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Title: Thermal Hydraulics Development for CASL

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Los Alamos
NATIONAL LABORATORY
EST. 1943

Thermal Hydraulics Development for CASL

This talk will describe the technical direction of the Thermal-Hydraulics (T-H) Project within the Consortium for Advanced Simulation of Light Water Reactors (CASL) Department of Energy Innovation Hub. CASL is focused on developing a ``virtual reactor'', that will simulate the physical processes that occur within a light-water reactor. These simulations will address several challenge problems, defined by laboratory, university, and industrial partners that make up CASL. CASL's T-H efforts are encompassed in two sub-projects: (1) Computational Fluid Dynamics (CFD), (2) Interface Treatment Methods (ITM). The CFD subproject will develop non-proprietary, scalable, verified and validated macroscale CFD simulation tools. These tools typically require closures for their turbulence and boiling models, which will be provided by the ITM sub-project, via experiments and microscale (such as DNS) simulation results. The near-term milestones and longer term plans of these two sub-projects will be discussed.

Thermal Hydraulics Development for CASL

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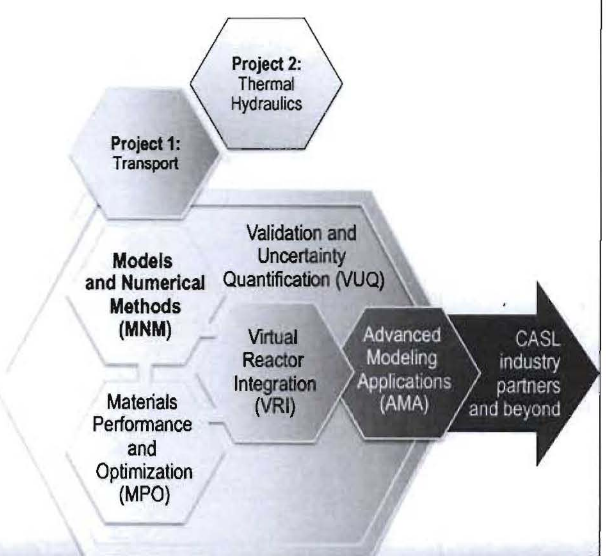
LA-UR-10-XXXX

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

MNM Thermal Hydraulics (T-H) will deliver state-of-the-art T-H simulation tools to the Virtual Reactor

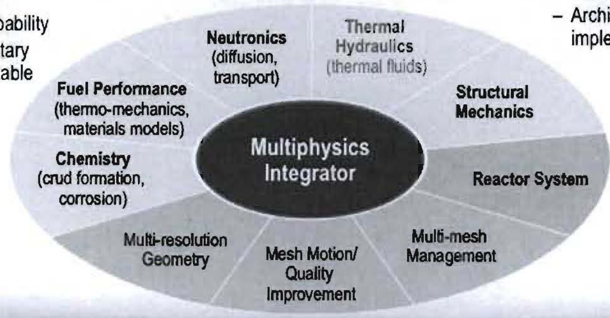
MNM T-H Ambitious Goals:

- Deliver next-generation, non-proprietary, scalable T-H simulation tools to VRI, interfaced with the latest VUQ technologies
- Accommodate tight coupling with other physics: conjugate heat transfer, structural mechanics (GTRF), neutronics, etc.



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



VERA builds initially on a foundation of mature, validated, and widely used software.

- Lattice physics + nodal diffusion: Current workhorse (Westinghouse)
- Deterministic transport: PARTISn (LANL), Denovo (ORNL), DeCART (UMichigan)
- Monte Carlo transport: MCNP5 (LANL), SCALE/KENO (ORNL)

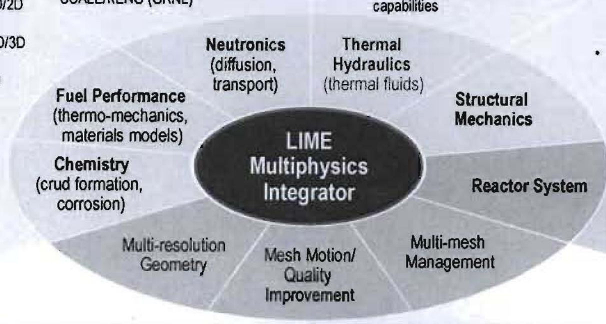
- VIPRE-W: Current subchannel flow workhorse (Westinghouse)
- ARIA (SNL), Charon (SNL), NPHASE (RPI): Initial 3D flow capability
- STAR-CCM+, TransAT: commercial capabilities

- FALCON: Current 1D/2D workhorse (EPRI)
- BISON: Advanced 2D/3D capability (INL)
- AMP FY10: Initial 3D capability (NEAMS)

- SIERRA (SNL)

- BOA: Current CRUD and corrosion workhorse (EPRI)

- RETRAN (EPRI)
- RELAP5 (INL)



Longer term, T-H development will require close multidisciplinary collaboration to take advantage of the tight coupling offered by VERA

