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CASL Institutional Computing Report, CY2013

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

LA-UR-xx-xxxx

Materials Performance Optimization (MPO)

Chris Stanek (MST-8)

Consortium for Advanced Simulation of LWRs

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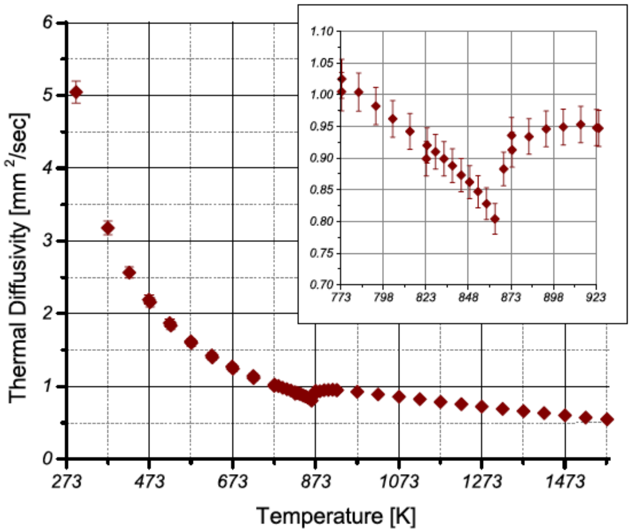
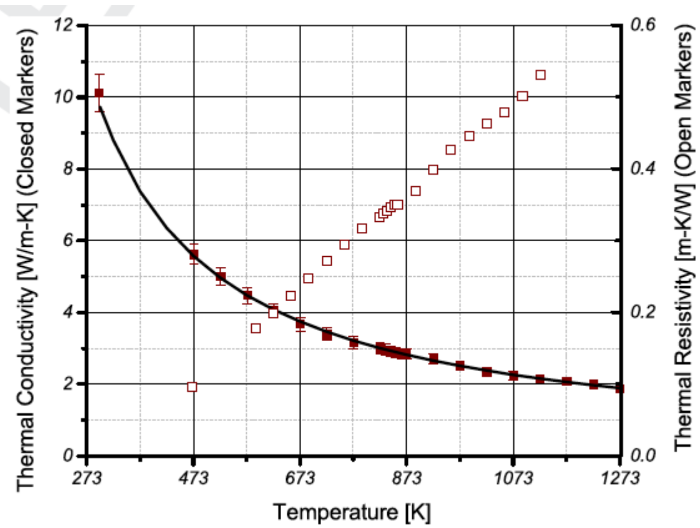
Thermal conductivity (κ) of $NiFe_2O_4$

Thermal diffusivity (α) and conductivity (κ) of $NiFe_2O_4$

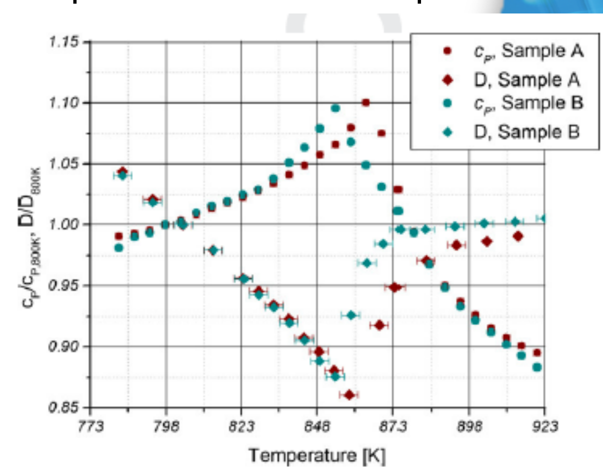
$$\kappa = \alpha \, \rho \, C_p$$





- DFT calculations were used for interrogating the thermal diffusivity and heat capacity at the Curie temperature as well as the variation between samples due to slightly different synthesis conditions.
- Calculations show that the sample variation are related to non-stoichiometry.

