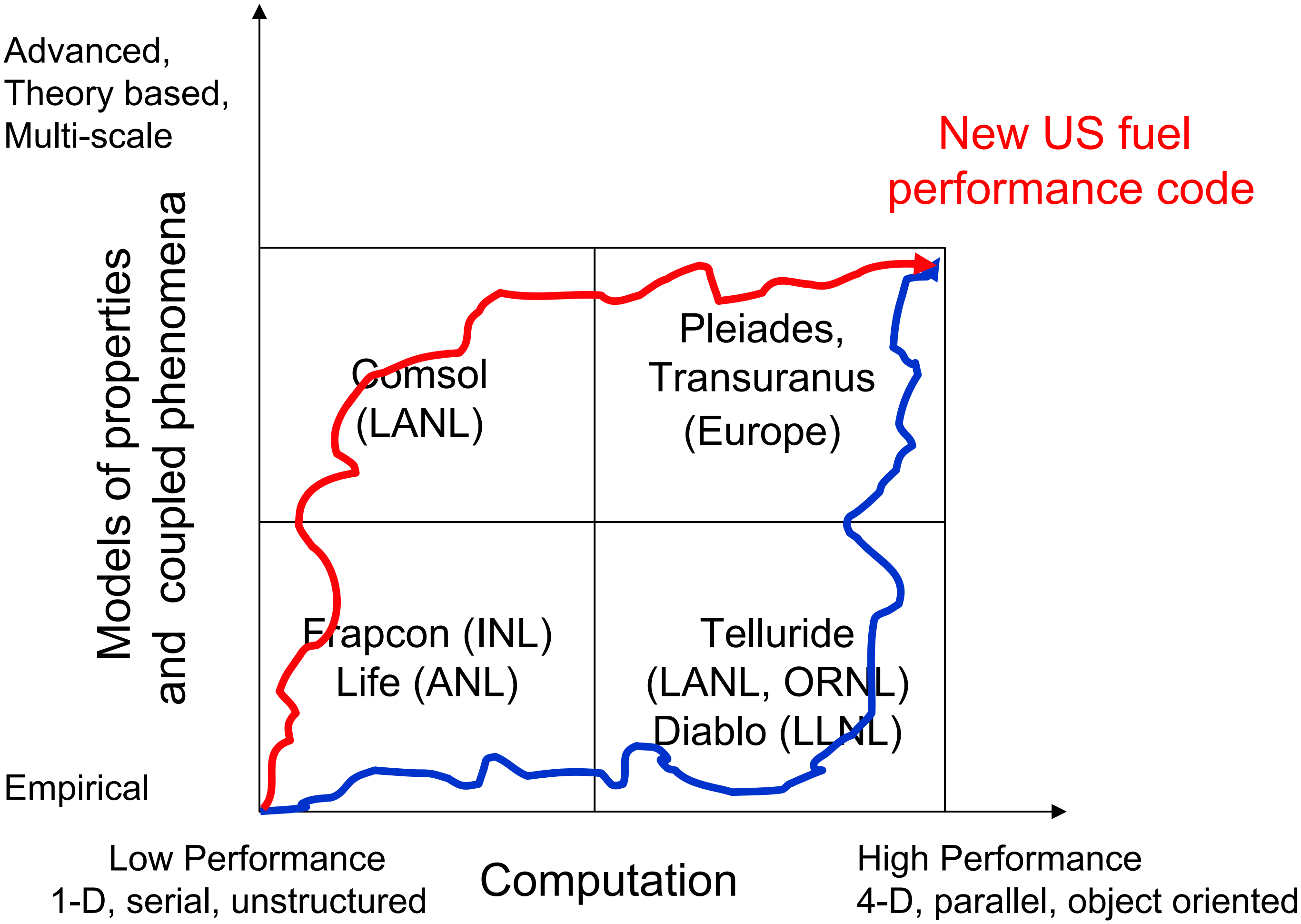

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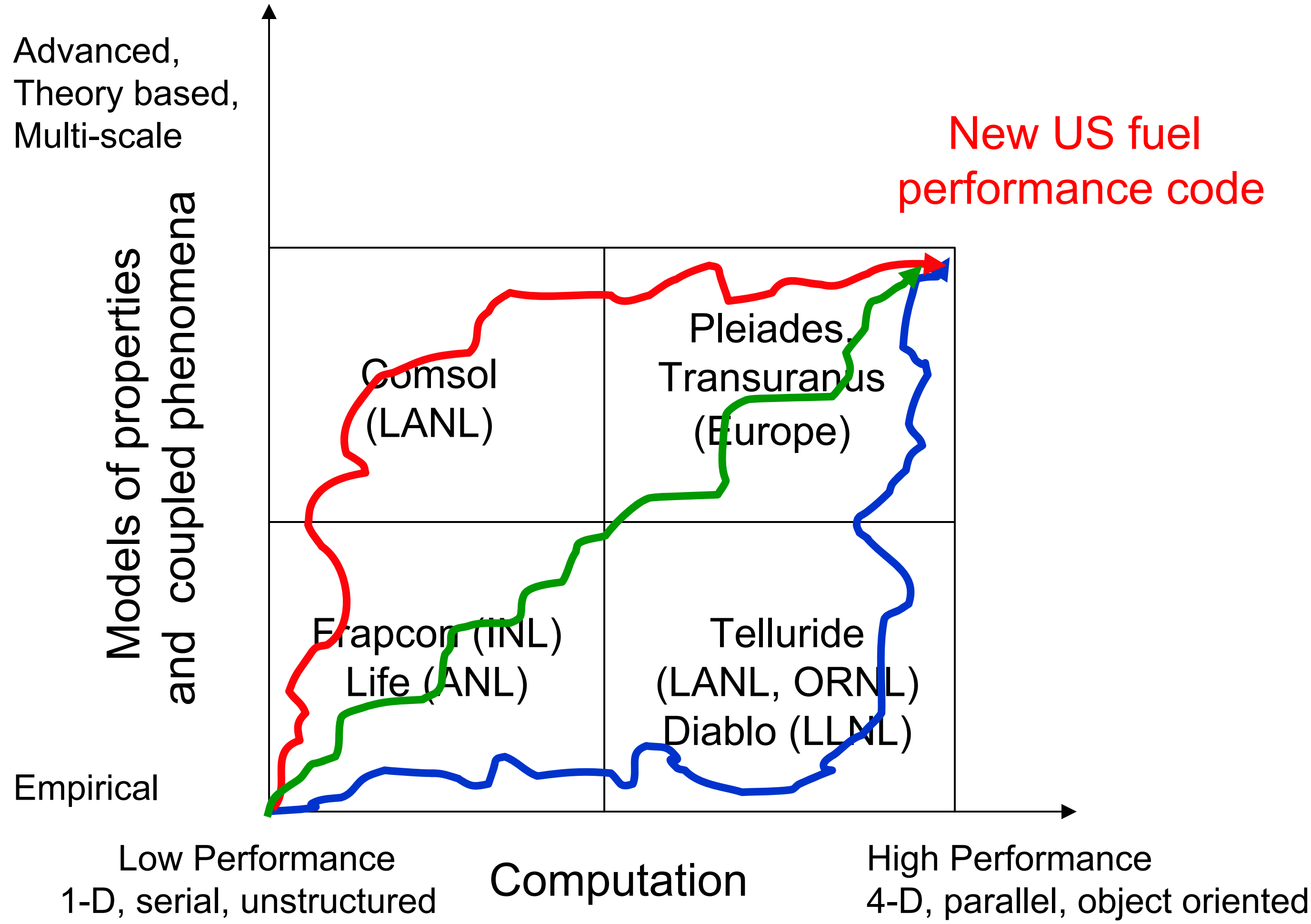

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Strategies for Fuel Performance Simulations

A) Improve on Existing Fuel Performance Codes (FRAPCON/FRAPRAN)

- Most important models are there
- Very difficult to turn into 3-D and parallel
- Good short-term, modest long term results