Key challenges for T-H to address CASL Challenge Problems

- Fluid mechanics challenges
  - Turbulence and two-phase flow modeling (all Challenge problems)
  - Complex geometries; meshing often labor-intensive (all Challenge problems)
  - Multiple length and time scales (all Challenge problems)
  - Interfacial phenomena in two-phase flows (CRUD, DNB)
  - Sub-cooled boiling (CRUD, DNB)
  - Boiling crisis (DNB)
- Coupling with other physics, such as
  - Conjugate heat transfer (CRUD, DNB)
  - Neutronics (CRUD, DNB)
  - Structural mechanics (GTRF)
  - Material modeling (all Challenge problems)
- Software challenges (all Challenge problems)
  - Intrusive UQ support
  - Advanced architectures
  - Extensibility to allow future advances in modeling

Addressing these challenges will require leveraging and collaboration outside of CASL

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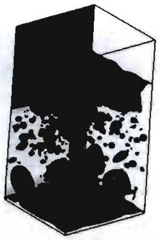
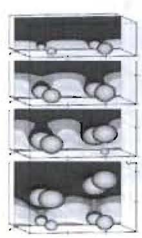
MNM T-H has two primary sub-projects

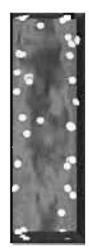
1. **Computational Fluid Dynamics (CFD)**: Development of non-proprietary, scalable, verified and validated *macroscale* CFD tools, that complement capability in existing commercial codes
2. **Interface Treatment Methods (ITM)**: Generate *microscale* simulation results and experimental data for CFD closure models and validation



Simulation of film boiling from a flat surface (D. Lakehal)



DNS simulation of bubbles growing and detaching from four prescribed nucleation sites (G. Tryygvason)



Wall-peaked low quality bubbly flow (M. Podowski)

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There are 2 primary paths within the CASL overall T-H strategy

1. Leverage existing T-H codes, such as STAR-CD/CCM+
   - These efforts within CASL are mostly outside of MNM T-H
2. Develop VERA-CFD: A focus of MNM T-H
   - Non-proprietary T-H capability, open to outside collaboration
   - Complements capability in existing commercial codes
   - Take advantage of our current code base (*e.g.*, NPHASE, Charon, ...)
   - Scalable to billions of degrees-of-freedom
   - Amenable to efficient, tight physics coupling within VERA (neutronics, FSI, MPO output, etc.)
   - Accommodate upscaling of ITM/DNS results
   - Use latest *intrusive* VUQ technologies (sensitivities, adjoint, MMS, ...)
   - Targeted towards latest computer architectures
   - Extensible to new models and numerical algorithms

ITM and experimental efforts will contribute to both of these paths

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MNM T-H Team

The Team is made up of experts in simulation, modeling, and experiments

Organization	Primary Focus in MNM T-H
MIT	Experiments, ITM, modeling
RPI	ITM, CFD, modeling (PHASTA, NPHASE-CMFD)
City College NY	Experiments, ITM simulation (FELBM)
Notre Dame	ITM simulation (FTC3D)
Texas A&M	Experiments, modeling
NC State	Upscaling CFD to sub-channel
U. Michigan	Uncertainty quantification
ASCOMP	ITM/CFD Simulations (TransAT), modeling
Sandia N.L.	CFD development, scalable algorithms
Idaho N.L.	Multiphase flow methods development
Oak Ridge N.L.	CFD methods and development
Los Alamos N.L.	CFD methods and development, multiphysics
Westinghouse*	CFD simulation, modeling
CD-Adapco*	CFD simulation, modeling

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MNM L2 Milestones: Year 1 (due 6/30/2011)

1. Full-core 3D transport (2D/1D, pin-resolved) capability with single-phase T-H coupling
   - T-H capability will be a commercial code (STAR-CD/CCM+)
2. Quantify scalability of CFD capability on a leadership system and document path forward for future needs
   - Will aid down-selecting current and future algorithms and codes
3. Establish CFD, ITM, and coupled physics benchmark problems to address Challenge Problems
   - Will aid down-selecting current and future algorithms and codes

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L2 Milestones - MNM	Yr	Link to L1
Full-core 3D transport (2D/1D, pin-resolved) capability with single-phase T-H coupling	1	CASL.Y1.02
Quantify scalability of CFD capability on a leadership system and document path forward for future needs	1	Outyear L1
Establish CFD, ITM, and coupled physics benchmark problems to address Challenge Problems	1	Outyear L1
Initial incompressible, single-phase, with sub-cooled boiling flow capability targeted to VRI	2	Outyear L1
Determine development paths for MOC (3D vs 2D/1D), Sn (unstructured grid vs cut-cell), Monte Carlo decomposition (domain vs data), and transient methodology	2	Outyear L1
Full-core 3D pin-resolved deterministic transport capability	3	Outyear L1
Full-core 3D pin-resolved deterministic transport capability with T-H coupling	4	Outyear L1
Deliver multiscale approach for upscaling and downscaling of microphysics subgrid models	4	Outyear L1
Full-core 3D domain/data-decomposition hybrid Monte Carlo transport capability	5	Outyear L1
Demonstrate ability to capture heat transfer and bubble condensation with advanced numerical methods and coupling	5	Outyear L1

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ITM Subproject: Year 1 Objectives

- Defining ITM benchmark problems, generate initial ITM results and experimental plans.
- L3 milestone:
  - Define interface treatment method (ITM) benchmark problems and metrics for guiding methodology down-select (6/30/2011)
- 11 L4 milestones that support this L3 and future work.