Variation in thermal diffusivity between samples at the Curie temperature



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 for CASL THM Milestones: 5 – L3, 3 – L2, 1 – L1 (L1 & L2 DOE reportable)
- s11_casl usage from 1/1/2013 – 1/1/2014
  - 3.35 Million cpu-hours used in 2011 (2.7% Utilization)
  - 18.58 Million cpu-hours used in 2012
  - 5.91 Million cpu-hours used in 2013

Machine	Hours Used	Percent Used
conejo	3,392,262.5	9.3%
mapache	926,131.0	3.0%
pinto	1,140,217.8	6.3%
mustang	450,875.4	0.4%

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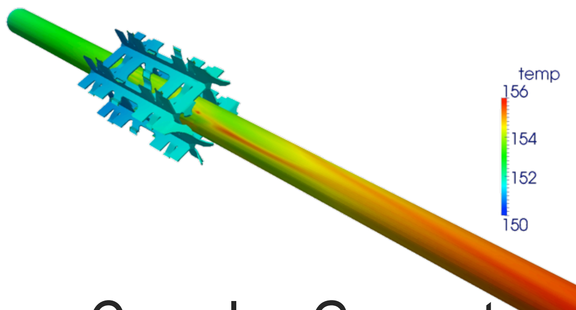
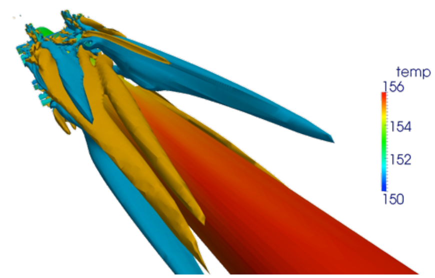
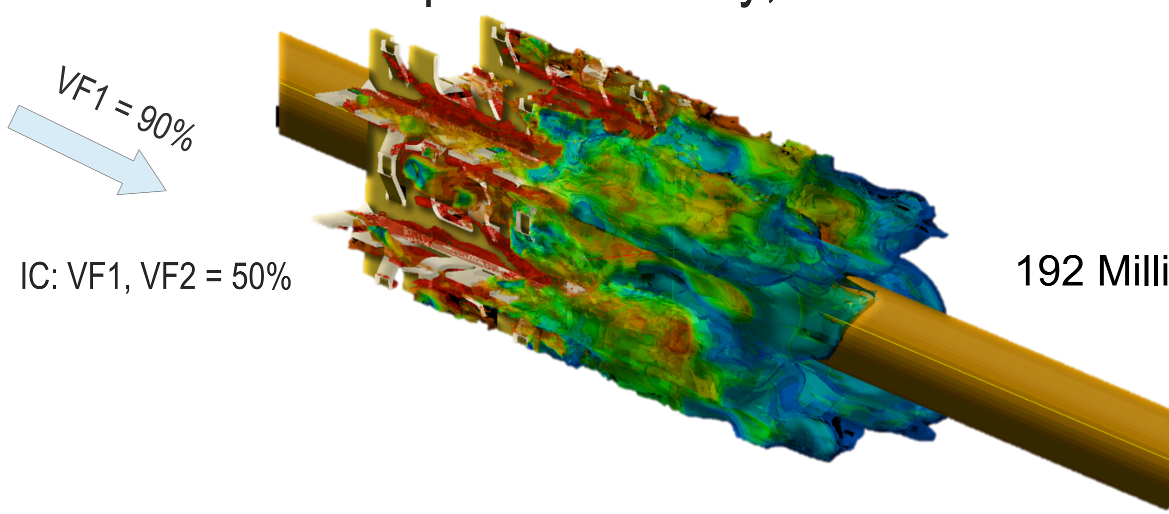
Impact on CASL Hydra-TH milestones

- Turquoise machines used for L1, L2 DOE reportable milestones, and supporting L3 milestones
  - Mesh scaling up to ~200 Million cells, two-phase flows
- Fully-implicit projection, RNG k-e model, Re ~ 4.0×10^5, $q_w = 10^6$ W/m^2





- MultiPhase Flow – Complex Geometry, Reactor Flow Conditions



Publications

- Selected Publications
  - CFD turbulence force calculations and grid-to-rod fretting simulation, R.Y. Lu, Z. Karoutas, M.A. Christon, J. Bakosi and L. Pritchett-Sheats, CASL-I-2012-0165-000, Consortium for Advanced Simulation of LWRs, Oak Ridge, Tennessee, Dec. 2012.
  - Hydra-TH advanced capabilities, J. Bakosi, M.A. Christon, L.A. Pritchett-Sheats, and R.R. Nourgaliev, LA-UR-13-20572.
  - Solution Algorithms for Multi-Fluid-Flow Averaged Equations, R. R. Nourgaliev, M. A. Christon, INL/EXT-12-27187.
  - 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, V. 262, pp 544-561, 2013.
  - Application of Hydra-TH, the CASL T-H code, for computing nuclear reactor spacer grids, E.L. Popov, M.A. Christon, and J. Bakosi, 2014 ANS Annual Meeting, Reno, NV, June, 2014.

