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NEAMS - Validation Needs for Computational Fluid Dynamics

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Flow in a Pebble bed lattice next to a vessel wall

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Introduction

Thermal and Fluid Flow phenomena involve a wide range of length and time scales.

Resolving all scales for a realistic engineering system of interest is often computationally not feasible (*time scale separation*)

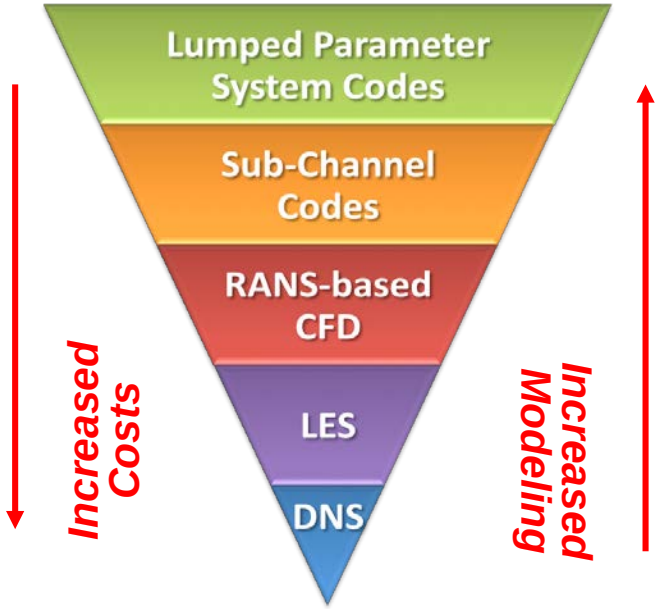
Hierarchical: validation requirements depend upon resolution of the technique.

e.g., PIV data for CFD, integral test data for system codes.

But Validation overall driven by specific problem, application, NOT the tool.

Validation for Multiscale modeling (involving more than one scale) completely unexplored.

Need for CONCURRENT validation data at multiple levels.



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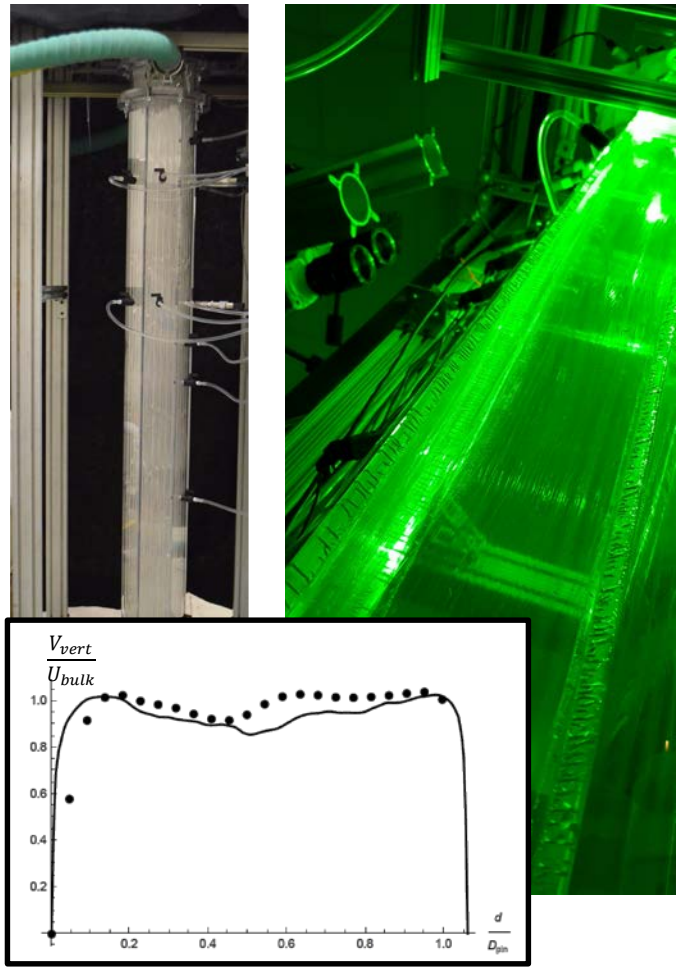
CFD-specific validation



PIV experiment 61-pin wire-wrapped fuel assembly and comparison.

