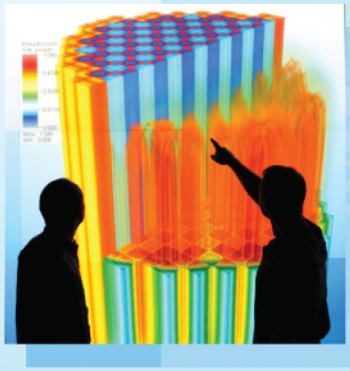
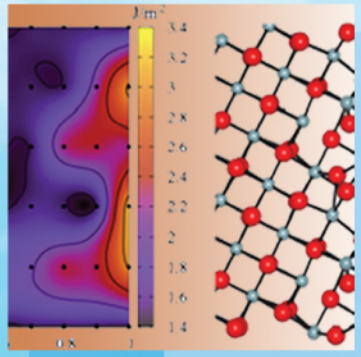
CASL-U-2013-0192-000-b

Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

A Study of the Role of Adjoint-Equipped CFD in VUQ Analysis of Channel Boiling Simulations

Krzysztof Fidkowski

University of Michigan

Milestone L3:THM.CFD.P7.08

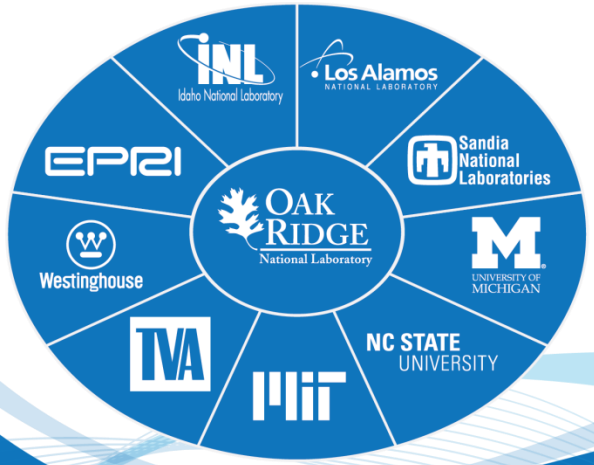
November 21, 2013

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

L3-THM-CFD-P7-08
A Study of the Role of Adjoint-Equipped CFD in VUQ Analysis of Channel Boiling Simulations

Milestone owner: Krzysztof Fidkowski, U. Michigan

Additional personnel: Isaac Asher, U. Michigan



U.S. DEPARTMENT OF ENERGY
Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

Milestone Execution Responsibility & Personnel

- Contact: Krzysztof Fidkowski, U. Michigan
- Focus Areas (FAs): THM
- Graduate Student: Isaac Asher, U. Michigan

Milestone Description

- **Goal:** Study the use of adjoint methods in numerical simulations of boiling flow for sensitivity calculations and error estimation
- **Context:** 1D drift flux model discretized with a discontinuous FEM
- **Assessment:**
  - Can we estimate numerical errors accurately?
  - Can we adapt to predict outputs better than uniform mesh refinement?
- **Relevance:** we need a handle on numerical errors to assess modeling errors in boiling simulations, which have complex physics
- **Timeliness:** we are running boiling simulations as part of CASL

Milestone Linkages

- No direct linkages

Milestone Execution Plan and Technical Approach

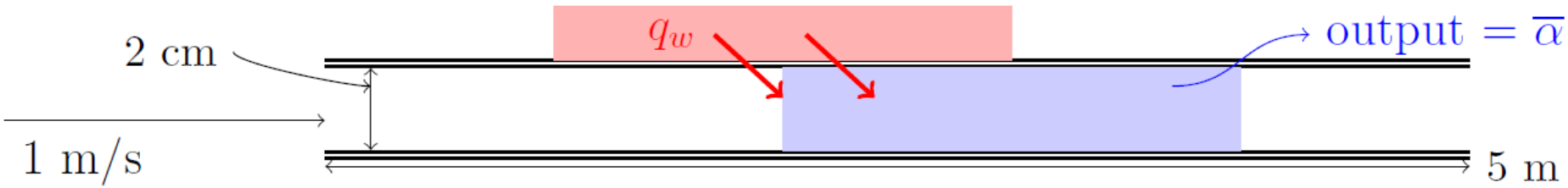
- 1D multiphase CFD model implemented and verified [Nov.30, 2012]
- Discrete adjoint implemented in the 1D code [December 31, 2012]
- First version of 2D multiphase CFD code implemented [March 31, 2012]
- Discrete adjoint for 2D multiphase code implemented and tested [April 30, 2012]
- Local sensitivity studies of 1D and 2D boiling using adjoint information [May 31, 2012]
- Error estimation using adjoints in 1D and 2D simulations [July 31, 2012]
- Preliminary results for parameter design optimization of a channel flow problem using adjoint-derived gradients [August 31, 2012]
- Milestone writeup [September 30, 2012]

Limited resources prevented 2D extension or optimization application; these are ongoing now as part of another project.

