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CASL Institutional Computing Report, CY2012

Stephen Lee
CCS Division Leader
(for Bruce Robinson, CNP-PO)

LA-UR pending

Materials Performance Optimization (MPO)

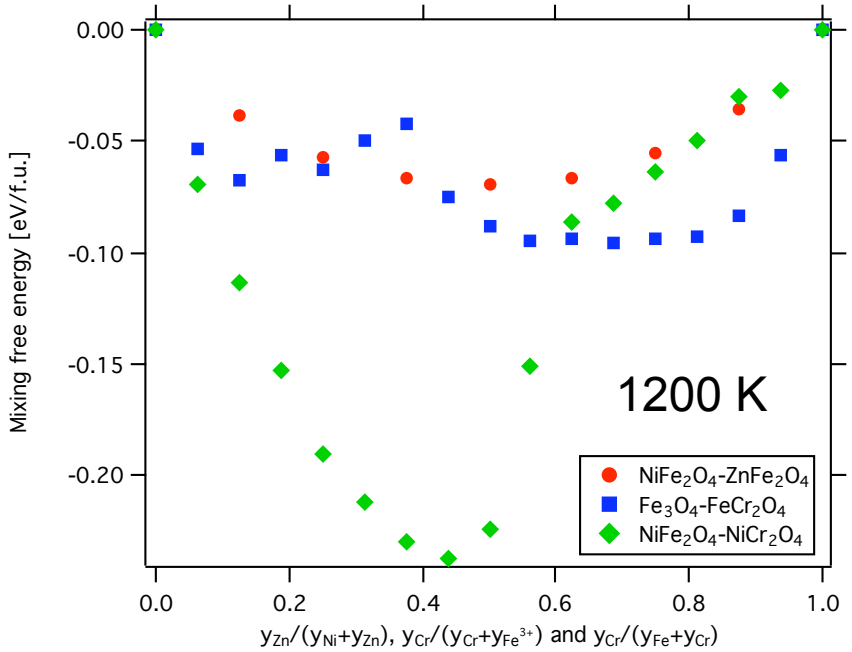
Chris Stanek (MST-8)

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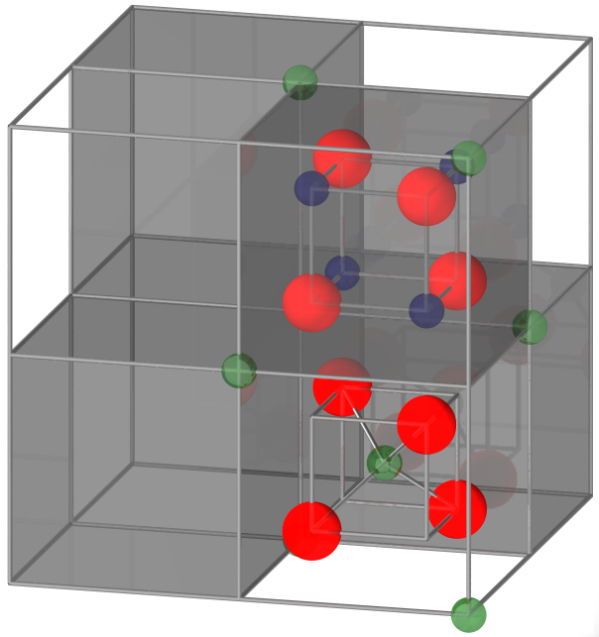
Density functional theory (DFT) study of CRUD thermodynamics

- The free energy of inverse-normal spinel mixtures was approximated by adding the configuration entropy derived from the spinel crystallography and DFT mixing rules to the enthalpies calculated from DFT.