B) Modify ASC codes (TRUCHAS, DIABLO)

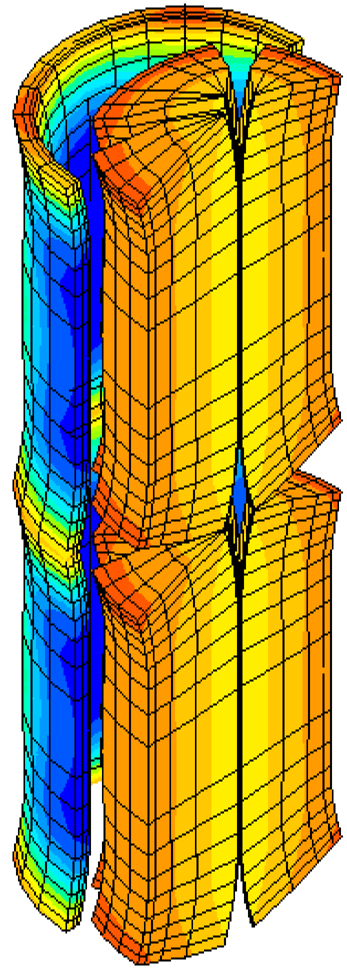
- Some models are there, adding new models is cumbersome
- Already 3-D and parallel
- Modest short-term, good long term results

C) Use commercial software (COMSOL, ABAQUS)

- Models are easy to implement
- Already 3-D, not parallel
- Good short-term, good long term results

D) Build a new code from scratch.