CFD validation needs differ depending on turbulence modeling approach.

(1) **RANS** validation needs involve detailed, high resolution velocity fields and rms of the velocity components and the shear stress.

(2) **LES/DNS** benefit from additional time resolved data (spectra, time histories) and higher momenta (skewness, kurtosis) as well as Probability density functions. Proper Orthogonal Decomposition.

Additional needs come from heat transfer/two-phase/FIV:

(1) **Heat transfer**: information on thermal stresses is very valuable especially for non-unity Prandtl number fluids. CONCURRENT temperature and velocity measurements are preferred.

(2) **Two-phase**: high-resolution void fraction measurements (more later).

(3) **FIV**: time resolved acceleration, high-resolution pressure and shear measurements at the wall.

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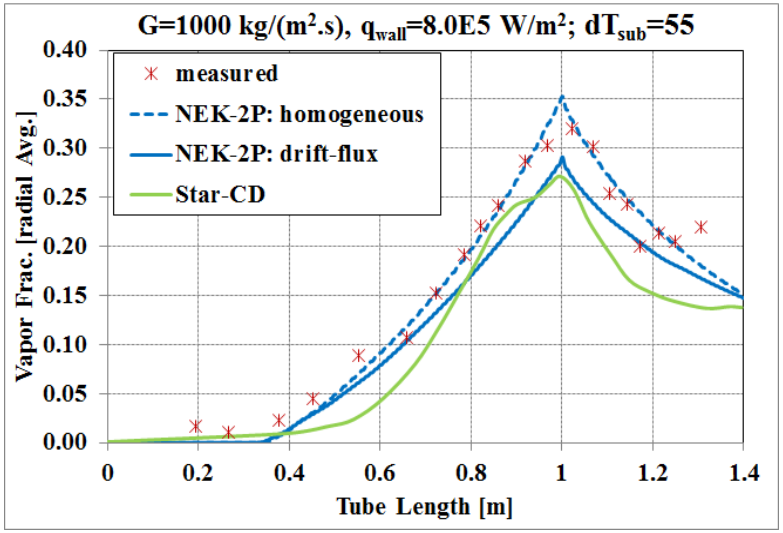
Two-phase flow validation needs for CFD (Eulerian-Eulerian)

- **High resolution void fraction**
- **Nucleation site density, Bubble departure size, Bubble departure frequency.**
  - The above three measured simultaneously in an experiment with a well characterized surface
  - Forced convection, or at least oriented vertically. The current state of boiling modeling relies on correlations developed for pool boiling conditions.
- Need for **high-quality experiments performed at high pressures** in the presence of boiling.



Nek-2P (Nek5000 two-phase flow version) results for the Bartolomei experiment

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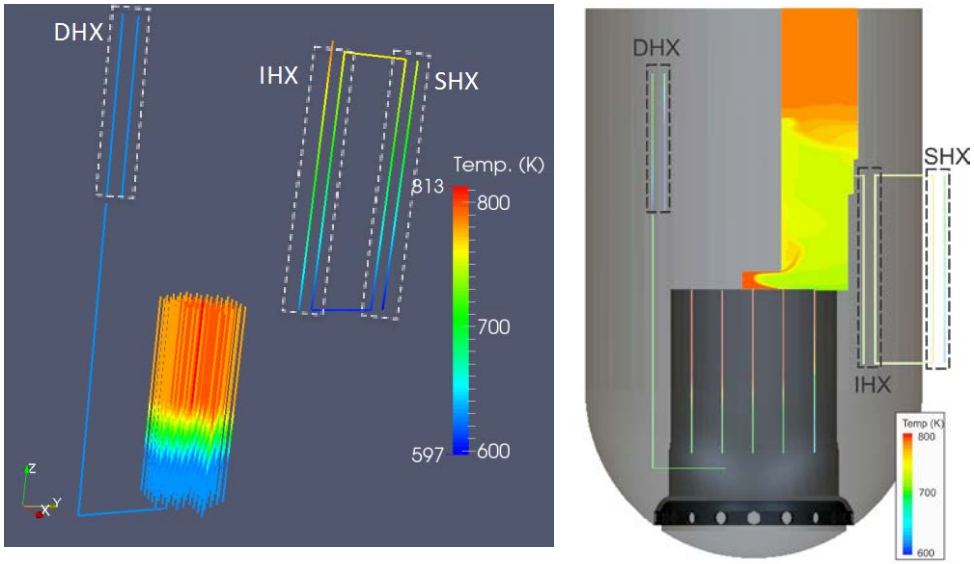
Multiscale validation needs

