Advanced Simulation: applications for fast reactors

Andrew Siegel
Argonne National Laboratory

Two approaches to reactor modeling

Yesterday's
computers

"*I would rather have today's algorithms on yesterday's computers than vice versa.*" --- Phillipe Toint

Supercomputers

Device modeling

Physics modeling

Modern
Desktop

Clusters

Empirical *models* describe observed behavior of as a function of key parameters based on experimental correlations. Relationships specific to design details.

- ✓Nusselt vs. Peclet numbers for different P/D
- ✓Gap conductance vs. burnup
- ✓Fuel-to-cladding gap vs. linear heat rate to incipient melting
- ✓Effective friction factor vs. Reynolds Number
- ✓% fission gas release vs. burnup
- ✓Fuel conductivity vs. burnup
- ✓Cross-flow in pin bundles
- ✓Turbulent diffusion

Mixed physics/empiricism
- sub-channel models
- homogenized transport
- 1.5-D fuels codes

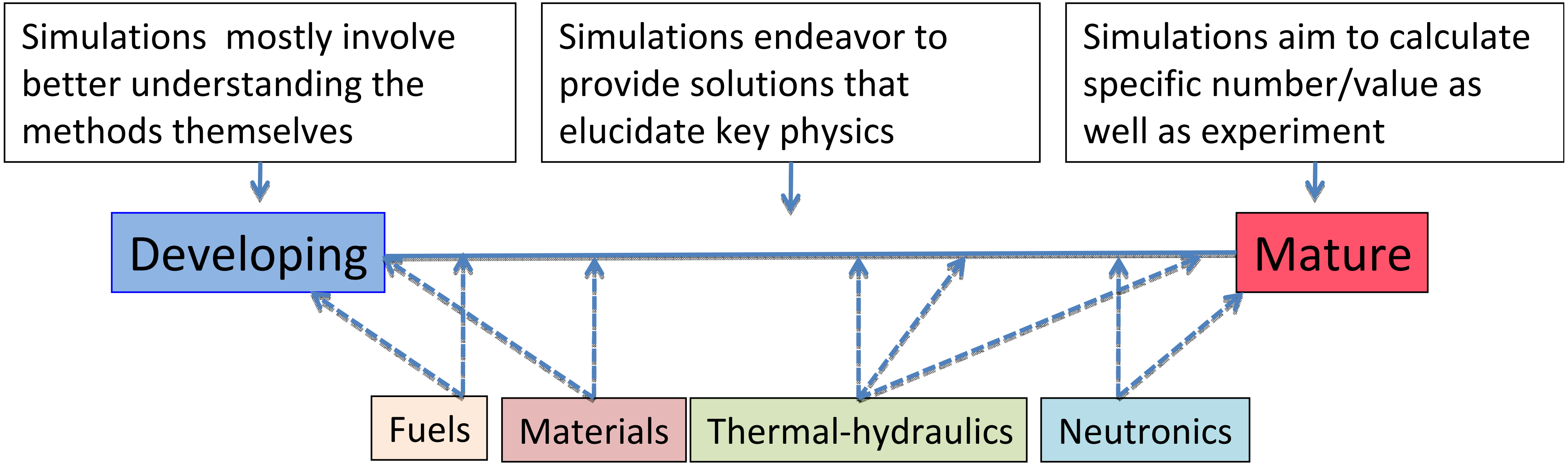
Most successful models

Governing physical equations
Solved numerically on 3d meshes

- ✓ Navier Stokes equations
- ✓ Non-homogenized transport
- ✓ Monte Carlo transport
- ✓ 3D finite element fuels codes informed by atomistic modeling
- ✓ Chemistry

Increasing work in this area -- some successes and many challenges. High potential.