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Sample ITM L4 Milestones	Organizations	Due Date
3. Deliver plan for ITM development	MIT, RPI, TAMU, ASCOMP	3/31/2011
4. Report on ITM benchmark problems including experimental plan	MIT, RPI, TAMU, ASCOMP	6/30/2011
5. Define an experimental plan for adiabatic air-water two-phase flow and subcooled flow boiling of a refrigerant inside a heated tube or rod bundle with or without Westinghouse-design spacers...	City College NY	12/31/2010
8. Compute the growth and detachment of one vapor bubble in the turbulent flow examined above.	Notre Dame	3/31/2011
11. Identify multiphase CFD closure relations to be developed and improved by ITMs	MIT, Umich, ASCOMP	6/30/2011

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CFD Subproject: Year 1 Objectives

- Defining CFD benchmark problems, assessment of current codes, plan forward for development
- L3 milestones:
  1. Document implementation plan for next-generation flow simulation capability (12/31/2010)
  2. Quantify scalability of existing CFD codes (6/30/2011)
  3. Define thermal fluid-flow benchmark problems and metrics for guiding methodology down-select (6/30/2011)
- 20 L4 milestones that support these L3's and future work.

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Sample CFD L4 Milestones	Organizations	Due Date
5. Deliver the Requirements Section of the documentation of implementation plan for next-generation flow simulation capability	ORNL	12/31/2010
10. Documentation of uncertainty sources and system response quantities in T-H simulations	Umich	12/31/2010
13. Demonstrate large-scale parallel solution of unstructured mesh stabilized FE CFD capability...	SNL	3/31/2011
15. Quantify scalability of NPHASE-CMFD	RPI	6/30/2011
16. Contribute to definition and documentation of CFD benchmark problems	LANL, ORNL, SNL, RPI, ASCOMP	6/30/2011

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Two examples from our team of including microscale physics into macroscale CFD models

1. Experimental determination of closure parameters for heat flux models (J. Buongiorno, MIT)
2. Coupling a microscale ITM/DNS code with a macroscale CFD code (M. Podowski, RPI)

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Example Use of Measurements to Provide CFD Closures

Heat transfer relation used by Star-CD code (Kurul & Podowski 1990, "RPI model"):

$$q''_{tot} = q''_e + q''_q + q''_c$$

$$q''_e = \frac{\pi D_b^3}{6} \rho_g h_{fg} f_b N_{SD}$$

$$q''_q = (t_w f_b) A_q \frac{2k_l (T_w - T_{sat})}{\sqrt{\pi \alpha_l t_w}}$$

$$q''_c = A_{1\phi} h_{turb} (T_w - T_{sat})$$

Requires input for:

- bubble departure diameter
- bubble departure frequency
- bubble growth and wait times
- nucleation site density
- areal void fraction

- Parameters depend on surface characteristics (roughness, wettability, porosity, composition) and coolant chemistry
- Generally parameters are not available analytically
- **Must measure and/or simulate with ITM**

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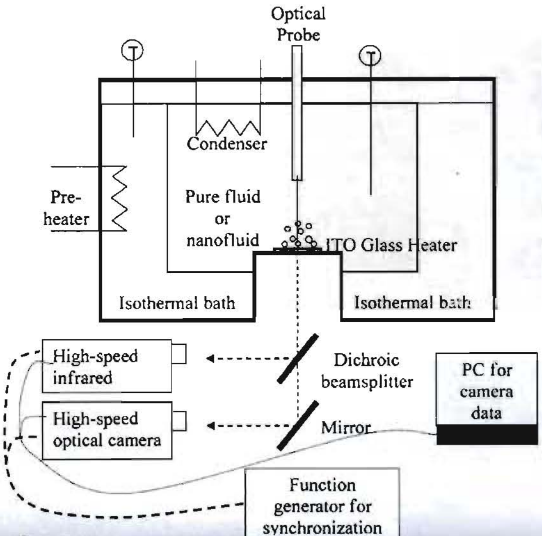
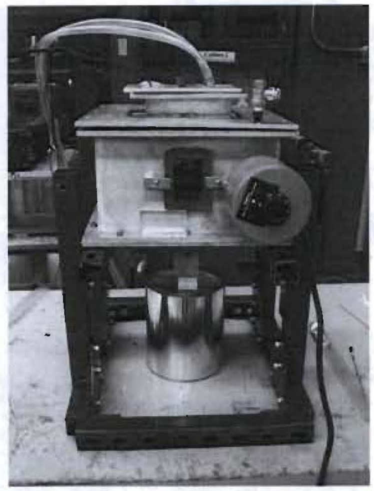
courtesy of J. Buongiorno