- Ideally, need for CONCURRENT validation data at multiple levels. Integral test facilities instrumented to provided local data in a component. Very little available. In general very little available at large scale (e.g., pools).

- Other specific needs for SAM and its multiscale capabilities (they will help for CFD too):
  - 3D flow and thermal mixing and stratification data in large enclosures for SAM 3D reduced-order model
  - System-level natural circulation loop data;



Simulation of ABTR PLOF (Coupled CFD+SAM)

- **SAM is A trustworthy and practical plant-level system analysis tool for advanced reactors** (SFR, LFR, MSR/FHR);
- Built-on MOOSE framework and other modern software libraries;
- Flexible multi-scale multi-physics integration with other high-fidelity tools.

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Nek5000: Open Source Spectral Element Code

Spectral Element Discretization: High accuracy at low cost

- Highly respected code in Fluid Dynamics Community. > **300 registered users**. Europe and United States mostly.
- Open source.
- Portable: runs on a laptop as well as a supercomputer.

Particularly well suited to LES and DNS of turbulent heat and flow transfer

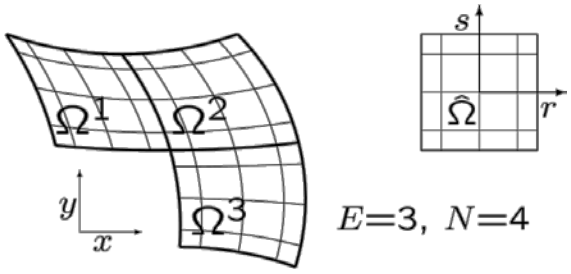
- Incompressible and Low-Mach, combustion, MHD, conjugate heat transfer, moving meshes, RANS, two-phase, CHT, buoyancy, adjoints,…
- New features in progress: compressible flow (GE), LBM, AMR, other meshing options.
- **LES typically done with explicit filtering (~hyper-viscosity), wall-resolved**

Exceptional **scaling**

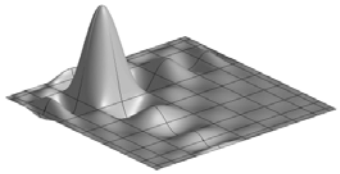
- 1999 Gordon Bell Prize.
- recently run with > 106 MPI processes.
- R&D100 awards in 2016.

High order method

- Local Polynomial Nodal Basis: Lagrange polynomials on Gauss-Lobatto-Legendre (GLL) quadrature points. for stability (not uniformly distributed points). **Implies a 2 level mesh.**
- Exponential convergence (100x reduction in error for 2x increase in resolution).
- Fast operator evaluation.



Example of the "2-level" mesh typical of Nek5000



2D basis function, N=10

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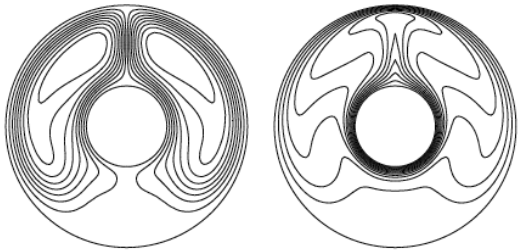
Nek5000: Resources and Verification

Code can be downloaded at:

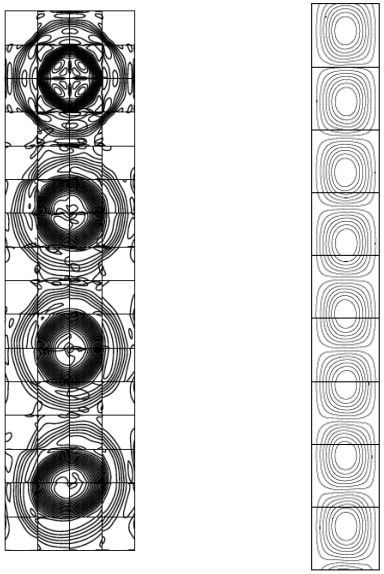
https://nek5000.mcs.anl.gov

Also available is a **manual** on the same website.