Presentations

- Selected Presentations
  - Thermal Hydraulics Methods Focus Area, M. A. Christon, E. Balgietto, CASL Science/Industry Council Meeting, ORNL, Sept. 10-11, 2013.
  - Overview of Thermal Hydraulics and Hydra-TH Capabilities, M. A. Christon, PWROG Meeting, Westinghouse Electric Co., Cranberry, PA, Dec. 3, 2013.
  - Overview of Thermal Hydraulics Focus Area, M. A. Christon, CASL-NEAMS Technical Exchange, Argonne National Laboratory, April 22, 2013.
  - Projection (Based) Methods for Industrial Single and Multi-Phase Flows, M. A. Christon, J. Bakosi, R. R. Nourgaliev, R. B. Lowrie, L. A. Pritchett-Sheats, MIT, Applied Computational Fluid Dynamics and Heat Transfer Lecture Series, March 19, 2013 (Invited).

Observations & Concerns

- Slight downturn in use of resources for 2013, but anticipate increased use for 2014 as complete multiphase capabilities are rolled out
- ParaView support has improved slightly, but still relies heavily on views project for builds
- Desirable to have better support of ParaView on Turquoise machines
  - Large-scale problems require running ParaView on the clusters
- Desirable to open access to post testing results on Hydra/Hydra-TH to Hydra dashboard(s) in the future

Verification and Uncertainty Quantification (VUQ)

Brian Williams (CCS-6)

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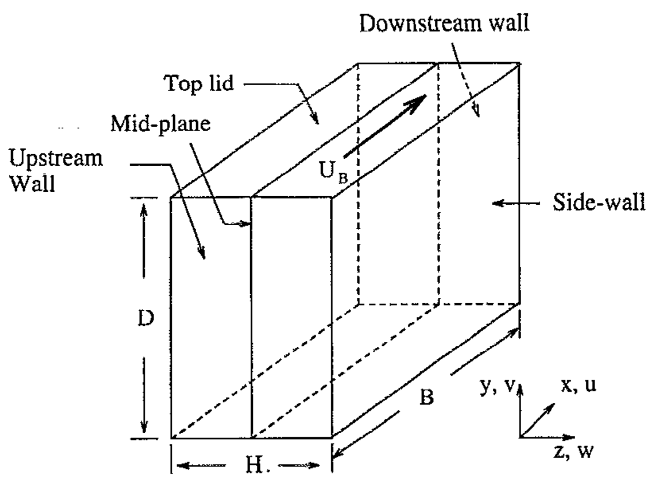
Deployment of VUQ Tools



Zang, Street, and Koseff (1993)
Lid-Driven Cavity

Large-eddy simulation of a lid-driven cavity flow at Reynolds number of 10,000

- **Hydra-TH** used for calculations
- **Smagorinsky (SSGS)** and **WALE** turbulence models
- **Percept** used to demonstrate solution verification
- **Dakota-QUESO-GPMSA** used to demonstrate surrogate-based model calibration

Smagorinsky (SSGS)			
Parameter	Nominal	Minimum	Maximum
C_s	0.18	0	0.36
Prandtl	0.8889	0.8	1
Schmidt	1	0.5	1.5

WALE			
Parameter	Nominal	Minimum	Maximum
C_w	0.5	0	0.6
Prandtl	0.8889	0.8	1
Schmidt	1	0.5	1.5