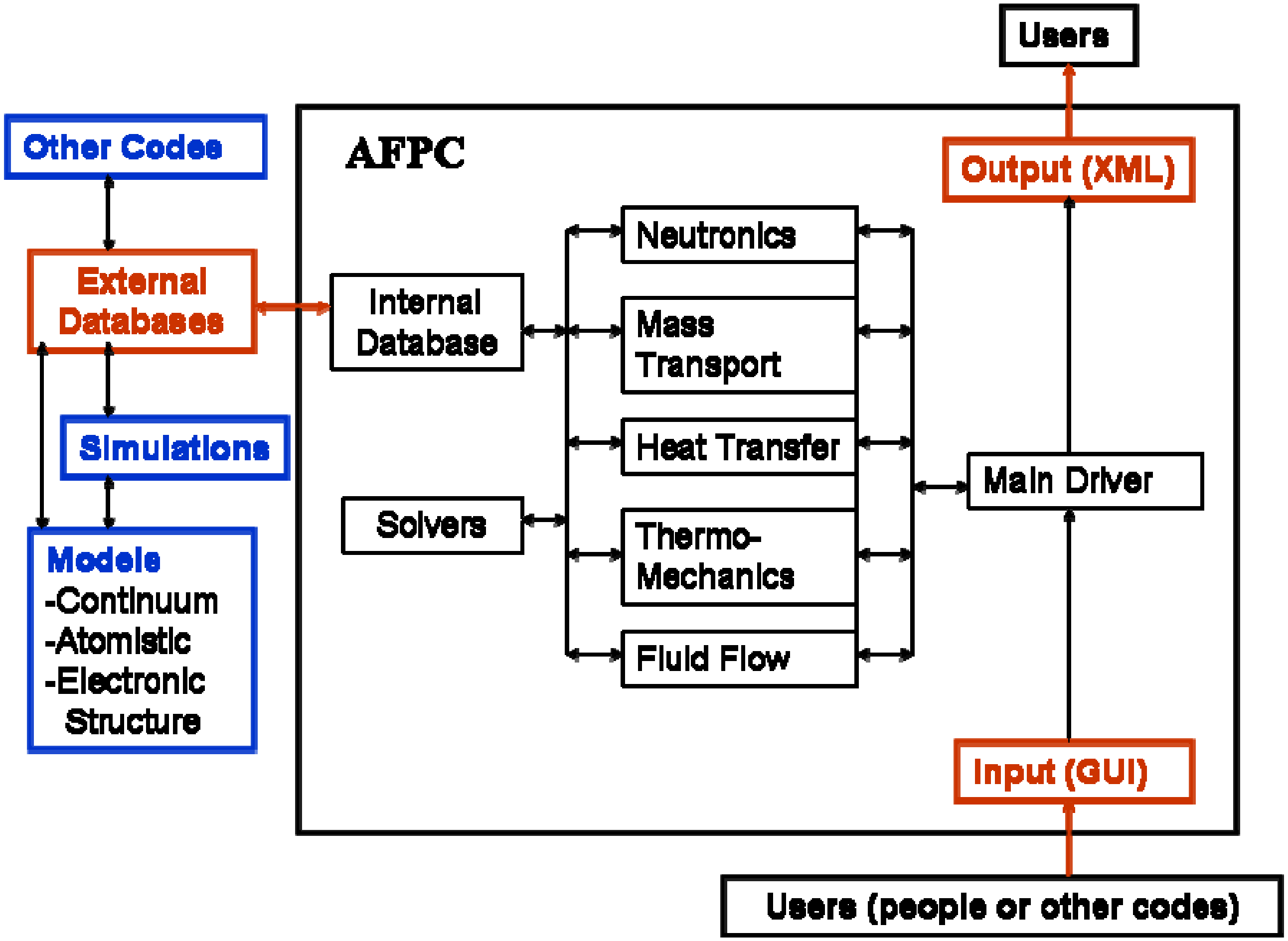
- Best design, will include all models
- Truly coupled physics, 3-D, parallel, optimized
- No short term, excellent long term results



Stress Field in a Fuel Element Simulations performed with PLEIADES, part of the SALOME integrating platform (CEA, France)

Design an Develop an Advanced Fuel Performance Code (AFPC)

New, interactive, 3-D code that includes experimental data and theory-based models[1].



AFPC will be developed in collaboration with national laboratories, universities, utilities, vendors, and the National Regulatory Committee (NRC).

[1]M. Stan, *Materials Models and Simulations in Support of Nuclear Fuels Development*, Los Alamos National Laboratory Report, LA-UR-05-4069.

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Uncertainties in nuclear energy applications

Regulators and reviewers:

- U.S. Nuclear Regulatory Commission (NRC)
- International Atomic Energy Agency (IAEA)
- Nuclear Energy Agency (NEA/OECD)
- Performance Assessment Peer Review Panels

International nuclear power plant licensing environments offer two acceptable options for demonstrating that the safety is ensured with sufficient margin:

- use of best estimate computer codes combined with conservative input data.
- realistic input data associated with experimental evaluation of uncertainty of results

Major sources of uncertainty[1]

- Thermal-hydraulic system codes contain partial derivatives equations. Balance (conservation) equations are approximate. Not all the interactions between steam and liquid are included,
- The equations are solved in cylindrical geometries: no consideration of geometric discontinuities
- Imperfect knowledge of boundary conditions and initial conditions.
- The numerical solution is approximate, therefore, approximate equations are solved by approximate numerical methods.
- The need "to average" the fluid conditions at the geometry level makes necessary the '*porous media approach*'.
- The 2nd principle of thermodynamics is not necessarily fulfilled by codes.
- Extensive use of empirical correlations. These are needed 'to close' the balance equations and are also reported as 'constitutive equations' or 'closure relationships'.
- Often ranges of model validity are not specified.
- 'Steady State' & 'Fully Developed' (SS & FD) flow condition are necessary prerequisite or condition adopted when deriving correlations. However, almost in no region of the nuclear power plant those conditions apply during the course of an accident.
- The state and the material properties are approximate.
- Computer/compiler errors.
- Software errors.
- Different groups of users having the same code and the same information for modeling a Nuclear Power Plant do not achieve the same results.