Existing capabilities



Simulations mostly involve better understanding the methods themselves

Simulations endeavor to provide solutions that elucidate key physics

Simulations aim to calculate specific number/value as well as experiment

Developing

Mature

Fuels

Materials

Thermal-hydraulics

Neutronics

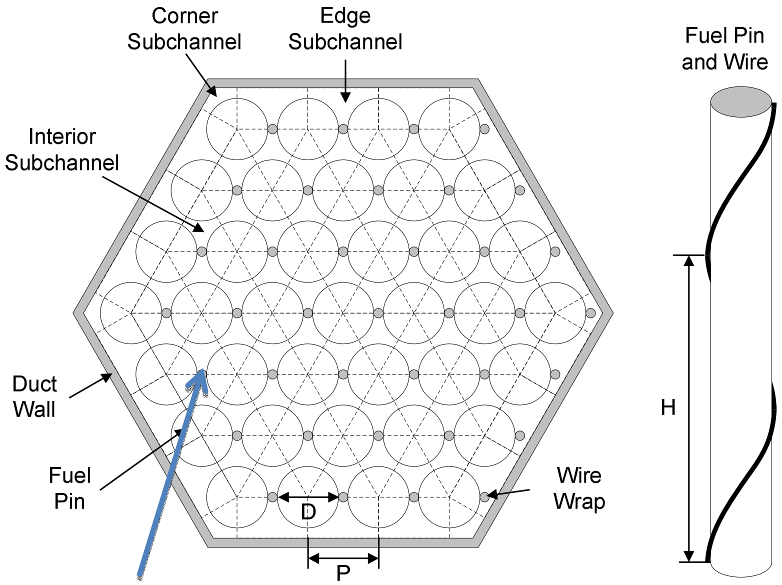
Must carefully distinguish proof of principle vs. direct applications of advanced methods

Example: Fast Reactor steady state core heat transfer

Device modeling

Physics modeling

- subchannel modeling: 1-d axial energy and momentum balance equations for each channel
- Relatively large number of parameters determined by experiments: diversion crossflow, turbulent mixing, shear forces
- Cobra, Super-Energy, etc. popular codes for fast reactors written in the 70s
- Couple to homogenized neutronics code

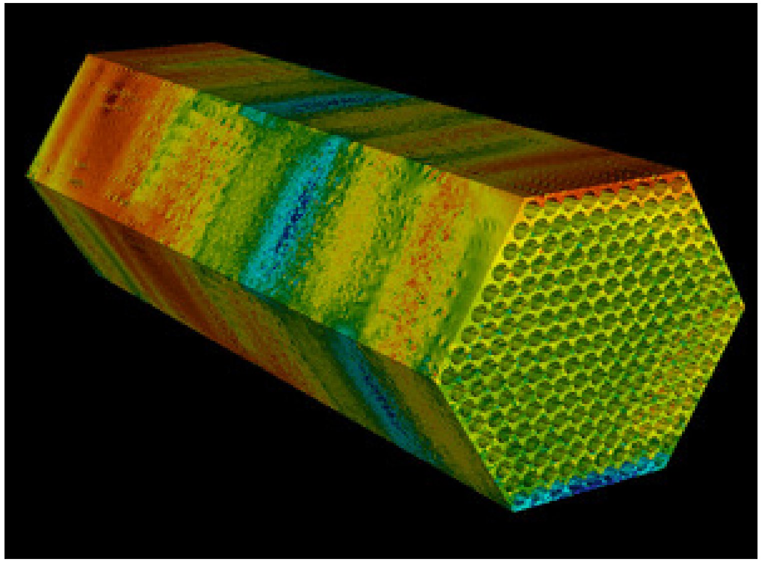


- Single phase
- Low Pr → more easily resolved thermal boundary layers
- Channel Re ~ 50,000
- Need to model turbulent energy transfer

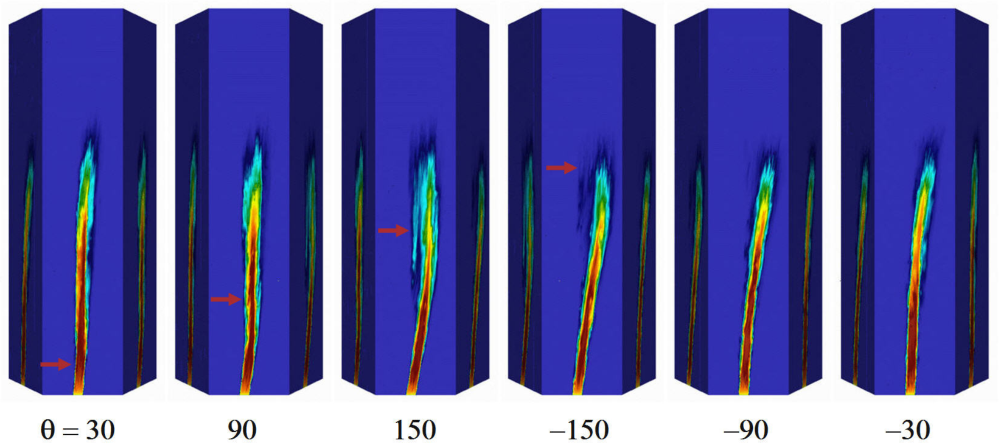
- Conjugate heat transfer with incompressible single phase N-S equations
- Treat fuel, gap, and cladding as material with known $\alpha = \alpha(T)$
- Mesh wire wrap, gap, cladding, and pin positions
- Inflow and outflow bc’s
- Non-linear heat transfer problem: Iterate source computation until convergence