Spinel mixing free energy



Spinel structure

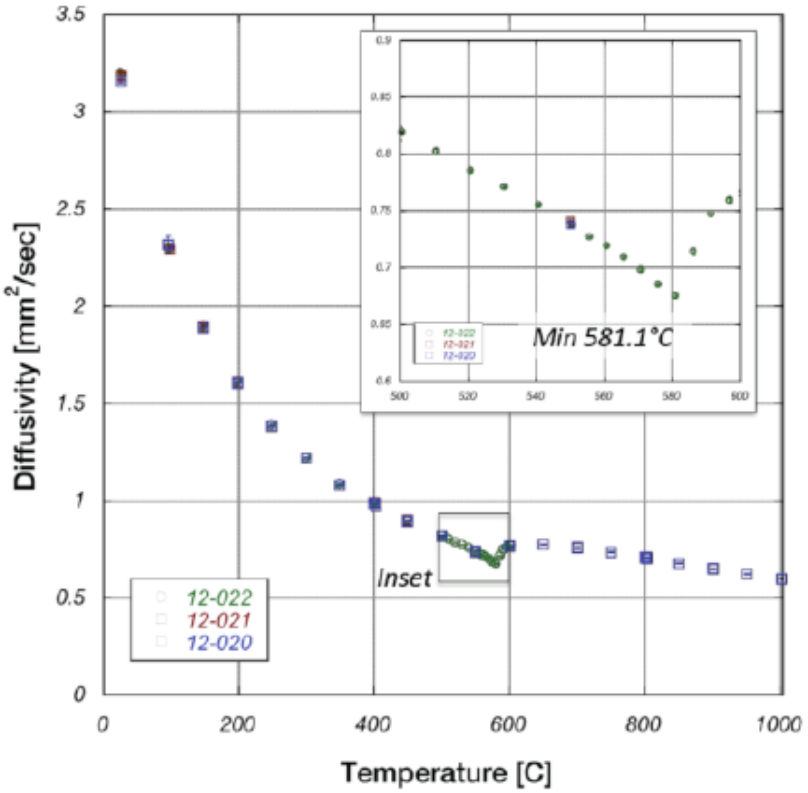


- These results enable us to better understand both the formation of protective films on corrosion sources and the chemistry of the CRUD that is deposited on the fuel pins.

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Thermal conductivity (κ) of $NiFe_2O_4$

Thermal diffusivity (α) of $NiFe_2O_4$ $\kappa = \alpha \rho C_p$



	ΔE^A [eV]	ΔE^B [eV]	E_g [eV]	$E_{e\text{-}h}$ [eV]	V [Å³]
Ferrimagnetic, ordered cations	-0.44/-0.44	-2.60/-2.74	1.91	1.47	593.5
Ferrimagnetic, disordered cations	0.00/0.00	-2.16/-2.30	1.60	1.14	593.95
Paramagnetic, disordered cations	2.16/2.30	0.00/0.00	1.53	1.12	599.18
Ferrimagnetic + Ni-Fe anti-site defect, disordered cations	0.86/0.86	-1.30/-1.44	1.46	0.65	596.84
Paramagnetic + Ni-Fe anti-site defect, disordered cations	2.74/3.02	0.58/0.62	1.43/1.27	0.79/0.62	601.55/601.84

Relative energies of ferrimagnetic and paramagnetic $NiFe_2O_4$ with and without anti-site defects (ΔE^A and ΔE^B). The band gap (E_g), electron-hole pair formation energy ($E_{e\text{-}h}$) and volume per supercell are also listed for these structures.

- DFT calculations of $NiFe_2O_4$ electronic defects show that the increase in thermal diffusivity at the Curie temperature must be related to non-stoichiometry and increased mobility of polarons (Fe^{2+}).

Thermal Hydraulics Methods (THM)

Mark Christon (CCS-2)

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CASL Usage of Turquoise Clusters

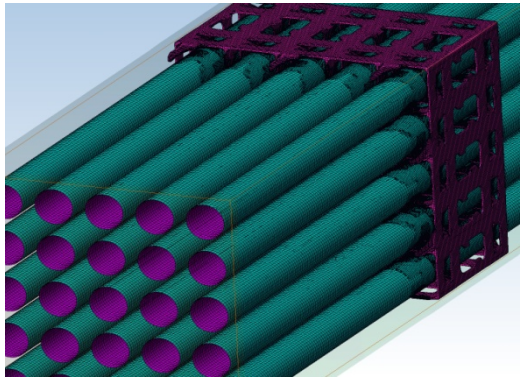
- Conejo, Mapache, Pinto and Mustang have been important computational resource for the thermal hydraulics methods (THM) development efforts
  - Used 4 CASL THM Milestones: 3 – L3, 1 – L2, 1 – L1 (L1 & L2 DOE reportable)
- s11_casl cluster usage from 1/1/2012 – 1/1/2013
  - 3.35 Million cpu-hours used in 2011 (2.7% Utilization)
  - 18.58 Million cpu-hours used in 2012