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[1]IAEA Report (authors: Allison C., Balabanov E., D'Auria F., Jankowski M., Misak J., Salvatores S., Snell V.) "Accident Analysis for Nuclear Power Plants" IAEA Safety Reports Series No 23, pp 1-121, ISSN 1020-6450; ISBN 92-0-115602-2, Vienna (A), 2002.

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- The need “to average” the fluid conditions at the geometry level makes necessary the ‘*porous media approach*’.
- **The 2nd principle of thermodynamics is not necessarily fulfilled by codes.**
- Extensive use of empirical correlations. These are needed ‘to close’ the balance equations and are also reported as ‘constitutive equations’ or ‘closure relationships’.
- Often ranges of model validity are not specified.
- ‘Steady State’ & ‘Fully Developed’ (SS & FD) flow condition are necessary prerequisite or condition adopted when deriving correlations. However, almost in no region of the nuclear power plant those conditions apply during the course of an accident.
- The state and the material properties are approximate.
- Computer/compiler errors.
- Software errors.
- Different groups of users having the same code and the same information for modeling a Nuclear Power Plant do not achieve the same results.

[1]IAEA Report (authors: Allison C., Balabanov E., D’Auria F., Jankowski M., Misak J., Salvatores S., Snell V.) “Accident Analysis for Nuclear Power Plants” IAEA Safety Reports Series No 23, pp 1-121, ISSN 1020-6450; ISBN 92-0-115602-2, Vienna (A), 2002.

Major sources of uncertainty[1]

- Thermal-hydraulic system codes contain partial derivatives equations. Balance (conservation) equations are approximate. Not all the interactions between steam and liquid are included,
- The equations are solved in cylindrical geometries: no consideration of geometric discontinuities
- Imperfect knowledge of boundary conditions and initial conditions.
- The numerical solution is approximate, therefore, approximate equations are solved by approximate numerical methods.
- The need “to average” the fluid conditions at the geometry level makes necessary the ‘*porous media approach*’.
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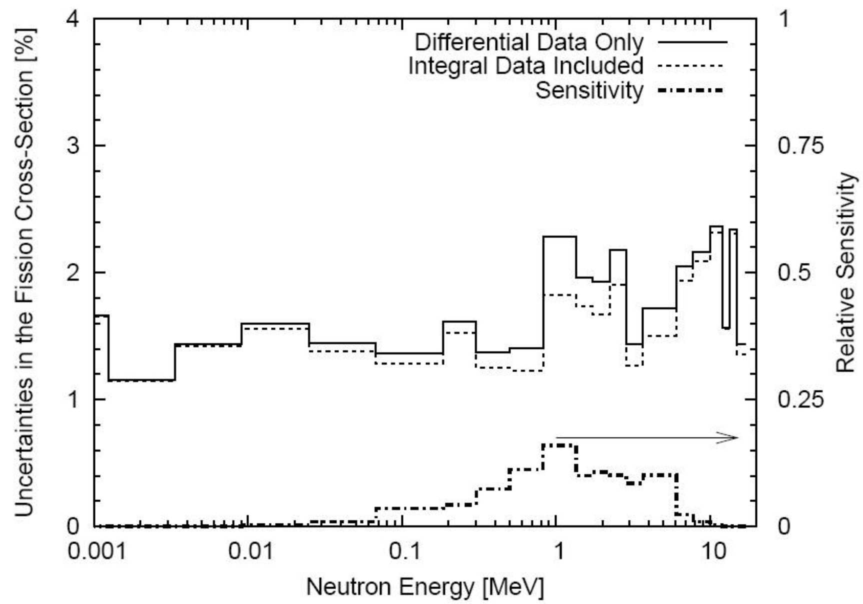
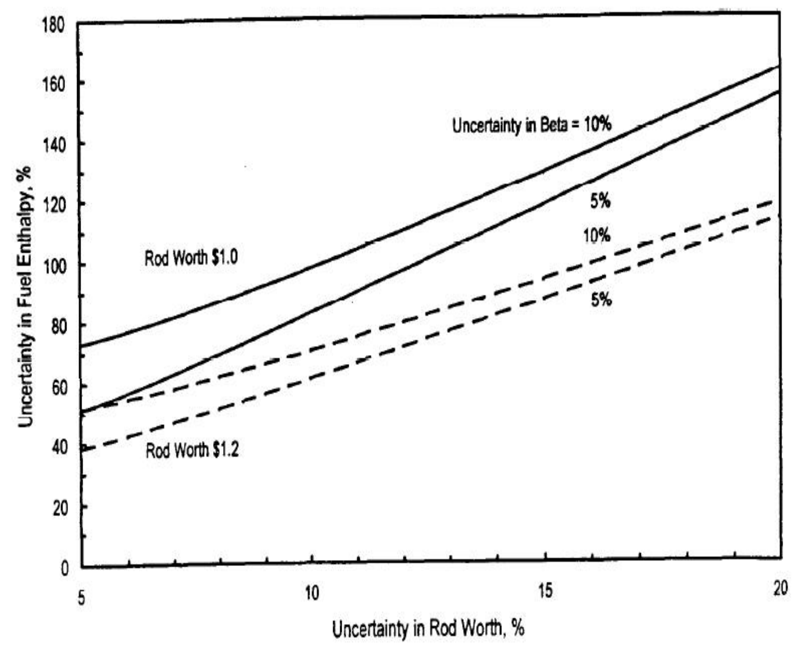
Uncertainty of Nuclear Data