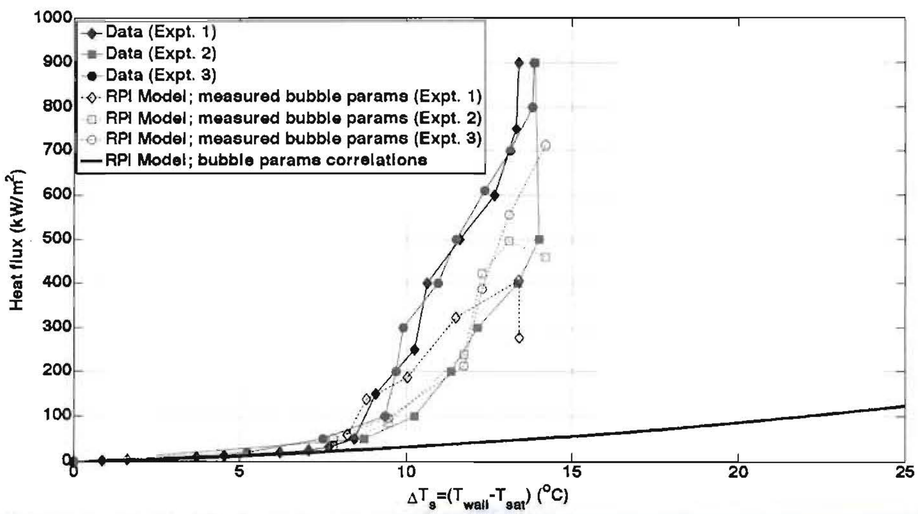
MIT's High-Speed IR Thermometry





courtesy of J. Buongiorno

Using measured bubble data in heat flux model is an improvement over default Star-CD parameters



courtesy of C. Gerardi, J. Buongiorno

Two examples from our team of including microscale physics into macroscale CFD models

1. Experimental determination of closure parameters for heat flux models (J. Buongiorno, MIT)
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Sample ITM Code: PHASTA (RPI)

- **P**arallel, **H**ierarchic, **A**daptive, **S**tabilized (finite element) **T**ransient **A**nalysis flow solver developed at RPI
- Effective tool for bridging a broad range of length scales in turbulent flows: RANS, LES, detached eddy simulation (DES), DNS
- Uses anisotropically adapted unstructured grids
- Capable of simulating two phase flows with level set method
- Highly scalable performance on massively parallel computers (e.g.,IBM Blue Gene)

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courtesy of M. Podowski

Sample CFD Code: NPHASE-CMFD (RPI)

- Computational Multiphase Fluid Dynamics solver
- Uses unstructured grids with arbitrary element types
- Capable of modeling an arbitrary number of fields (fluid components and/or phases)
- Has built-in mechanistic modeling, integrated with numerics
- Can be used to model gas/liquid interfaces using Level-Set method
- Uses state-of-the-art multiphase models which have been extensively validated

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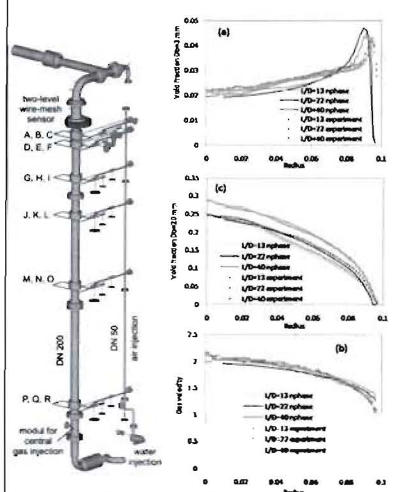
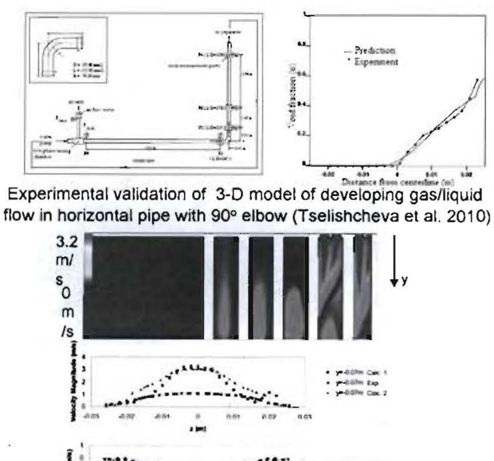
courtesy of M. Podowski

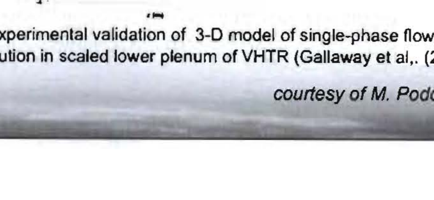
Examples of NPHASE-CMFD validation



- Validation of 3-D model of developing gas/liquid flow against TOPFLOW experiments (Tselishcheva et al., 2010)



Experimental validation of 3-D model of developing gas/liquid flow in horizontal pipe with 90° elbow (Tselishcheva et al. 2010)



Experimental validation of 3-D model of single-phase flow distribution in scaled lower plenum of VHTR (Gallaway et al,. (2007)