Discovery of new physics using more science-based simulation: “virtual experiments”

LES of a 217-pin LMFBR assembly



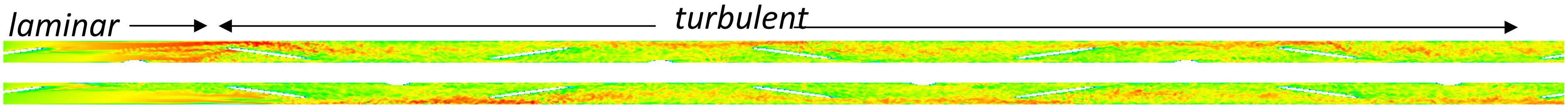
Passive scalar transport in an LMFBR assembly



Important discoveries of flow field from CFD: Pointer talk

- much different physics between 19 and 37 pin assemblies
- affect of wire wrap on turbulent transport

DNS of single pin



- Transition to turbulence with inflow/outflow boundary conditions in 7-pin x 3H configuration occurs at z ~ H/2:
  - use of periodic BCs is warranted,
  - significant savings (10 x)
  - to be verified for larger pin counts (edge effects)

Key parameters in T-H modeling

Multiscale simulation hierarchy involving:

Increased Costs

1. Experiments
2. DNS (direct numerical simulation of turbulence)
   ~50 M pt/channel (e.g., in subassembly simulation)
3. LES (large eddy simulation)
   ~5 *M pts/channel*
4. RANS (Reynolds-averaged Navier-Stokes)
   ~20,000 *pts/channel*
5. Subchannel or lumped-parameter models
   ~150 *pts/channel*

Increased Modeling (uncertainty)

Multiscale approach provides an important validation path:

- In the past, only Options 1 and 5 were available.

State of the practice

- **Several recent studies addressing issues related to applying CFD to reactor analysis (including fast reactors)**
  - ECORA Project: “Evaluation of Computational Fluid Dynamics for Reactor Safety Analysis”
    - *CFX, Fluent, Saturne, STAR-CD and Trio_U*
  - NEA/CSNI report “Best Practice Guidelines for the Use of CFD in Nuclear Reactor Safety Applications”
  - ASCHLIM Project: “Assessment of Computational Fluid Dynamics Codes for Heavy Liquid Metals”

Broad conclusions

- **Use of CFD codes is recommended if there are important 3-D aspects of the systems thermal-hydraulics that need to be resolved at smaller scales than can be handled by standard system and containment**

- **For foreseeable future CFD will be confined to specific isolated phenomena and sub-regions**

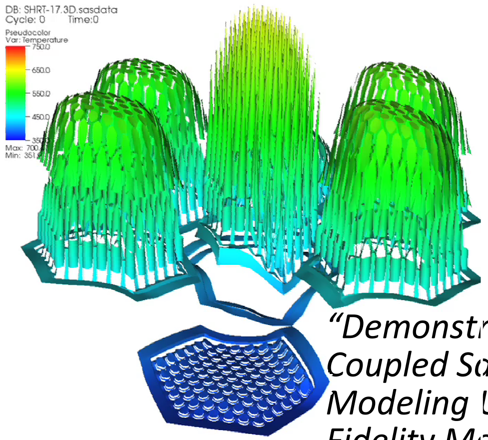
- **Typical instances for reactor safety problems include e.g.**
  - flow-induced vibration of structures
  - erosion of surfaces
  - mixing and stratification
  - heterogeneous flow situations
  - Sodium fires
  - Effect of fuel rod displacement on temperature profile
  - Sodium/water chemical reactor Induced by steam generator tube rupture
  - Thermal striping in T-junctions, upper plenum

Broad conclusions, cont.