Machine	Hours Used	Percent Used
conejo	3,464,213.7	1.7%
mapache	617,213.2	9.1%
pinto	957,456.4	4.9%
mustang	13,544,498.6	17.2%

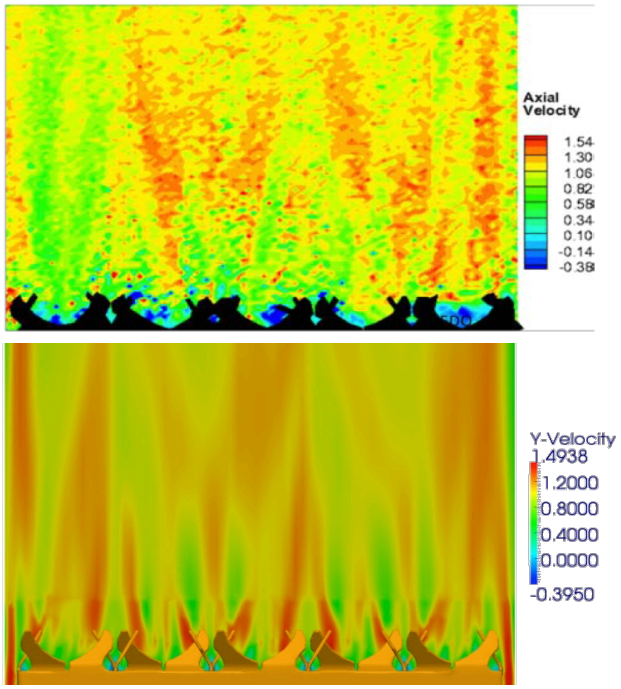
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Impact on CASL Hydra-TH milestones

- Turquoise machines used for L1, L2 and L3 milestones
  - Demonstrated scaling using hybrid meshes up to ~100 million elements with ILES
- L1 Milestone demonstrated effective use of ILES for grid-to-rod-fretting



- Predicted mean peak velocities within 5% of experiments





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Publications

- Publications
  - Integration of Hydra-TH in VERA (L2 Milestone), M. A. Christon, J. Bakosi, N. Barnett, M. M. Francois, R. B. Lowrie, R. Sankaran, LA-UR-12-22403
  - Hydra-TH User's Manual, M. A. Christon, J. Baksoi, and R. B. Lowrie, LA-UR-12-23181
  - Solution Algorithms for Multi-Fluid-Flow Averaged Equations, R. R. Nourgaliev, M. A. Christon, INL/EXT-12-27187
  - Hydra-TH Verification, Validation and Thermal-Hydraulics Benchmark Problems, J. Bakosi, M. A. Christon, L. Pritchett-Sheats, H. Luo, T. Xia and R. Nourgaliev, LA-UR-13-22017
  - Large-Scale Turbulent Simulations of Grid-to-Rod Fretting, J. Bakosi, N. Barnett, M. A. Christon, M. M. Francois, and R. B. Lowrie, CFD4NRS-4 conference, LA-UR-12-20281
  - Large-Eddy Simulations of Turbulent Flow for Grid-to-Rod Fretting in Nuclear Reactors, J. Bakosi, M. A. Christon, R. B. Lowrie, L. A. Pritchett-Sheats, R. R. Nourgaliev, submitted to Nuclear Engineering and Design, LA-UR-12-26572
  - Hydra-TH: A Thermal-Hydraulics Code for Nuclear Reactor Applications, R. R. Nourgaliev, M. A. Christon, J. Bakosi, R. B. Lowrie, L. A. Pritchett-Sheats, NURETH-15, Pisa Italy, May 12 - 17, 2013