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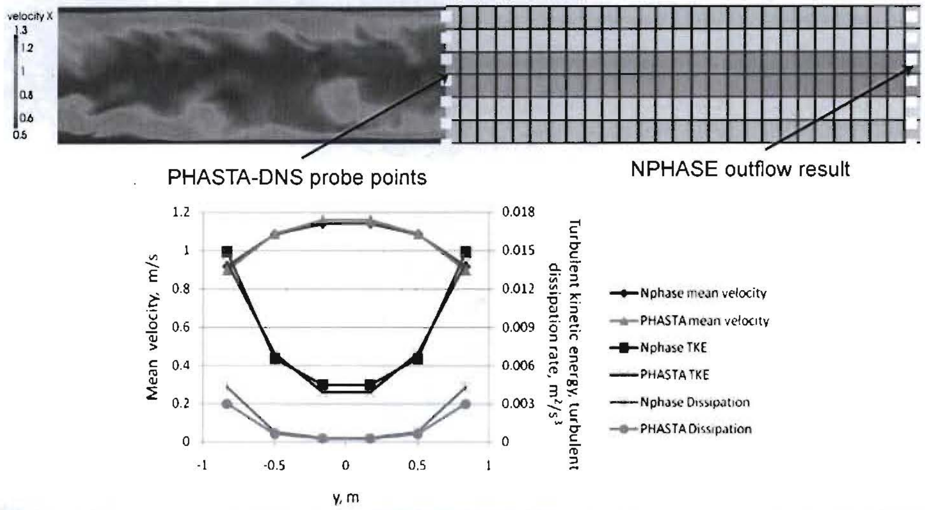
courtesy of M. Podowski

Single-phase channel flow: Link with high-Re k-ε model case

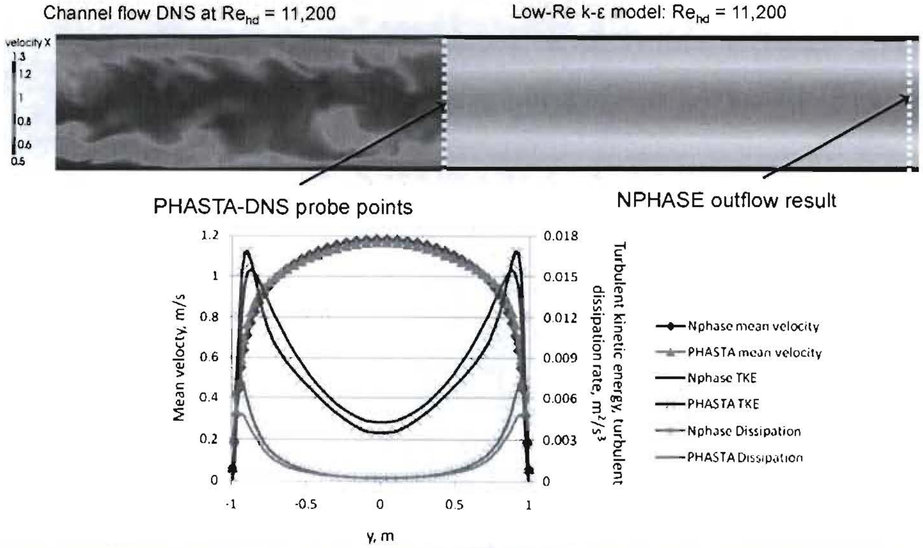
Channel flow DNS at Re_{hd} = 11,200 High-Re k-ε model: Re_{hd} = 11,200



courtesy of M. Podowski

Single-phase channel flow: Link with low-Re k-ε model case

Channel flow DNS at Re_{hd} = 11,200 Low-Re k-ε model: Re_{hd} = 11,200



courtesy of M. Podowski

Multiscale modeling example from M. Podowski (RPI)

- Simulation of Sodium Fast Reactor (SFR) during fuel rod failure
- Application of three existing computer codes
  - FronTier (SUNY-SB): models fission gas from fuel rod
  - PHASTA (RPI): ITM microscale modeling of gas bubble evolution into coolant
  - NPHASE-CMFD (RPI): Macroscale multiphase CFD modeling of coolant flow
- Currently, one-way coupling through BCs:
  - FronTier ➔ PHASTA ➔ NPHASE-CMFD
  - Ultimately, would like to use PHASTA to provide closure parameters for NPHASE-CMFD (see Lahey, Nuc. Eng. & Design, vol. 235, 2005; Podowski, Nuc. Eng. & Design, vol. 239, 2009)

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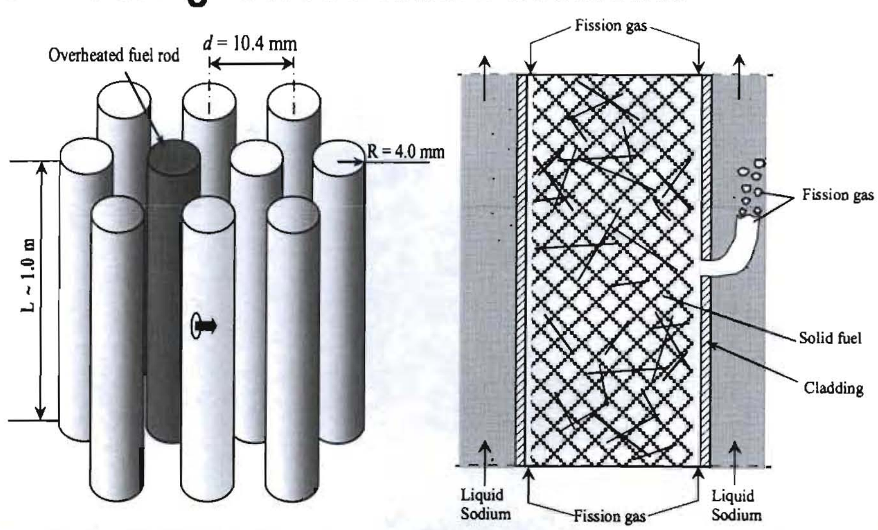
Schematic of fuel degradation and transport in SFR during fuel rod failure accidents