Demonstrate solution verification and model calibration tools

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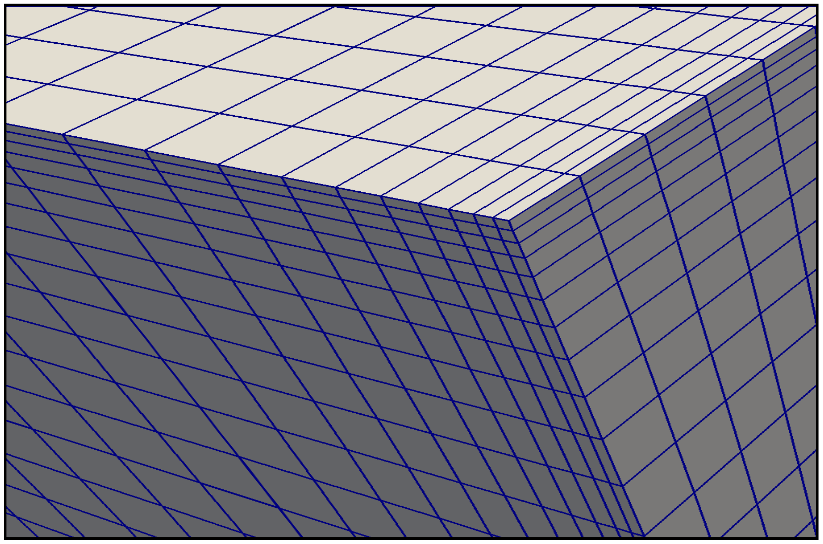
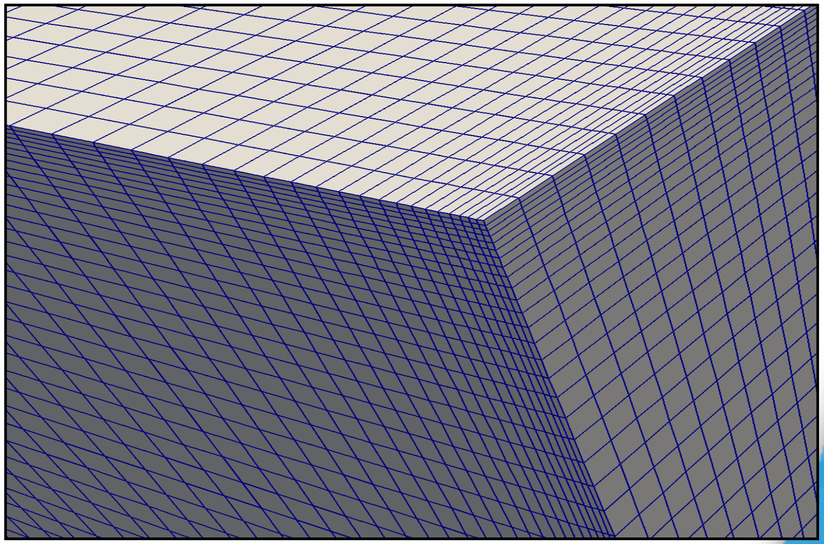
Solution Verification

Percept is a software package that provides tools for code and solution verification

In this study…

- Produce a uniformly refined sequence of grids
- Extrapolate the figure of merit (FOM) values as mesh size approaches zero
  - Mean velocity and Reynolds stress tensor
- Compute convergence rates of these FOMs with respect to mesh size





FY14: A Dakota/Percept interface is under development

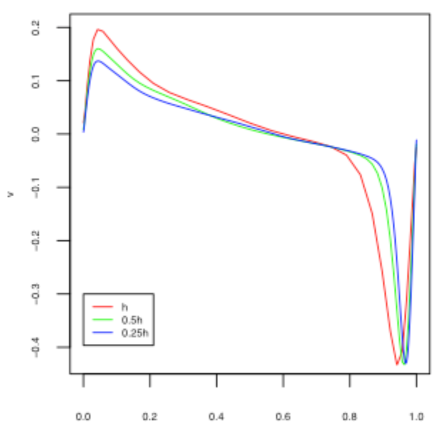
Convergence Analysis

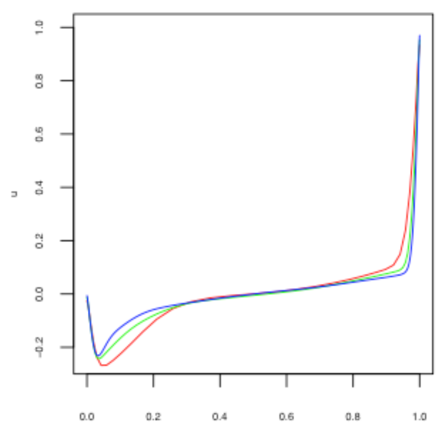
SSGS convergence rates	$v(x)$	<v'v'>(x)	<u'v'>(x)	u(y)	<u'u'>(y)	<u'v'>(y)
Median	1.0028	1.0056	1.0002	1.0002	N/A	N/A
Mean	1.0061	0.93699	0.75574	0.99905	.	.
Std. deviation	0.0081	0.32836	0.35614	0.011849	.	.