User community: mailing list, code snippets shared, regular user meetings (5th user meeting in 2016).



2 convection, vortex propagation, Rayleigh-Benard



Extensive Regression testing

- Small batch of regression test is run on each commit. Commits are accepted only if they clear the short regression test.
- **932** longer tests (verification, basic validation, performance) are performed overnight and continuously monitored.
- New features are associated to new tests. **Most new features are implemented through user code**.
- Stable releases.
- Bug fixes and new features documented on github.

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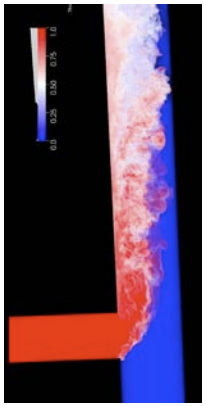
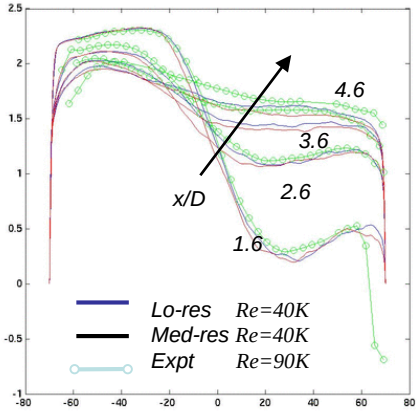
Current Validation Strategy

International Benchmarks

OECD blind benchmark against T-junction experimental data (Ranked #1 in temperature prediction).





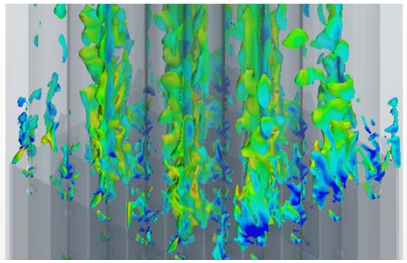
International Collaborations

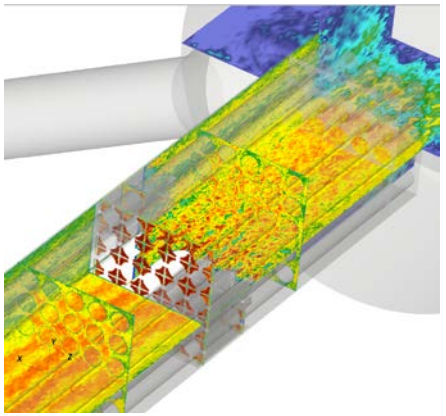
INERI, SESAME, …

Industrial Collaborations

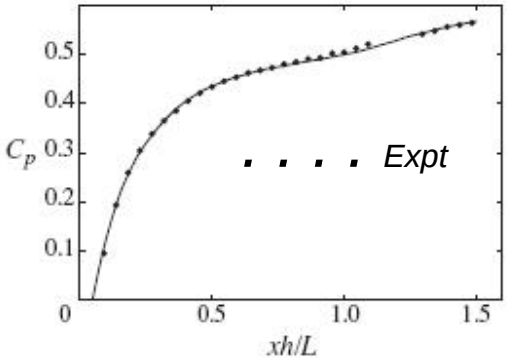
Example: collaboration with Westinghouse, **Nuscale**, etc..
NDA with several companies

OECD blind benchmark against fuel assembly experimental data (Ranked #1 in turbulence predictions)