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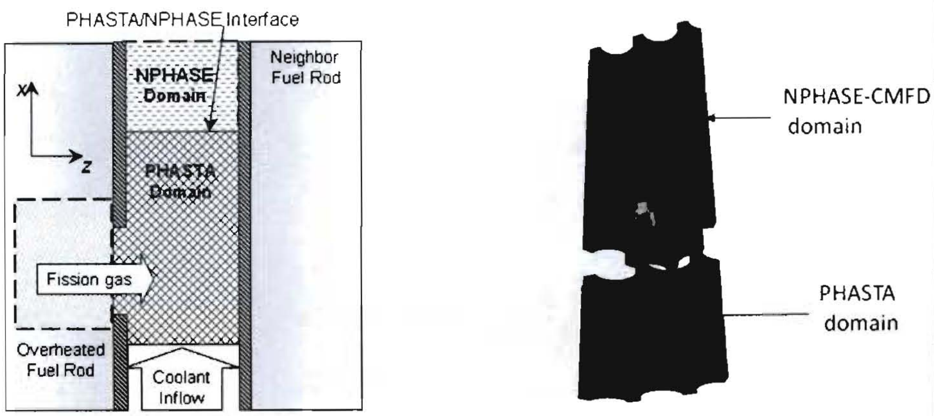
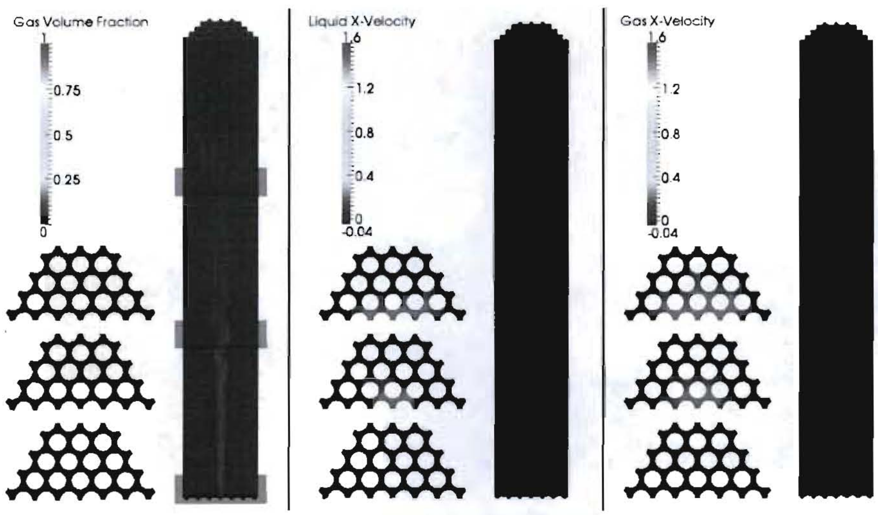
courtesy of M. Podowski

Computational domains overview



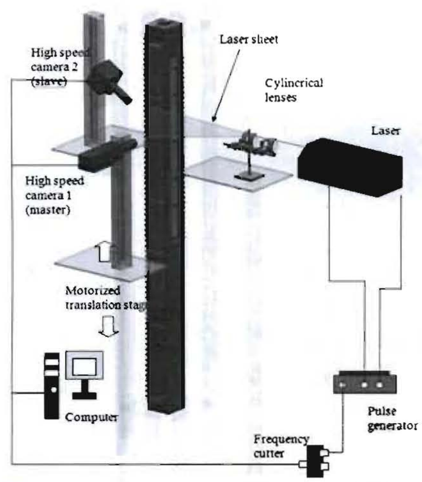
courtesy of M. Podowski

NPHASE-CMFD results for SFR bundle at final time: Inflow conditions provided by PHASTA



courtesy of M. Podowski

Texas A&M will provide state-of-the-art experimental results



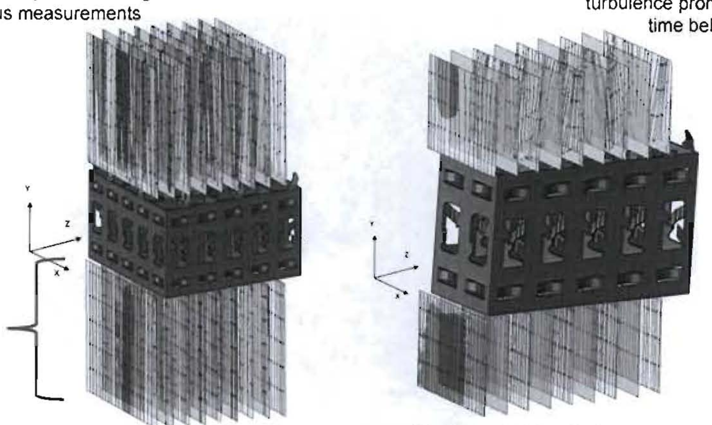
- Subcooled boiling experiment
- PIV measurements for grid spacers:
  - 5x5 rod bundle
  - High repetition laser (20 KHz, l=527 nm, 10 mJ).
  - High speed cameras
    - ➢800x600 pixels & 150,000 fps max., 14 bit.
    - ➢One color camera 1024x1024 pixels & 250,000 fps max., 12 bit.