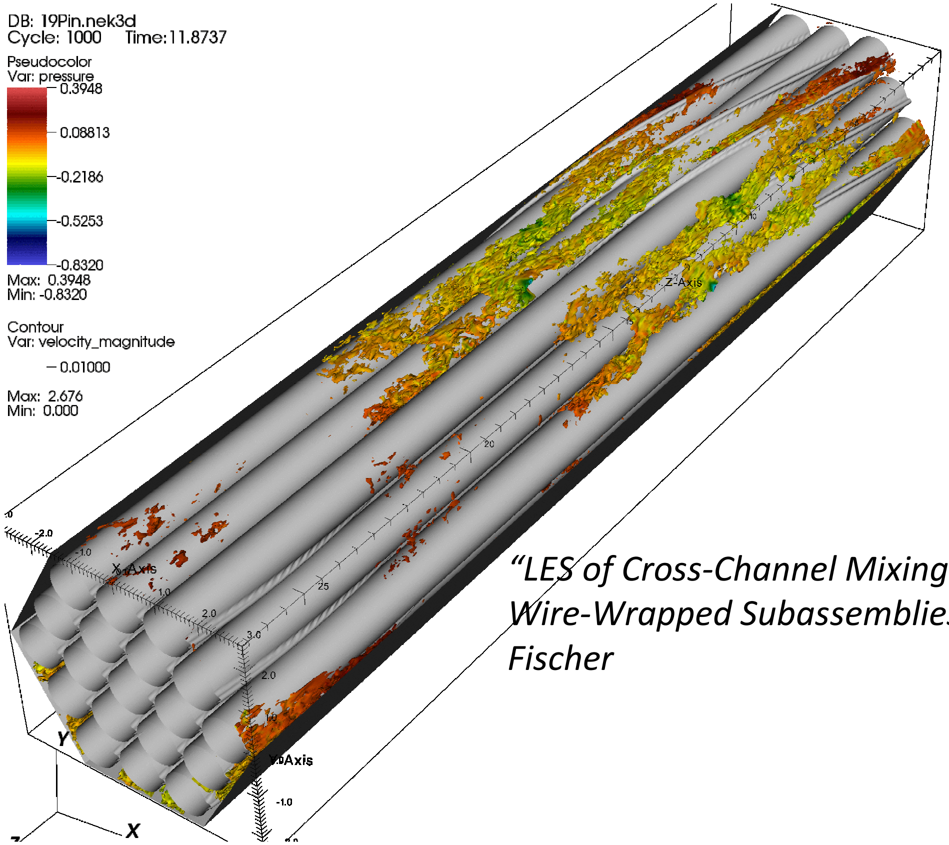
- **Most of value of CFD analysis will be derived from coupling to traditional system analysis codes to address very specific local problems.**
  - “Modeling of Thermal Stratification in Sodium Fast Reactor Outlet Plenums During Loss of Flow Transients”, T. H. Fanning and T. Sofu
  - "Evaluation on natural circulation behavior of the 4S by integrated analytical models", A.Matsuda, H.Watanabe, J.Ohno
  - Thermal-Hydraulic Calculation for Simplified Fuel Assembly of Super Fast Reactor Using Two-Fluid Model Analysis Code ACE-3D”, T. Nakatsuka, T. Misawa, H. Yoshida and K. Takase
  - “Development of computational method for predicting vortex cavitation in the reactor vessel of JSFR”, Hamada et al
  - Nature of coupling (on vs. two-way) can complicate analysis

- **Weak coupling to derive bulk parameters for sub-channel models**
  - *“LES of Cross-Channel Mixing in Wire-Wrapped Subassemblies”, Fischer*

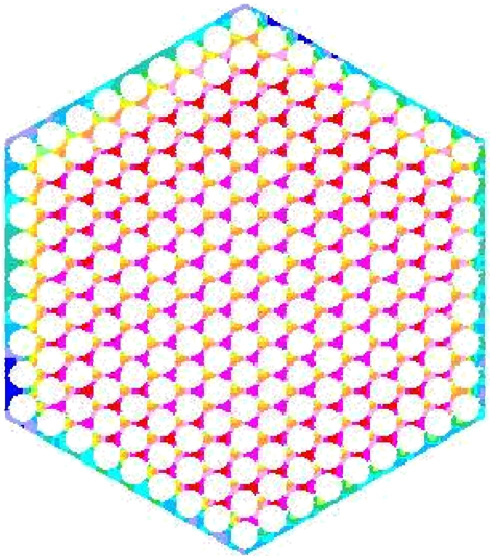
- **Modeling limitations that must be addressed**
  - Gas bubble two phase flows
  - Free-surface flows
  - Temperature gradients and related buoyancy flows:
    - *Turbulent liquid metal heat transfer along a heated rod within an annular cavity, R. Stieglitz, A. Batta, J. Zeininger*
  - Subgrid modeling issues for low-Pr flows
  - Sensitivity of solution to complicated gridding/numerical issues.