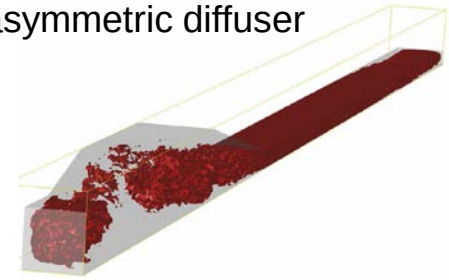




Users



Pressure Recovery in an asymmetric diffuser



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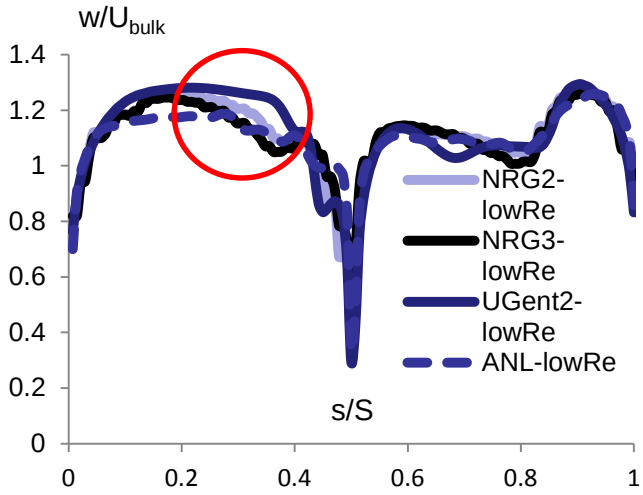
RANS: Lack of data leads to code-to-code comparison

For complex geometries CFD-grade data is often not available.

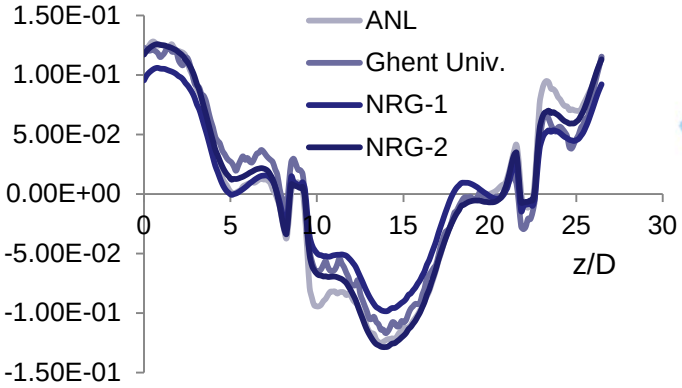
- RANS approaches can benefit from comparison with DNS/LES

International collaboration (INERI) centered on wire-wrappers.

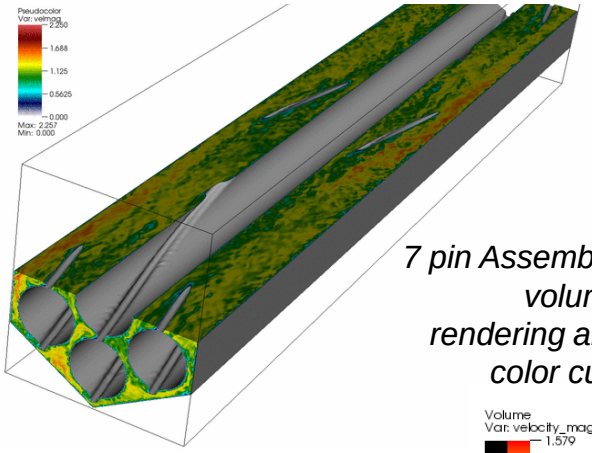
- Comparison between commercial codes and Nek5000
- Results are being used in the design of MYRRHA
- **Need for resolved velocity and rms data.**



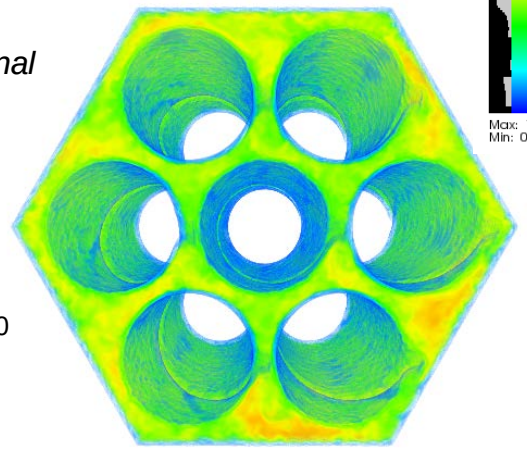
7 pin Assembly: streamwise velocity on diagonal