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Presentations

- Presentations
  - A Prototypical Workflow for Grid-to-Rod Fretting Analysis with Hydra-TH, M. A. Christon, J. Bakosi, R. B. Lowire and R. R. Nourgaliev, LA-UR-13-20102
  - Thermal Hydraulics Methods and Hydra-TH Development, M. A. Christon, CASL Site Visit, LA-UR-13-20093
  - A Hybrid FEM/FVM Approach for Fully-Coupled Incompressible and Multiphase Flows, M. A. Christon, J. Bakosi, R. B. Lowrie, R. R. Nourgaliev, Advances in Computational Mechanics – invited lecture, LA-UR-13-21552
  - Multiphase Flow in Hydra-TH, R. R. Nourgaliev, M. A. Christon, and R. B. Lowrie, Two-Phase Flow Workshop, NCSU, Raleigh, NC, July 12 -13, 2012
  - Large-Scale Turbulent Simulations of Grid-to-Rod Fretting, J. Bakosi, N. Barnett, M. A. Christon, M. M. Francois, and R. B. Lowrie, CFD4NRS-4 conference, LA-UR-12-24534
  - Hydra-TH: A Thermal-Hydraulics Code for Nuclear Reactor Applications, R. R. Nourgaliev, M. A. Christon, J. Bakosi, R. B. Lowrie, L. A. Pritchett-Sheats, NURETH-15, Pisa Italy, May 12 - 17, 2013

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Observations & Concerns

- HPC Staff has been very helpful in resolving issues on Turquoise clusters
  - Some problems with the file system affecting restarts on Pinto, but final cause has not been diagnosed
- Desirable to have better support of ParaView on Turquoise machines
  - Large-scale problems require running ParaView on the clusters
  - Outstanding conflics with gcc and paraview modules
  - Desirable to have newer versions of paraview server available from views project
    - Time-consuming to build our own versions of the paraview server, and doesn't leverage HPC/views expertise

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Validation and Uncertainty Quantification (VUQ)

Brian Williams (CCS-6)



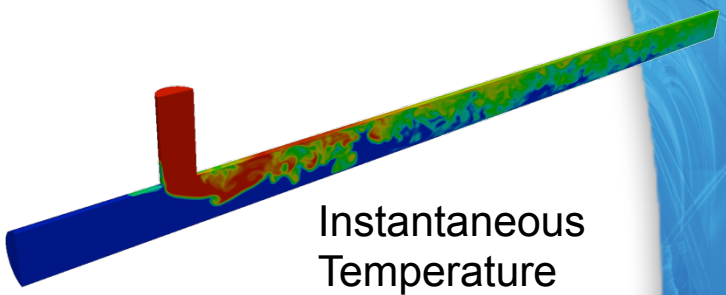


Separate Effects V&V for Hydra-TH
Brian Williams, L3.VUQ.SAUQ.P7.01

Description, Linkages, Completion Criteria

- Data-model integration for calibration and validation of the Hydra-TH LES turbulence model
- Milestone Linkages:
  - Support L3.THM.CFD.P7.02 “Single-Phase Benchmark Results with Hydra-TH”
- Completion Criteria
  - A report that describes implementation status, lessons learned and recommendations

Result Image or Graphic



Instantaneous Temperature

Technical Approach and Results

- Technical approach
  - Utilize data from a T-junction experiment
  - Conduct a mesh resolution study on Hydra-TH calculations of pressure differential across the junction
  - Calibrate four LES parameters (2 Reynolds numbers, 2 inlet temperatures) to temperature/velocity mean data
  - Validate calibrated Hydra-TH predictions of temperature/ velocity RMS data, with rigorous UQ
- Project schedule
  - Complete preparation of Hydra-TH input deck and DAKOTA scripts to drive VUQ studies, 03/29/2013
  - Complete Hydra-TH mesh resolution study, 05/31/2013
  - Complete Hydra-TH validation study, 09/30/2013

Personnel, Costs, Challenges/Issues

- Personnel
  - Brian Williams (Hydra-TH calibration/validation study)
  - Lori Pritchett-Sheats (Hydra-TH input deck, data)
  - Jozsef Bakosi (Hydra-TH turbulence modeling, statistics)
  - Mark Christon (study definition and guidance)
- Cost Estimate (person-months, dollars)
  - 20 person-weeks
- Issues and Challenges Encountered
  - Availability of computational resources
  - Troubleshooting Hydra-TH calculations