Personnel responsible: Krzysztof Fidkowski and Isaac Asher

Milestone Results: Problem Setup

- One-dimensional problem setup (*z* is to the right):



- Output, *J*, is a void fraction integral:

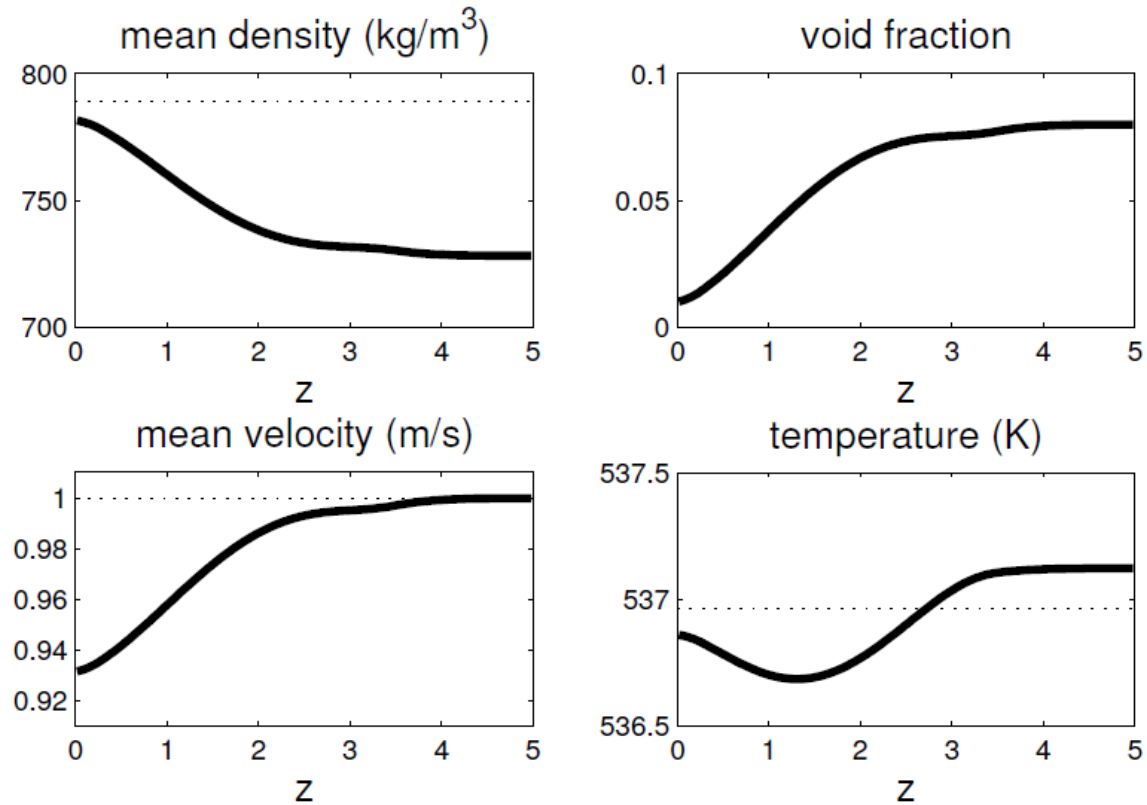
$$J = \int_2^4 \alpha(z)dz$$

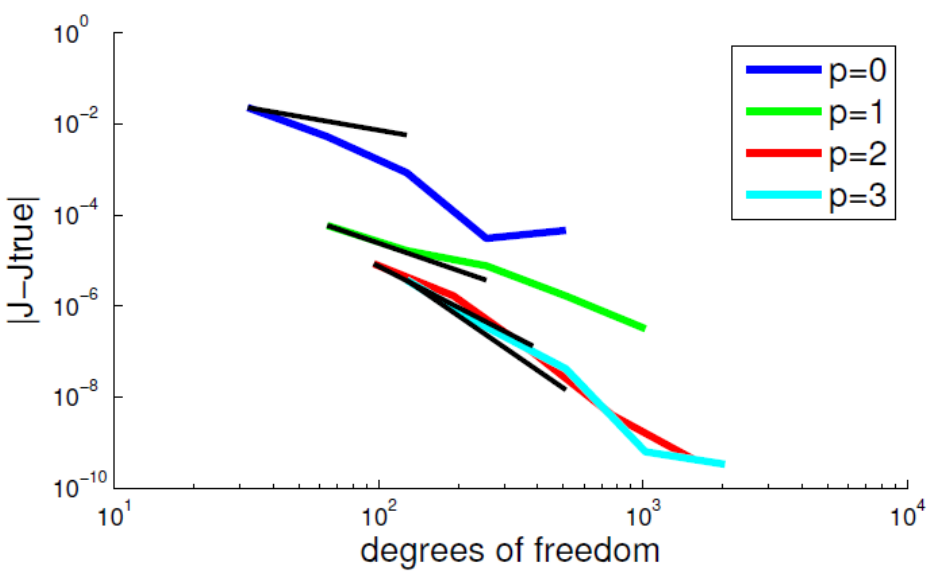
- Some details:
  - 4-eqn drift-flux model of Ishi and Hibiki (2006), subcooled boiling similar to PATHS
  - Local discontinuous Galerkin FEM discretization; steady-state Newton solver