7 pin Assembly: Average Cross-flow



7 pin Assembly: volume rendering and color cuts



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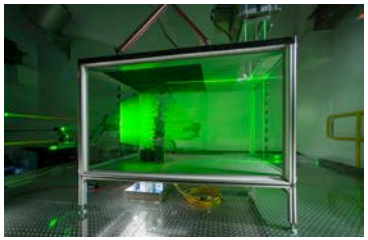
Thermal-striping and Mixing

Simulations of the MAX experiments

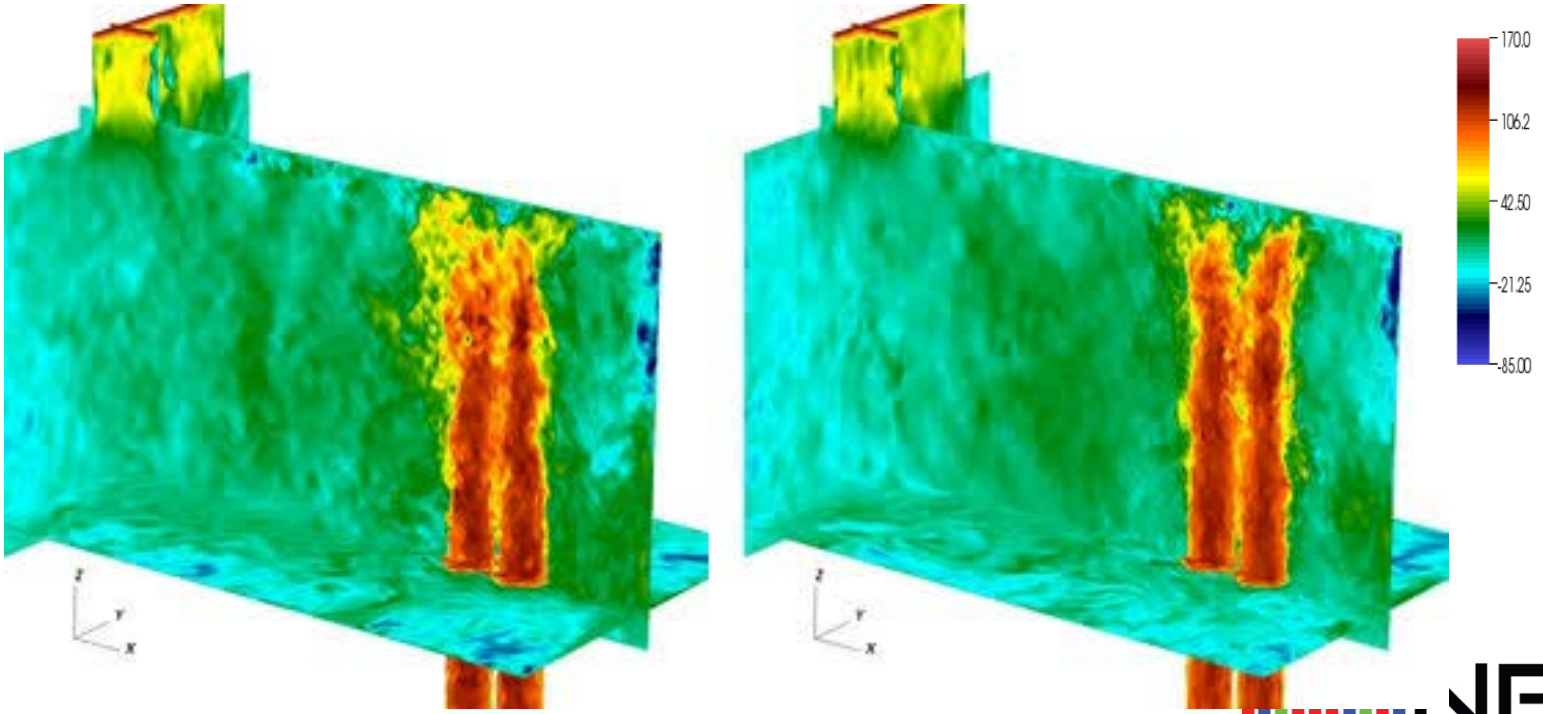
Accurate predictions of stability of the jects.