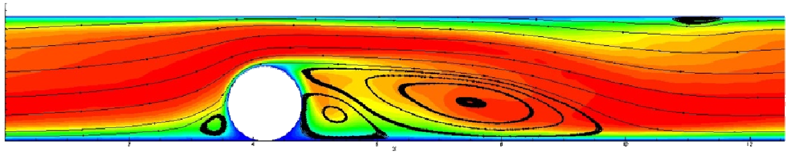
"Demonstration of Coupled Safety Modeling Using High Fidelity Methods", Fanning et al



"LES of Cross-Channel Mixing in Wire-Wrapped Subassemblies", *Fischer*



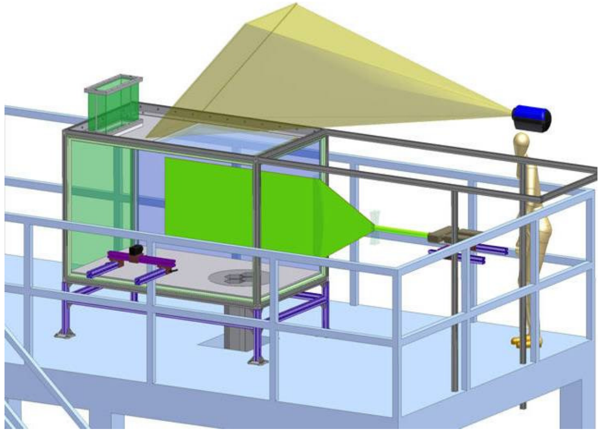
"RANS Simulations of Turbulent Diffusion in Wire-Wrapped Sodium Fast Reactor Fuel Assemblies", Pointer *et al*

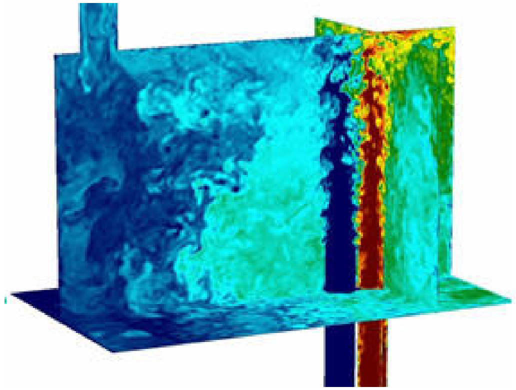


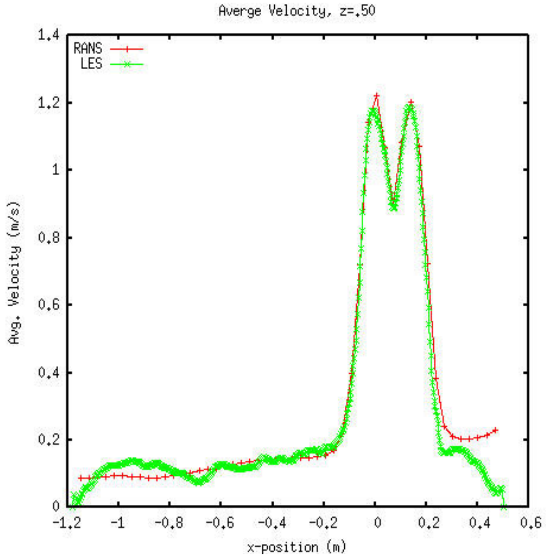
"Direct simulation of a passive scalar flow in a Turbulent swept flow over a wire in a channel", Pantano et al