courtesy of Y. Hassan

Sample PIV Measurements from Texas A&M

Transient studies possible using simultaneous measurements

Measurements near the turbulence promoters and its time behavior



Boundary conditions with high space and temporal resolution

Macro scale: Across rod bundle

Micro scale: Resolution to 5x Kolmogorov scale at Re=16,000

courtesy of Y. Hassan

Primary Goals for VERA-CFD

- Non-proprietary T-H capability, open to outside collaboration
- Complements capability in existing commercial codes
- Take advantage of our current code base (*e.g.*, NPHASE, Charon, ...)
- Scalable to billions of degrees-of-freedom
- Amenable to efficient, tight physics coupling within VERA (neutronics, FSI, MPO output, etc.)
- Accommodate upscaling of ITM/DNS results
- Verified, and validated on CASL Challenge Problems
- Use latest *intrusive* VUQ technologies (sensitivities, adjoint, MMS, ...)
- Targeted towards latest computer architectures
- Extensible to new models and numerical algorithms

Technology from Sandia N.L. will contribute to many goals above

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Sandia code base that will contribute to MNM T-H

Charon (2003, Templated C++)
- 2D, 3D CFD (Laminar)
- Flow/Transport/Reaction
- Drift-Diffusion Systems
- Multiphase (Gas-solid, aerosol)
- Resistive MHD
- Implicit Stabilized FE (Quad, Hex, ..)
- Parallel NK w/ AMG & Physics-based Demo to O(10^5) procs

Trilinos/Aztec00 (2000, C++)
- Preconditioned Krylov Solver Lib.
- Parallel Domain Decomp., AMG;
- R&D 100 (2004)
- Users: ~250 internal, 4000+ external

Trilinos/ NOX
Trilinos/LOCA

SIERRA/Aria (~2000)
- 2D/3D CFD
- Flow/Transport/Reaction
- Free Surface Flow
- Mesh Motion
- Level Sets
- Turbulent combustion w/soot
- High Mach CFD (reentry vehicles)

???? (2010, Templated C++, Expression-graph based)
- 2D, 3D CFD & Flow/Transport/Reaction (Laminar, Turb.)
- Extended MHD, 2T Shock-MHD, Multi-group Rad-Diff.
- Arbitrary no. of Momentum, energy, transport equations.
- ......
- Implicit Stab. FE; Mixed FE; Edge/face FE, FV
- Higher order methods (space and time)
- Heterogeneous Multiphysics (e.g. Conjugate Heat trans.)..

More Info: DOE Office of Science Sponsored Report –

Network Attributes Impacting the Generation and Flow of Knowledge within and From the Basic Science Community, Mohrman, Monge (2004)

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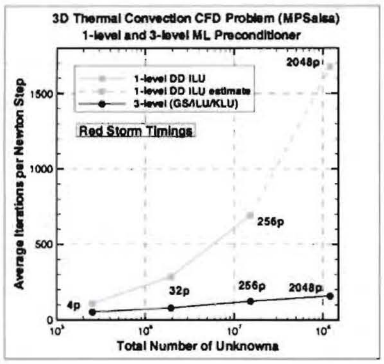
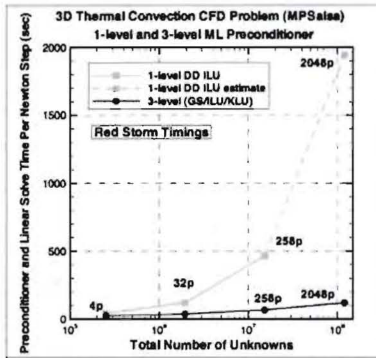
courtesy of R. Pawlowski, J. Shadid

Multilevel Preconditioner Scaling Study:
3D Thermal Buoyancy Driven Convection



(a)



(b)

Figure 8. Weak scaling for one-level and three-level preconditioners for the steady-state 3D thermal convection problem on the Cray XT3/4: (a) Iteration count (b) Linear solve time per Newton step

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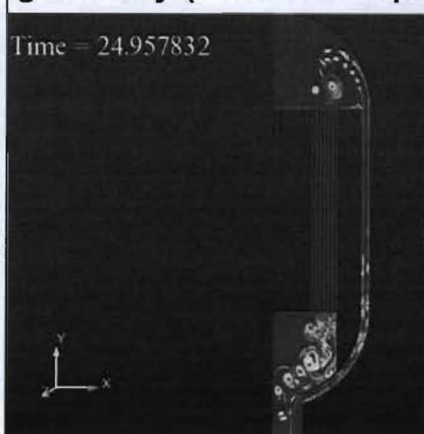
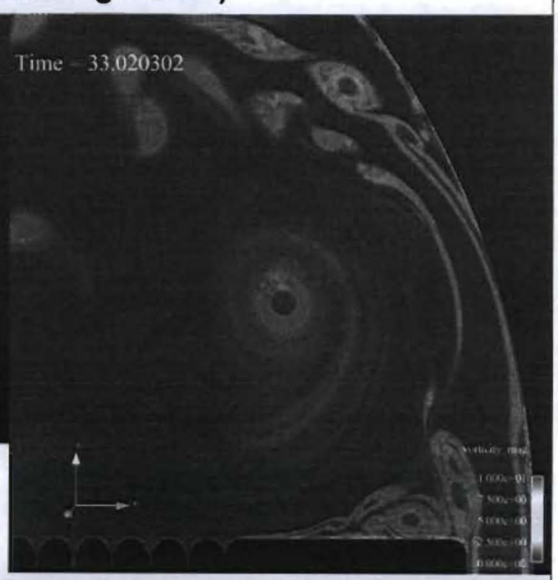
courtesy of J. Shadid

Start-up of Helium fluid flow in NGNP reactor geometry (not actual operating cond.)