Milestone Results: Primal Solution

Sample solution

- p=2 approximation
- 16 elements
- 7-9 orders of mag. residual drop





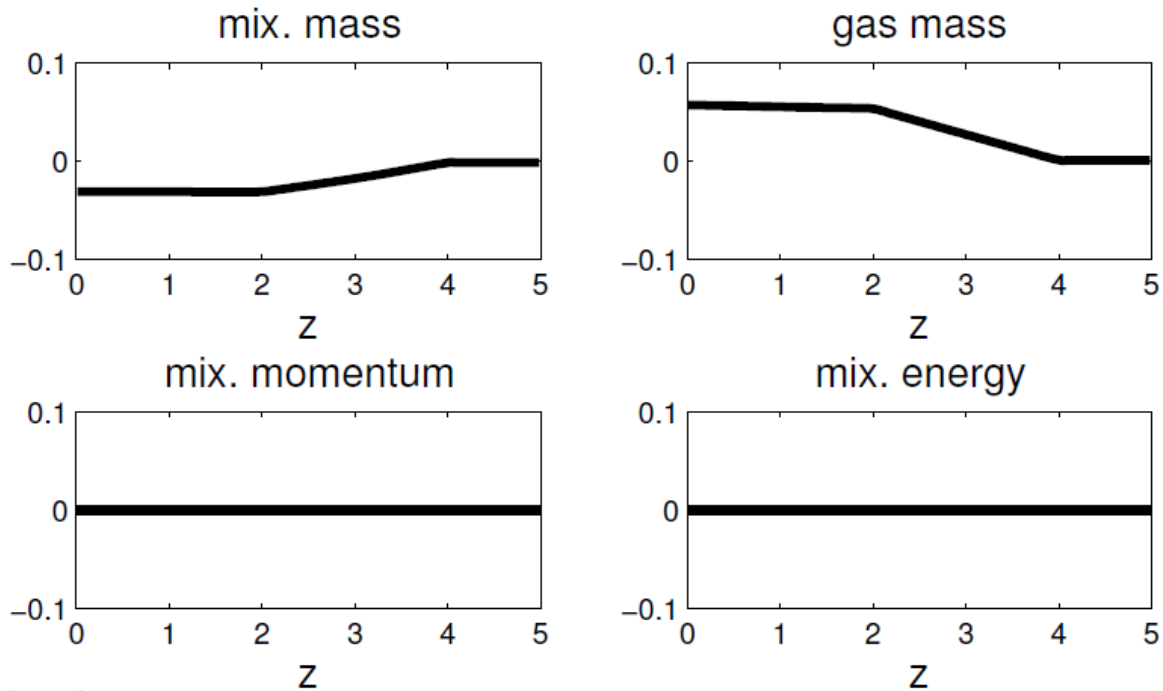
Convergence

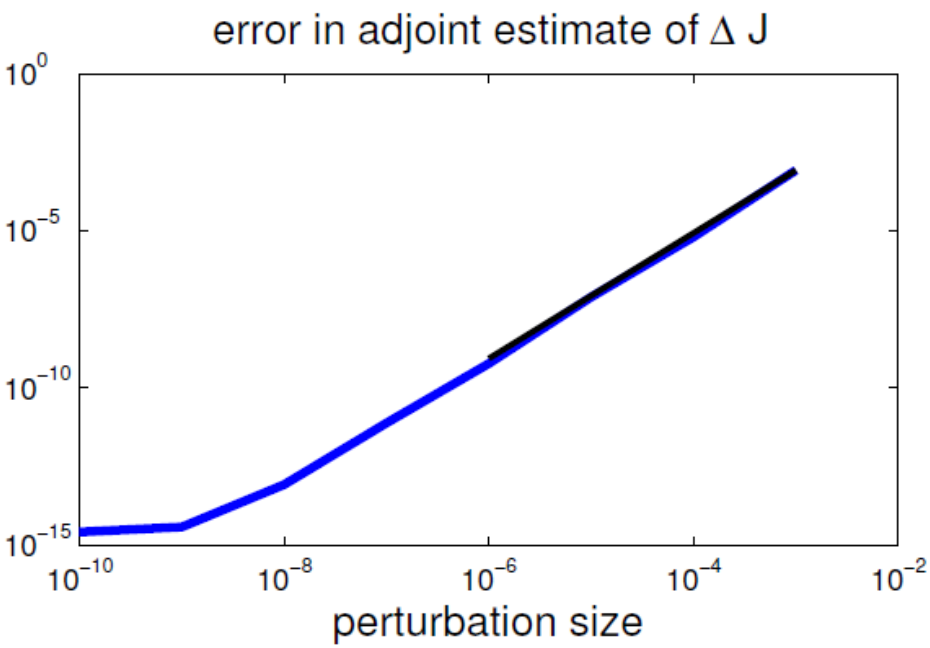
- Uniform mesh refinement
- Black lines: order p+1 rates
- Expected rates attained