Validation

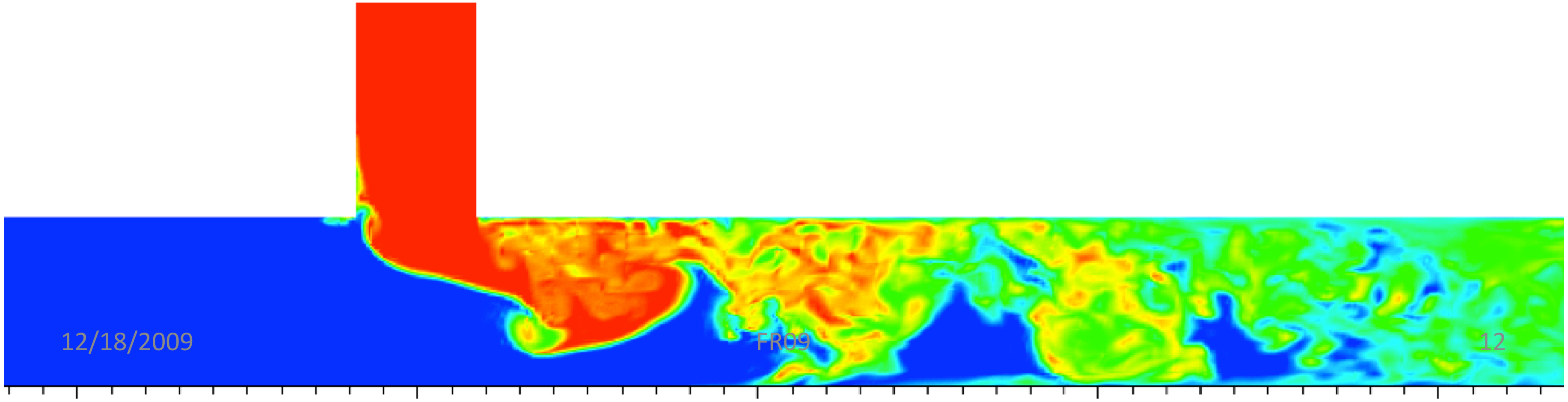
- Validation: Concerns attempts to build and quantify level of confidence in code predictions
- Should not be thought of as a binary “yes” or “no” decision.
  - Interpretation is problem-specific and depends heavily on intended use of code
- Takes place subsequent to *verification*
- More than sensitivity analysis for uncertain input parameters
- For science-based codes e.g. verification likely more critical
- No one-size-fits all: neutronics, T-H, and fuels modeling all treated differently
- Tiered approach: Complete system; subsystem, benchmarks, unit cases





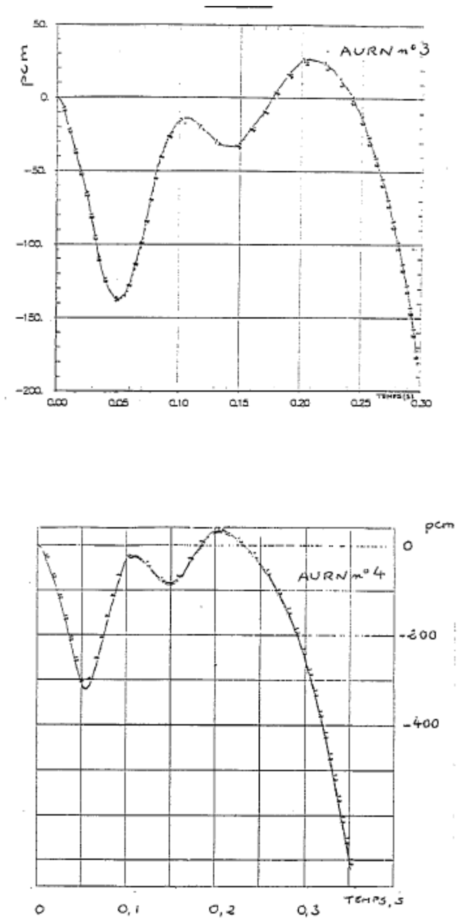


- *“Validation of fast reactor thermo-mechanical and thermo-hydraulic codes”*
  IAEA-TECDOC-1318,p. 13, November 2002.
  - First determine range of damaging frequencies for given wall thickness
  - Duration of simulation should be deduced from the lower bound of the range; transient duration should cover at least 10 periods of this low frequency
  - LES is recommended, requiring O[2] discretization schemes
  - Time step must resolve oscillations at higher bound of damaging frequencies
  - Boundary conditions should include possible secondary flows (e.g. swirl flow) and low-frequency variations of temperature and/or velocity
  - Boundary condition sensitivity analyses are critical
  - Care must be given to the transient behaviour of the computational mesh adjacent to the wall in association with a transient heat transfer coefficient with induced filtering of high frequencies.