Successful concurrent experiment with predictive simulations (heat transfer in ongoing)



Thermal striping

Prediction of creep (with Diablo)



Vertical velocity

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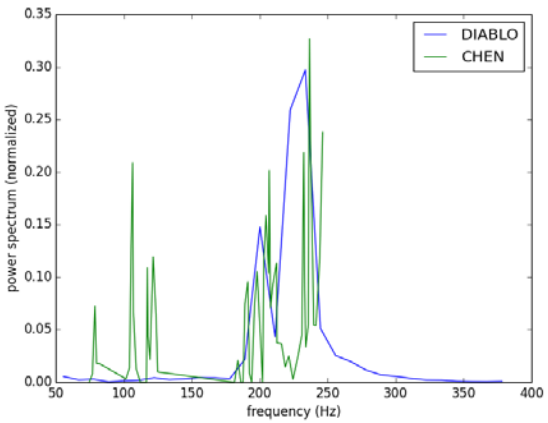
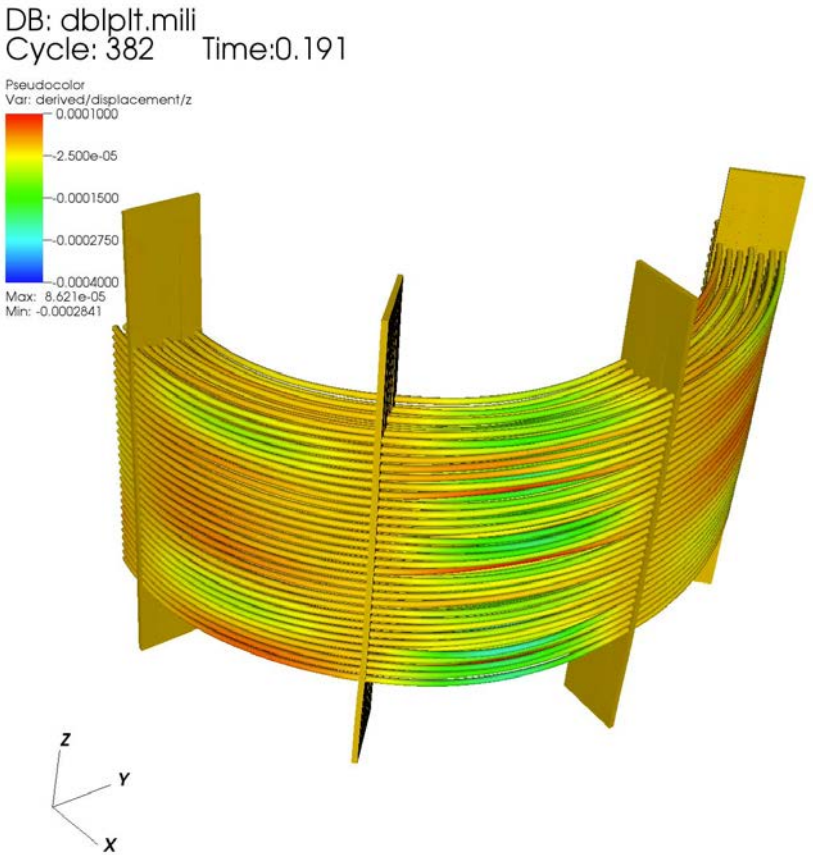
FIV: Validation on legacy data

- Use Nek data to drive dynamic simulations in Diablo.
- Data transferred (~150 Gb) over ~10M points.
- Reasonable PSD accuracy (huge geometric uncertainty in legacy experiments).
- New modern experiments needed (time resolved acceleration), detailed, resolved pressure and shear measurements at the wall.