- Uncertainty in fission cross sections is reasonably small
- Uncertainty in fuels and materials properties is often quite large



Examples:

- Top figure: Neutron-transport calculation with PARTISN and criticality measurement (Jezebel) using a Bayesian method[1].
- Bottom figure: Uncertainty in fuel enthalpy as function of the rod worth for various worth and beta parameters. The case of rod rejection accident[2].



Rod worth = density/beta

Beta = fraction of fissions caused by delayed neutrons

[1]T. Kawano, K.M. Hanson, S.C. Frankle, P. Talou, M.B. Chadwick, R.C. Little, Uncertainty Quantification for Applications of 239Pu Fission Cross Sections Using a Monte Carlo Technique, LANL report.

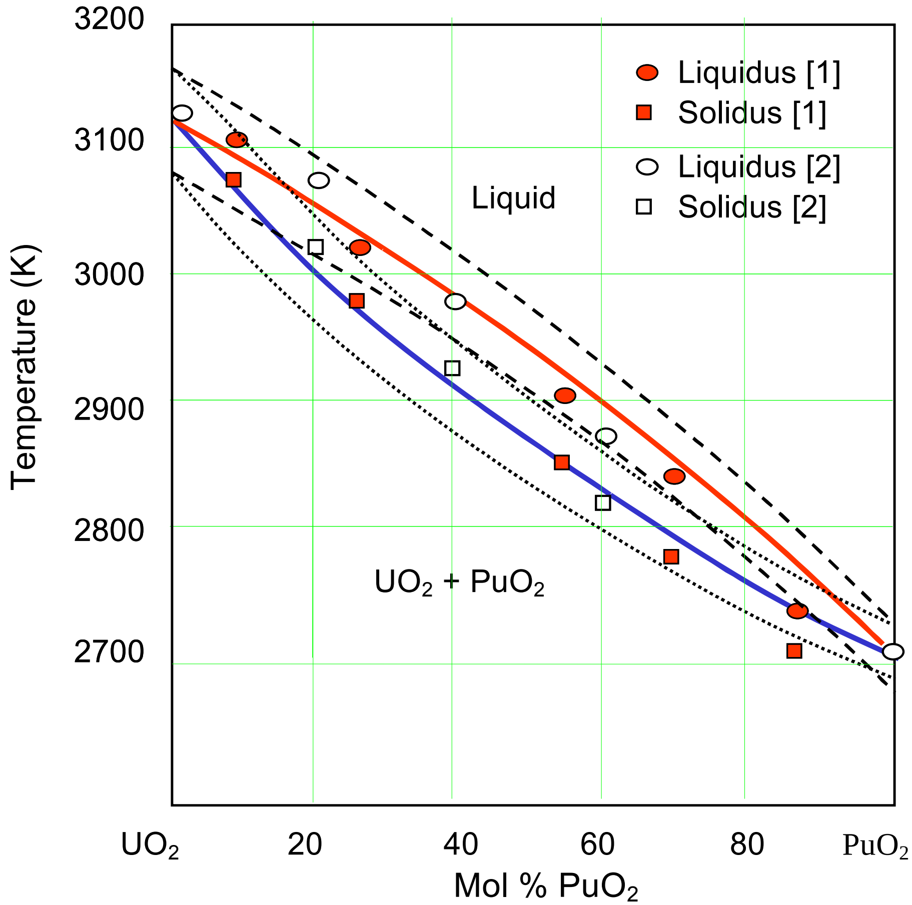
[2]D. J. Diamond, A. L. Aronson, and C. Y. Yang, BNL-NUREG-67430

Uncertainty of Nuclear Fuels Data

- Uncertainty in fuel thermo-mechanical properties is often >10%
- Uncertainty of chemical properties (free energy) can be 10-15 %

Example:

- Uncertainty quantification the UO_2-PuO_2 phase diagram*. DT = 50K, Dc = 3%
- Bayesian analysis of 15 data sets (melting temperatures and transformation enthalpies).
- Optimization via a genetic algorithm.



* M. Stan and B. J. Reardon, *CALPHAD*, **27** (2003) 319-323.

[1] M. G. Adamson, E. A. Aitken, and R. W. Caputi, J. Nucl. Mater., **130** (1985) 349-365.