NGNP Geometry: Rich Martineau (INL), Unstructured Quad Cubit Mesh SNL

CASL

courtesy of R. Pawlowski, J. Shadid

Use of C++ templates to generate derivatives

$$f_0 = 2x_0 + x_1^2 \qquad f_1 = x_0^3 + sin(x_1)$$

```
// double version
void computeF(double* x, double* f)
{
  f[0] = 2.0 * x[0] + x[1] * x[1];
  f[1] = x[0] * x[0] * x[0] + sin(x[1]);
}
```

```
void computeJ(double* x, double* J)
{
  // J(0,0)
  J[0] = 2.0;
  // J(0,1)
  J[1] = 2.0 * x[1];
  // J(1,0)
  J[2] = 3.0 * x[0] * x[0];
  // J(1,1)
  J[3] = cos(x[1]);
}
```

Writing derivatives in the context of multiphysics systems with changing dependency chains is difficult, error prone and a combinatorial explosion!

```
// ad version
template <typename ScalarT>
void computeF(ScalarT* x, ScalarT* f)
{
  f[0] = 2.0 * x[0] + x[1] * x[1];
  f[1] = x[0] * x[0] * x[0] + sin(x[1]);
}
```

ScalarT → double	**Residual**
ScalarT → Dfad<double>	**Jacobian**

Machine precision accuracy: No FD involved!

courtesy of R. Pawlowski, J. Shadid

Summary of MNM T-H Efforts

- ITM subproject will generate microscale simulation results and experimental data for CFD closure models and validation
- CFD subproject will develop next-generation CFD tools:
  - Complement existing commercial capability
  - Non-proprietary
  - Verified, and validated on CASL Challenge Problems
  - Goals: Scalable, tight physics coupling, intrusive VUQ, extensible, target latest computer architectures
- Other contributors only briefly mentioned here: ORNL, INL, LANL, City College NY, Notre Dame, Michigan, NC State, ASCOMP

Questions?

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Extras

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Success of MNM T-H will require leveraging with activities outside of CASL

Interfaces with other NE activities:

- NEAMS Fuel Performance (Pannala ORNL) and Safeguard & Separations (Francois LANL)
- Tokyo Electric Power Company project on BWRs (Buongiorno MIT)
- Areva project on DNS and ITM (Buongiorno MIT)
- Westinghouse project of experiments of flows in fuel bundles with mixing vanes using Particle Image Velocimetry technique (Hassan TAMU)
- NRC Thermal-hydraulics projects on simulations and experiments (Banerjee, Kawaji, Lee CCNY)
- NASA Thermal LBM simulations of nucleate boiling (Lee CCNY)
- NSF DMS Unstructured LBM simulations of wetting (Lee CCNY)
- NURISP EU funded Project: simulations of multiphase, phase-change heat transfer systems (Lakehal ASCOMP)
- THINS EU funded Project: simulations of turbulent free-surface flows and single-phase non-unity Prandtl number flows (Lakehal ASCOMP)
- INL project on development of a multiscale simulation capability for multiphase flow equipment; also other RPI projects on DNS and CMFD (Podowski, RPI)

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External Interfaces: Other applications

- NSF Multiscale simulations of multiphase systems (Tryggvason Notre Dame)
- ASCR Applied Mathematics research (Shadid SNL)
- ASCR UQ funded project (Shadid SNL)
- Office of Science Climate CFD (Lowrie LANL)
- Environmental Management ASCEM (Lowrie LANL)
- NNSA ASC PSAAP CRASH Project, adapative UQ (Fidkowski Umich)
- NNSA ASC (LANL & SNL)

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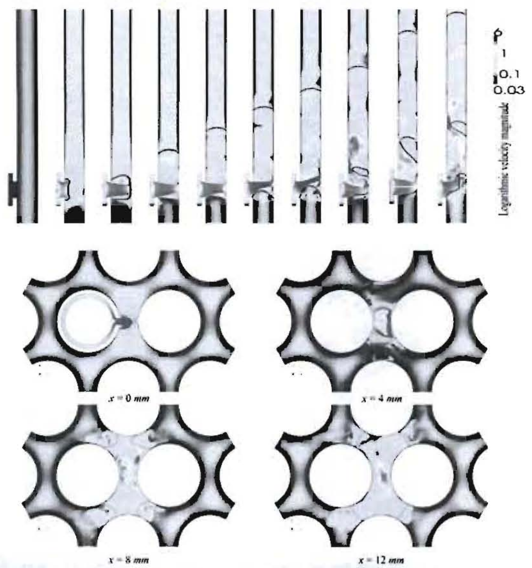
Instantaneous fission-gas/liquid-sodium velocity field



- Time evolution of fission gas propagation along coolant channels
- Lateral two-phase velocity distribution around fuel rods at different axial locations

courtesy of M. Podowski