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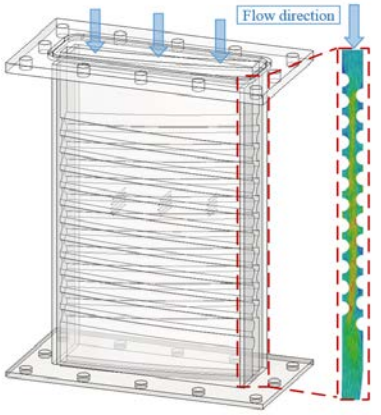
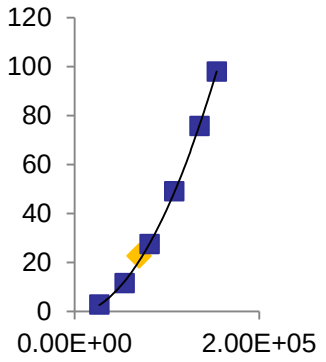
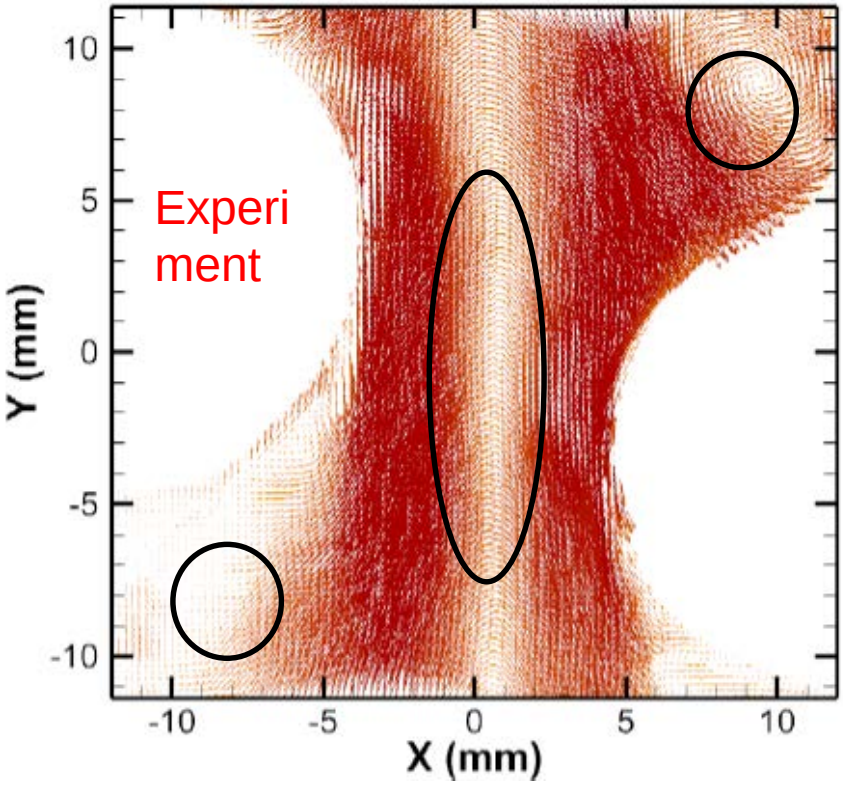
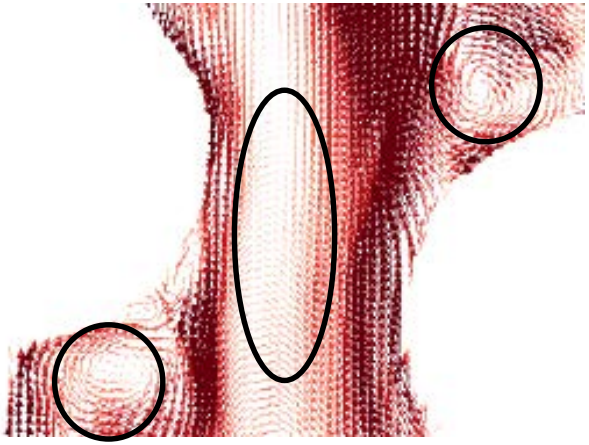
More than line comparisons: POD

- Flow in a helical coil steam generator.
- Complex, pulsatile behavior. Vortices change size. Good comparison between principal POD modes.









Nek5000

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