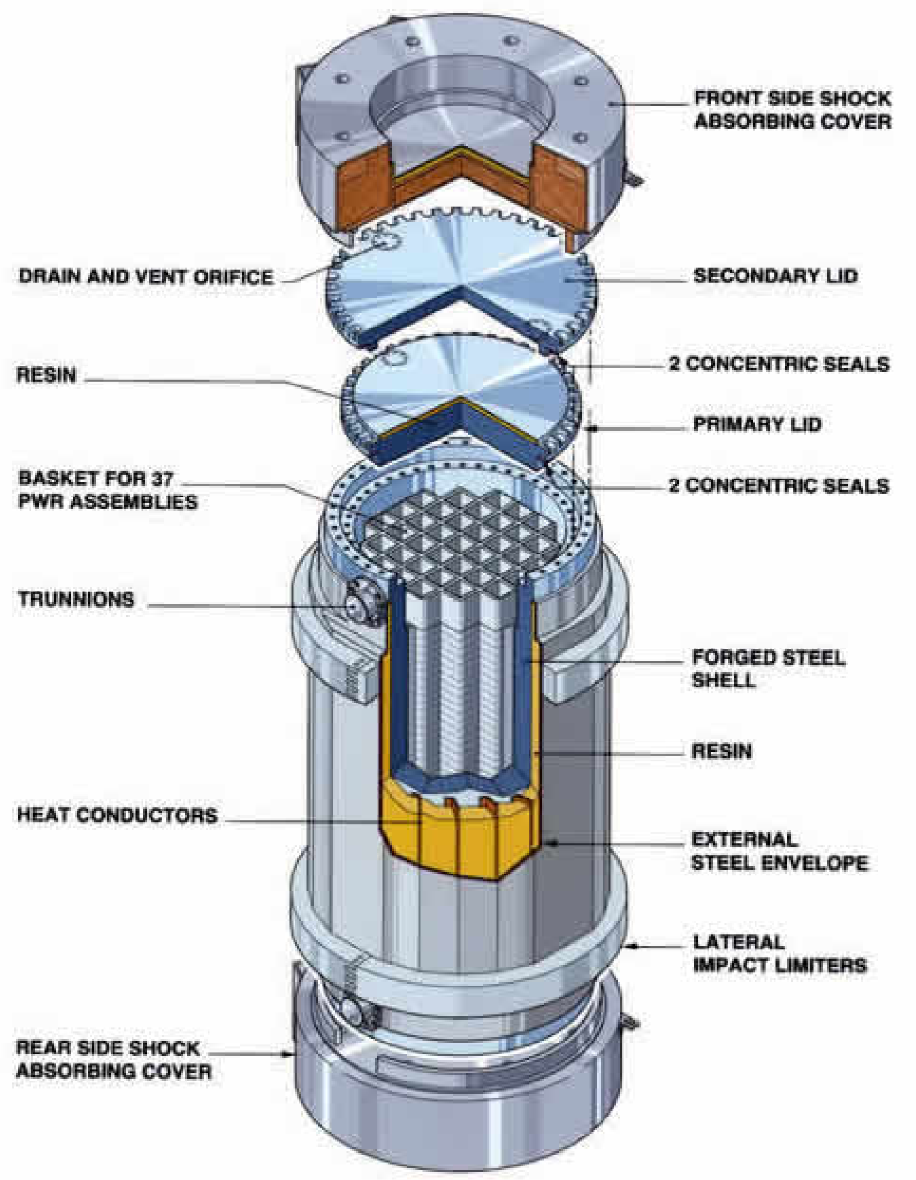
[2] T. D. Chikalla, J. Am. Ceram. Soc., **47** (1964) 309-309.

Waste management

- NRC requirements specified in **CFR 63.304**
  - Total System Performance Assessment (TSPA) methodology
  - Alternative conceptual models (ACM)

- National storage:
  - WIPP (Waste Isolation Pilot Plant) still running.
  - The Yucca Mountain repository project still uncertain (dead?).

- Local storage, example:
  - Uncertainty analysis for corrosion depth of the spent nuclear fuel canister has been studied using differential analysis[1].
  - It shows that the mean value presents a second-order linear increase while the variance demonstrates a first-order linear increase in 1000-year time.



Schematic design of the spent nuclear fuel canister.

[1] D. K-F. Shih, WM'02 Conference, February 24-28, 2002, Tucson, AZ

The Case for Science-Based Models and High-Speed Simulations (1)
Saving Time and Money

Science-based models and high performance simulations coupled with solid uncertainty quantification have the potential to save millions in nuclear plant licensing and fuel qualification.

Example: Nuclear Fuel Qualification takes 10-15 years
and costs over $100 mil (materials, labor, facility access)

• Fabrication specifications: composition, density, thermal conductivity, linear power generation.
• Post irradiation examination: deformation, mechanical integrity, fission gas accumulation, creep.
• See: ASTM C1068 - 03 Standard Guide for Qualification of Measurement Methods by a Laboratory Within the Nuclear Industry.