WALE convergence rates	$v(x)$	<v'v'>(x)	<u'v'>(x)	u(y)	<u'u'>(y)	<u'v'>(y)
Median	1.0007	N/A	1.0029	0.99965	N/A	N/A
Mean	1.1677	.	0.88577	0.75059	.	.
Std. deviation	0.3722	.	0.28467	0.35247	.	.

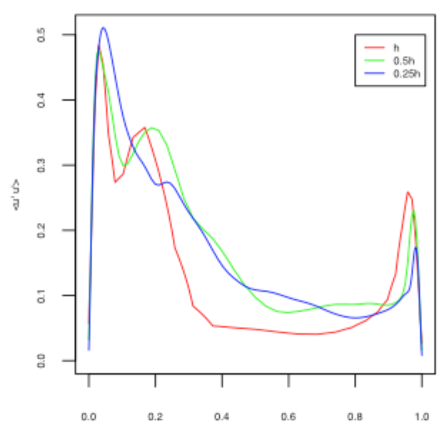
SSGS L2 norms mesh size	$\|\| \bullet \|\|_{L^2}$ $v(x)$	<v'v'>(x)	<u'v'>(x)	$u(y)$	<u'u'>(y)	<u'v'>(y)
h	0.018665	0.065560	0.030541	0.025155	0.033246	0.006287
½ h	0.012596	0.064237	0.018513	0.017049	0.045295	0.012929
¼ h	0.010043	0.033335	0.003693	0.012755	0.044755	0.005896

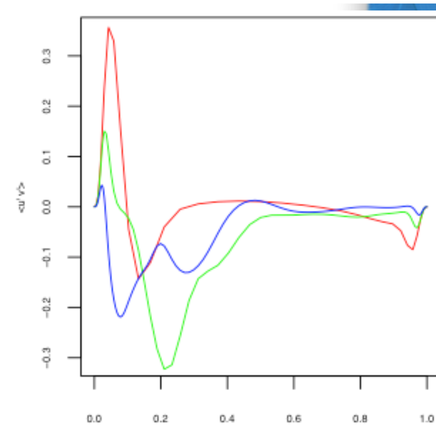
WALE L2 norms mesh size	$\|\| \bullet \|\|_{L^2}$ $v(x)$	<v'v'>(x)	<u'v'>(x)	$u(y)$	<u'u'>(y)	<u'v'>(y)
h	0.013202	0.045993	0.019010	0.009378	0.012933	0.000375
½ h	0.009515	0.049642	0.015989	0.010031	0.033860	0.007982
¼ h	0.008970	0.020846	0.001710	0.010648	0.028179	0.006516





SSGS mean velocity profiles





SSGS Reynolds stress tensor profiles

Percept uses the L2 norm to assess convergence

Probabilistic Model Calibration

Dakota is a software package that provides a unifying framework for optimization, sensitivity analysis, surrogate modeling, and uncertainty quantification (UQ)

QUESO provides sampling tools for exploring the probability distribution of uncertain model parameters that is consistent with experimental data and its errors