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Separate Effects SA/UQ/DA for Advanced VERA for CIPS
Brian Williams, (was) L3.VUQ.SAUQ.P5.04

Description, Linkages, Completion Criteria

- Calibrate Denovo to benchmark experimental data, varying thousands of uncertain cross-section (e.g. fission, scattering) and fission yield inputs
- Milestone Linkages:
  - Support L2.VUQ.P7.02, "UQ/DA study on a VERA Core Simulator component for CRUD analysis"
  - L2.VUQ.P4.01 for benchmark data ("Separate effects UQ/calibration/validation for Advanced VERA (Denovo) for CIPS")
- Completion Criteria
  - A report that describes implementation status, lessons learned and recommendations

Result Image or Graphic

	PSRF (Regular)	PSRF (ESM)
$\Sigma_{s,0}^{1\to1}$ (MOX)	1.04	1.01
$\Sigma_{s,0}^{1\to1}$ (Uranium)	2.39	1.01
$\Sigma_{s,0}^{1\to1}$ (H_2O)	2.15	1.00
$\Sigma_{s,0}^{1\to2}$ (MOX)	1.41	1.24
$\Sigma_{s,0}^{1\to2}$ (Uranium)	1.74	1.38
$\Sigma_{s,0}^{1\to2}$ (H_2O)	1.25	1.10
$\Sigma_{s,0}^{2\to2}$ (MOX)	23.91	1.00
$\Sigma_{s,0}^{2\to2}$ (Uranium)	15.62	1.00
$\Sigma_{s,0}^{2\to2}$ (H_2O)	18.34	1.00
Σ_f^2 (MOX)	4.73	1.00
Σ_f^2 (Uranium)	1.64	1.02
Multivariate	28.6	1.39

Table 1: Comparison of results for traditional method versus ESM

MCMC Convergence Assessment

Technical Approach and Results

- Technical approach
  - Utilize benchmark experimental data
    - LEU-COMP-THERM-008 (k-eff and relative pin powers)
  - Use Efficient Subspace Method for dimension reduction
  - Randomly sample gradients from input space to identify active subspace
  - Input calibration via Markov Chain Monte Carlo
  - MCMC efficiency via transformation of input parameters to active subspace and its orthocomplement
- Project schedule
  - Complete build of Denovo SUQ root, 02/28/2013
  - Complete MCMC implementation and testing, 04/30/2013
  - Complete calibration study and report, 05/31/2013

Personnel, Costs, Challenges/Issues

- Personnel
  - Brian Williams (MCMC methodology, implementation)
  - Bill Rust (LANL Denovo build)
  - Jason Hite (NCSU Denovo build, MCMC implementation)
  - Hany Abdel-Khalik (data, study guidance)
- Cost Estimate (person-months, dollars)
  - 20 person-weeks
- Issues and Challenges Encountered
  - Build of Denovo SUQ root
  - Availability of computational resources
  - Troubleshooting Denovo calculations

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Integration of Emulator-based Model Calibration Methodology into VERA

- Subcontract with UT-Austin PECOS Center to leverage Quantification of Uncertainty for Estimation, Simulation and Optimization (QUESO) library
  - Translate Matlab-based Gaussian Process Models for Simulation Analysis (GPMSA) software into the C++/MPI QUESO framework
  - Interface QUESO MCMC capabilities with GPMSA
  - Output MCMC and prediction results on a test case
  - Interface GPMSA/QUESO capability with DAKOTA
  - Performance period expires December 2012
- UT Subcontract continues through September 2013 under ORNL supervision
  - Complete integration of GPMSA capabilities into QUESO
    - Simultaneous calibration to multiple experiments
    - Metropolis within Gibbs GPMSA MCMC methodology
    - More flexible discrepancy modeling
    - Global sensitivity analysis via Sobol' decomposition
    - Emulator cross-validation
  - Integrate new MCMC capabilities into QUESO
    - DREAM
  - Interface new GPMSA/QUESO capabilities with DAKOTA
  - Demonstrate DAKOTA/GPMSA/QUESO on Hydra-TH T-junction application
  - Release to VERA (through DAKOTA)!!

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