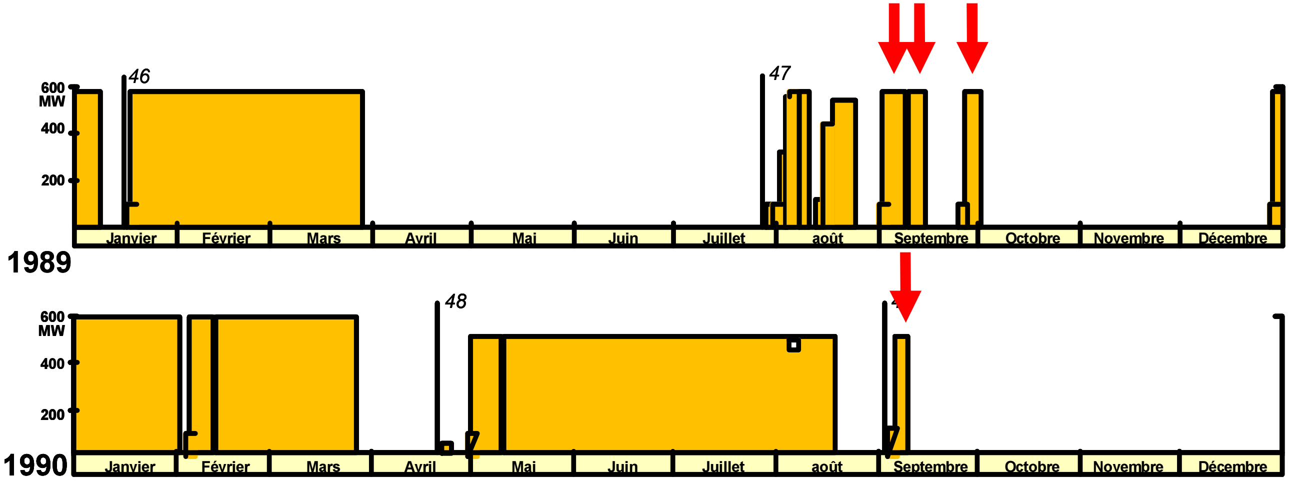


Neutronics

- **Methods improvements need to be guided by solution to real problems**
- **Good example: negative Reactivity Transients of PHENIX**
  - Four unexpected scrams occurred in 1989 - 1990 due to short negative reactivity transients (200 ms) with the same signal shape
  - Several potential explanations were given, but not satisfactory
  - Experiments are planned for PHENIX end-of-life tests for further investigation