GPMSA implements a particular surrogate-based calibration methodology

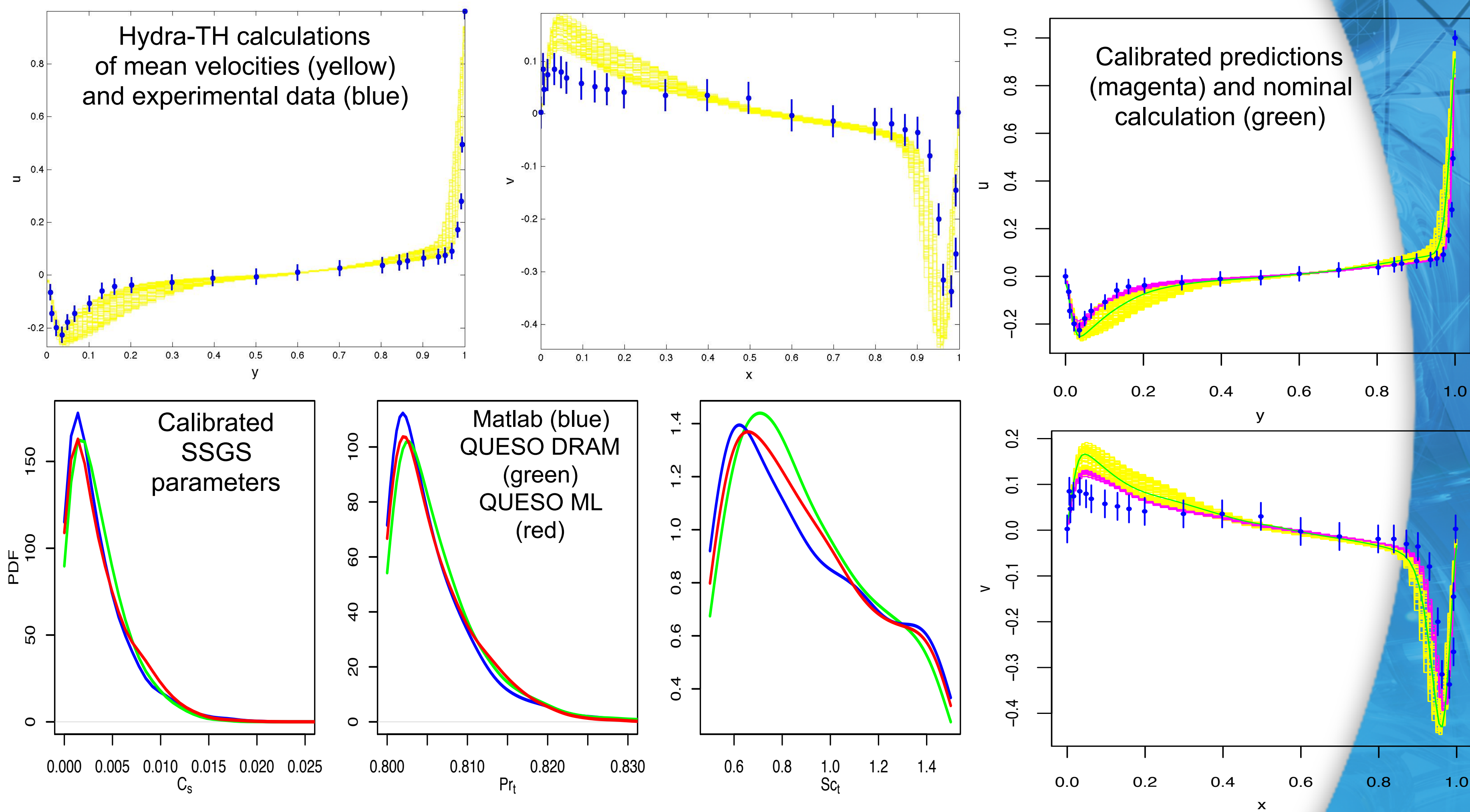
- FY13: Most GPMSA functionality interfaced with QUESO
- FY14: Dakota-QUESO interface completed

In this study…

- Dakota manages and processes results from multiple Hydra-TH runs
  - Generate 50-run Latin hypercube samples of SSGS/WALE parameters
  - Create Hydra-TH input decks for each run and a job list for user submittal
  - Extract FOMs from each Hydra-TH run via ParaView script
- QUESO-GPMSA produces calibrated parameter samples for UQ studies

FY14: Verified probabilistic model calibration capability

Calibration of SSGS Turbulence



Probabilistic calibration provides basis for FOM UQ studies

Looking Forward: FY15 and Beyond

- FY14: Mini-PIRTs conducted on challenge problems to provide subject matter input on important physics models, experimental data, and figures of merit
  - Progression problem 6, CIPS, PCI
  - RIA and LOCA up next
- Tailor “generic” VUQ plan (FY14 milestone) to each challenge problem
  - Appendix to challenge problem charters
- FY15: Full implementation of probabilistic model calibration capability
  - Complete implementation of GPMSA in QUESO
  - Complete verification tests of sampling algorithms in QUESO
  - Complete Dakota-QUESO interface
- FY15: Demonstrate dimension reduction capability for large input spaces
  - Hybrid sampling methods for ESM dimension reduction and probabilistic calibration

VUQ efforts are expanding to coupled codes and multiple data sources