•Accelerated development of new fuels will shorten R&D by 1-2 years.
•Elimination of 1 destructive irradiation and PIE will save $1-5 million (NRC).
→ Estimated savings: $10-20 million per fuel type, over two years (GE, Westinghouse reports)

•"Shaving off" 5 years will allow faster starting of operation
→ Estimated $100 mil in profit over 5 years

More impact and saving:
• Design of proliferation resistant fuels
• Simulations of accident scenarios

The Case for Science-Based Models and High-Speed Simulations (2)
Expanding the investigation space to identify and resolve new scientific problems

High-speed computing will allow for simulations of physics, chemistry, and materials science phenomena that are not accessible today:

- Quantum Mechanical electronic structure calculations on millions of atoms to predict properties of multi-component materials, such as free energy of formation of alloys and compounds.
- Quantum Mechanical electronic structure calculations on millions of atoms to predict properties at finite temperature, such heat capacity and stress-strain curves.
- Atomistic (MD) simulation of a much larger number of atoms (10^20) compared to the current state of the art (10^8) to capture whole grains, interfaces, and heterogeneous regions of materials and simulate radiation effects.
- Atomistic (MD) simulations that cover much longer real times (seconds) compared to the current state of the art (nano-seconds) to simulate fission products diffusion, gas bubbles nucleation and swelling.
- Many-body, parallel Monte Carlo simulations of coupled neutron transport and radiation cascades on trillions of atoms for hours or days to capture the interplay between the neutron flux and the changes in materials properties, such as simulations of stress corrosion cracking.
- Multi-scale embedded simulations, building on the Car-Parrinello example but covering larger time and space domains, to improve on the “first principles” character of the meso-scale simulations.
- Deterministic and stochastic simulations of neutron transport fully coupled with the irradiation effects on material properties, for a more accurate neutron and thermal balance of the reactor and studies of accident scenarios.
- …etc

The Case for Science-Based Models and High-Speed Simulations (3)
Increasing the predictive character of models and simulations.

In USA, one of the most important drivers for high-speed (performance) computing is to create predictive simulation capabilities to certify nuclear weapons and maintain good knowledge and expertise in the area without nuclear tests..

Building upon the ASCI experience:
• Extraordinary advances made in computational power (speed) and methods. We are currently using these capabilities for nuclear energy simulations.
• Outstanding contributions in uncertainty validation (QMU). Similar approach can be used for uncertainty analysis and predictions in reactors, even nuclear plants.
• Visionary leadership.

Differences and opportunities:
• There is no ban on experiments for (Nuclear) Energy applications. We should become knowledgeable and get involved in experiments.
• This is unclassified research. We compete and must partner with universities, private companies,…etc
• Visionary Leadership.

New Driver: Create predictive simulation tools to assist the discovery and design of new energy sources, improved energy transportation, and high capacity energy storage.

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The Case for Science-Based Models and High-Speed Simulations (4)
Inspiring new ways of doing science.

High-speed simulations will expand our investigation space and generate ideas that will lead to completely new ways of doing science. Monte Carlo was possible because of advanced (for that time) computers. What will be next?

- Quantum Mechanical inspired new theory going beyond Density Functional Theory to predict materials properties from 'first principles"?

- New bio, nano, ..(?), … materials that morph into new structures to accommodate the local radiation environment?

- Self-healing nuclear reactor that never suffer accidents?

- Your turn: …

The Case for Science-Based Models and High-Speed Simulations (5)
Initiatives

The goal is to control the properties and phenomena in irradiated materials for fission nuclear energy. To achieve this goal, we propose to develop theory-based models that enhance the understanding of irradiation effects on materials properties, to perform petascale/exascale simulations of heat and species transport in reactor materials, and to create an integrated theoretical, experimental, and computational validation process.

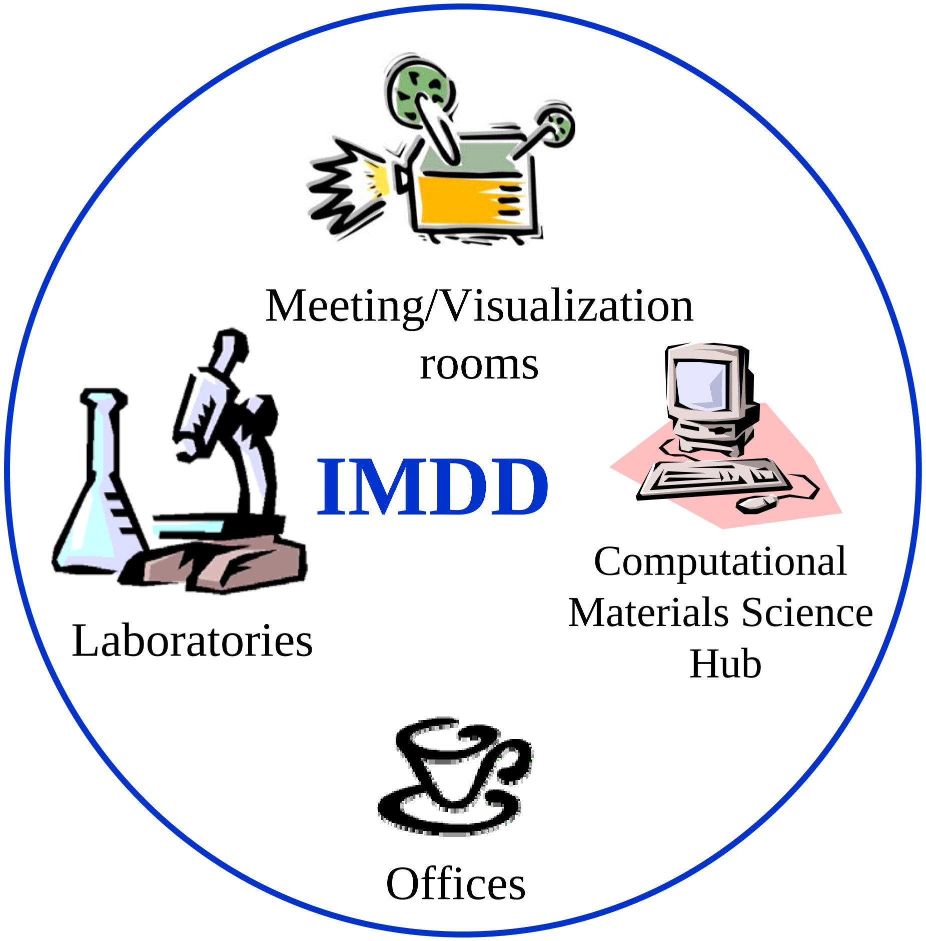
INITIATIVES:

1. **Create Energy Institutes (Centers, Lablets, Hubs…) for theory-based model development, high-performance simulations, and experimental validation.** The models will cover a wide range of space and time scales, starting with the nucleus and the atomic electronic structure (nm) all the way to the reactor components (meters), and from defect formation (pico-seconds) all the way to the operating characteristic times (months, years). Participants will collaborate in developing and performing atomistic, meso-scale, and continuum simulations of irradiation effects in reactor materials, to predict and control point defect formation, microstructure evolution, and materials performance in reactor environments.
2. **Develop and maintain a National Knowledgebase of data, models, and simulation results.** Besides maintaining a close collaboration with the existing databases, we propose to create, update, and maintain an international "knowledgebase" that includes experimental data, models (mathematical expressions), and simulation results (tables, graphs, diagrams), all linked to publications and web sites. The knowledgebase will have a friendly user interface and will use advance query techniques capable of retrieving numbers, text, and images.

The Future: Institute for Materials Discovery and Design (IMDD)

The institute will integrate experiment, theory, and computation. The scientists will be trained in all areas and experts in one of them.

- State of the art laboratories for small-scale experiments
  - A “home made” ion implanter can lead to an idea for a new radiation resistant material that will be further developed using the intense neutron source.
- A computational materials science hub for model development and small-scale simulations
  - Complex, multi-physics models and simulations can be tested before running on high-performance computers.
- Meeting rooms equipped with visualization capabilities for discussions
  - Discussions are the catalyst of scientific progress in both discovery and design.
- Offices for staff, guest scientists and students
  - It is critical for IMDD to bring together mature and early career scientists, both from US and the international community.



International Collaborations
Materials Models and Simulations for Nuclear Fuels (MMSNF) Workshops

The MMSNF Workshops aim at stimulating research and discussions on models and simulations of nuclear fuels and coupling the results with the fuel performance codes.

SESSIONS:

- Fundamental models of fuel properties.
- Fuel performance codes and their validation.
- Collaborations and integration of activities.

MMSNF-6, University of Tokyo, Japan, Dec. 14-15. 2007 (Dr. Motoyashu Kinoshita and Dr. Kazuo Minato, JAEA)

MMSNF-7, Karlsruhe, Germany, Sept. 29-30, 2008 (Dr. Paul van Uffelen, EC)

MMSNF-8, Albuquerque, NM, U. S. A, Oct. 19-21, 2009 (Timothy Bartel, SNL)

MMSNF-9 will be part of the Nuclear Materials Congress, Europe, Oct 2010 (R. Konings, ITU)

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The Organization for Economic Cooperation and Development (OECD)
The Nuclear Energy Agency (NEA)
Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems (WPMM)

- WPMM was established to deal with scientific and engineering aspects of fuels and structural materials, aiming at establishing multi-scale models and simulations as validated predictive tools for the design of nuclear systems, fuel fabrication and performance.
- **The main WPMM tasks are:**
  - Identification of fundamental problems.
  - Development of *Ab-initio* and *Atomistically-informed* models and simulations of nuclear fuels and structural materials properties.
  - Integration of results from multi-scale modelling and simulation into *performance codes.*
  - Validation of simulations and model predictions by benchmarking.
  - Creating and maintaining synergy with experimental work.
  - Development of new applied mathematics and software tools.
- **Five Expert Groups have been defined:** A) Nuclear Fuels B) Structural Materials C) Multi-Scale Methods D) Validation Experiments E) Uncertainty Evaluation.
- **Next meeting (WPMM-3) will be in Paris, Fall of 2009.**

Summary

- Science-Based models predict radiation effects better than Empirical models.
- New, Science-Based, codes are necessary to predict and control properties and phenomena in the nuclear reactors.
- This approach builds on ASC but is different:
  - Experiments are possible, desirable
  - New competition, partnership in the open
  - New driver: Discovery and Design
- Exascale computing and uncertainty quantification can and will:
  - Save millions in nuclear plant licensing and fuel qualification
  - Allow for simulations of physics, chemistry, and materials science phenomena that are not accessible today
  - Change the way we do science
- International collaborations are critical.
- Must use high-speed computing to develop high-speed understanding.
- Must create a Moore's law for understanding.
- All this involves changes in thinking, rhetoric, and the actual methodology.

Future US nuclear plant (not in my backyard)

To assist the discovery and design of new materials for energy applications we must understand, predict, and control one mole of substance (10^26 atoms or molecules), for one second, before 2015.

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