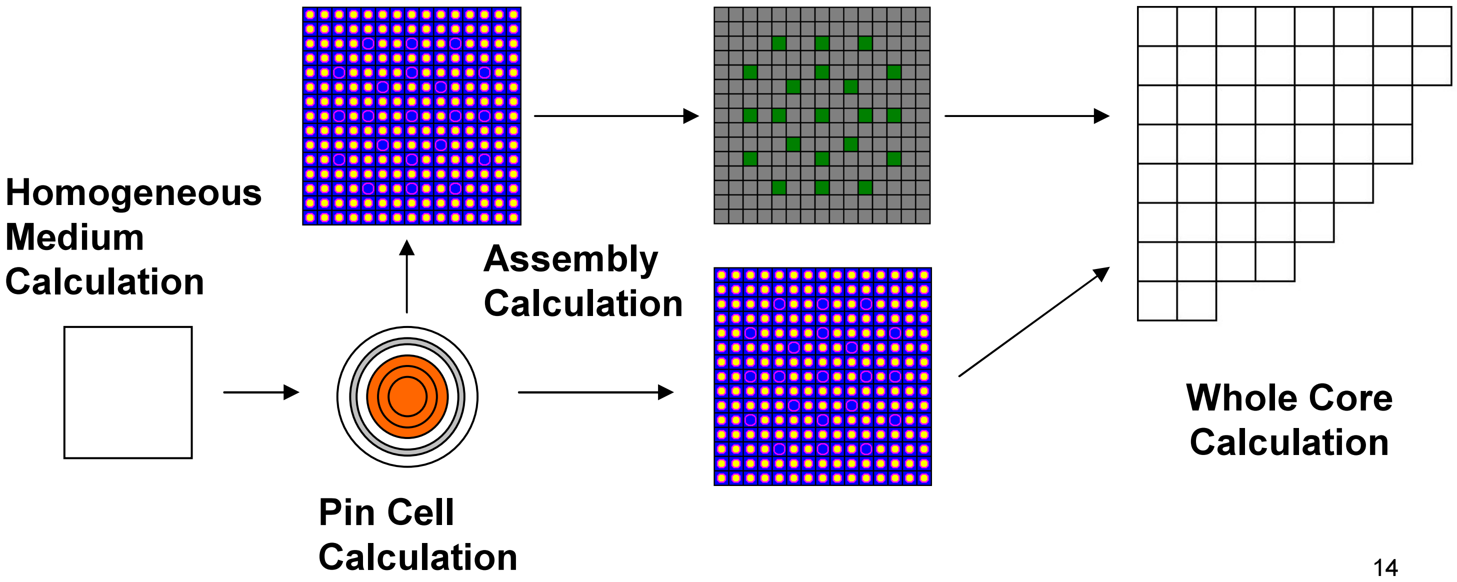


AURN n^{os} 3 et 4 : évolution de la réactivité



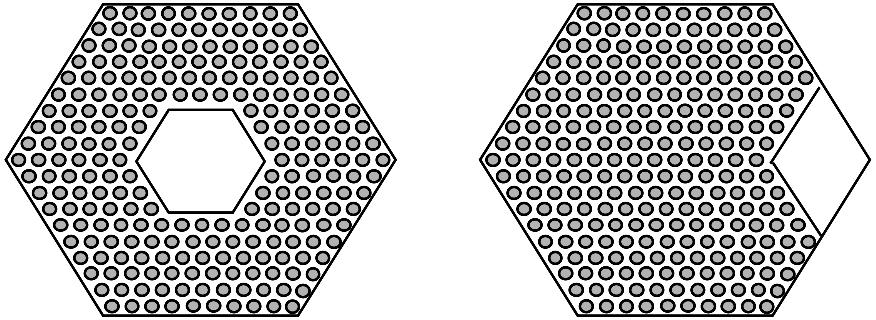
Status of Deterministic Design Analysis Tools

- **Current tools are judged to be adequate to begin the ABR design process**
- **However, based on various approximations and sophisticated multi-step procedures**
  - Average parameters for whole-core calculations are determined by a series of sub-domain calculations with increased modeling details and approximate boundary conditions
  - Detailed information is approximately recovered by reconstruction (de-homogenization) method



Status of Deterministic Design Analysis Tools

- **Improved accuracy is needed to meet burner design challenges**
  - Radial blanket is typically replaced by reflector
  - High leakage configurations also challenge design methods
  - Improved pin power and flux distributions
- **Applicable range of problems needs to be extended**
  - Possibly different assembly geometry (e.g., grid spacer for low CR core)
  - Modeling of structure deformation (for accurate reactivity feedback)
  - Neutron streaming in voided coolant condition
  - Control assembly worth (relatively large heterogeneity effects)



Assembly design concepts of JSFR

Status of Monte Carlo Codes

- **Monte Carlo method can represent these details geometric complexity and complicated energy dependence of nuclear data**
  - Need sufficiently low uncertainty, reliable variance estimates and uncertainty propagation
  - Fission source convergence
  - Error prediction accuracy
- **Computing resource requirements still remain unmanageable for many types of routine design analyses, including**
  - Accurate estimation of local reaction rates
  - Effects of small perturbations,
  - Transients analysis
  - Error propagation via depletion
  - Thermal feedbacks
- **Thus, the current design tools heavily rely on deterministic methods**
  - Monte Carlo methods are typically used for steady-state reference solution

Benefits of Advanced Simulation Tools

- **A modern, integrated design tool is crucial to improve the current design procedure, which is time-consuming and inefficient**
  - Eliminate piecemeal nature vulnerable to shortcomings in human performance, organizational skills, and project management
    - *Improved automation of data transfers among codes/modules*
  - Greatly improve the turn-around time for design iterations
  - Utilize advances in computer science and software engineering

- **Improved modeling in the integrated design tool would allow radical improvements**
  - Reduced reliance on costly experiments
    - *Integral mockup experiments*
    - *Thermal-hydraulic experiments to derive correlations*
  - Remove unnecessarily conservative design margins
  - Ability to optimize the design (e.g., reduce nominal peak temperatures)
  - New knowledge to alter and redirect the design features and approach

Conclusions

- Increasing interest internationally in advanced simulation reactor design/safety
- Much of this is enabled by HPC
- Science-based methods range tremendously from speculative to nearly mature
- Most critical aspect of approach is to define project with clear goals, metrics for success, and