Milestone Results: Adjoint Solution

Sample discrete adjoints

- Components associated with equations
- Tell us sensitivity of J to residual perturbations in those eqns





Adjoint verification

- How accurate are our sensitivities?
- Black line: 2nd order
- Expected rates attained until machine precision

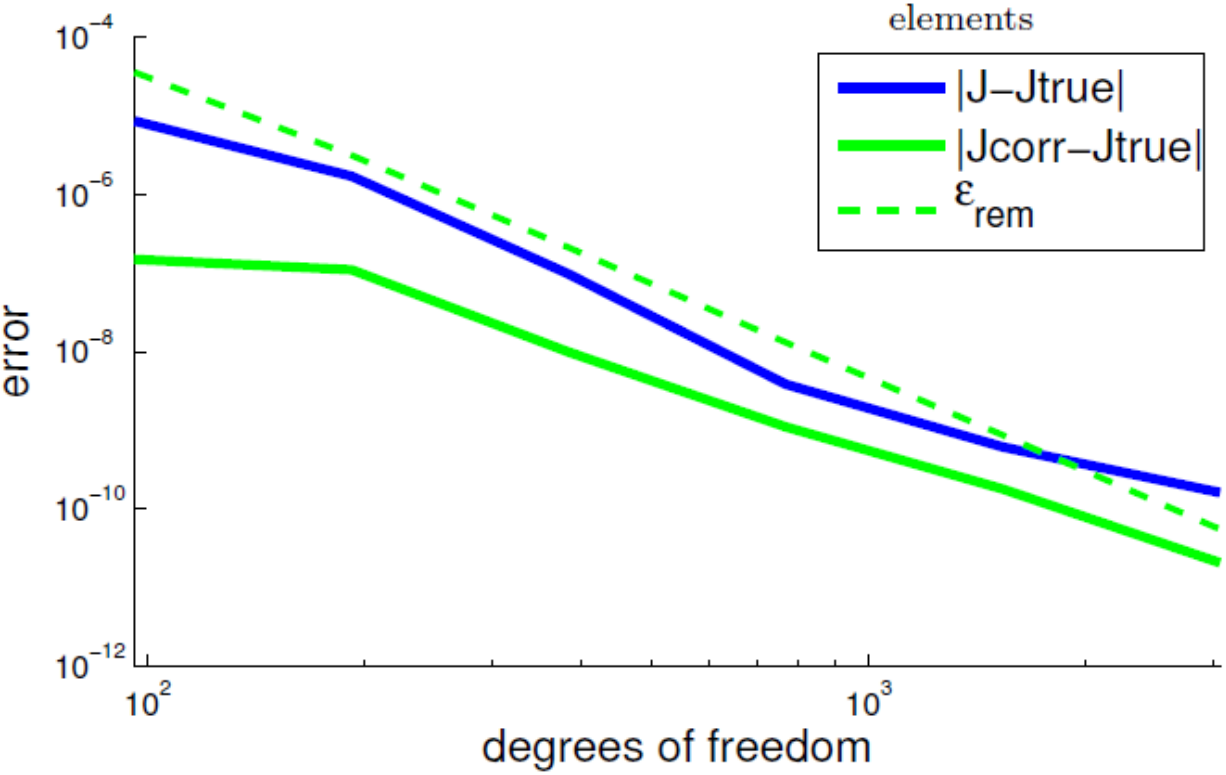
Milestone Results: Output Error Estimates

We solve for a discrete adjoint (on a fine space, p+1)

$$\Psi = \left(\frac{\partial R^T}{\partial U}\right)^{-1} \frac{\partial J}{\partial U},$$

and use it to estimate the output error:

$$J_{\text{true}} - J(U) \approx \sum_{\text{elements}} \Psi_{\text{fine}}^T R_{\text{fine}}(U)$$



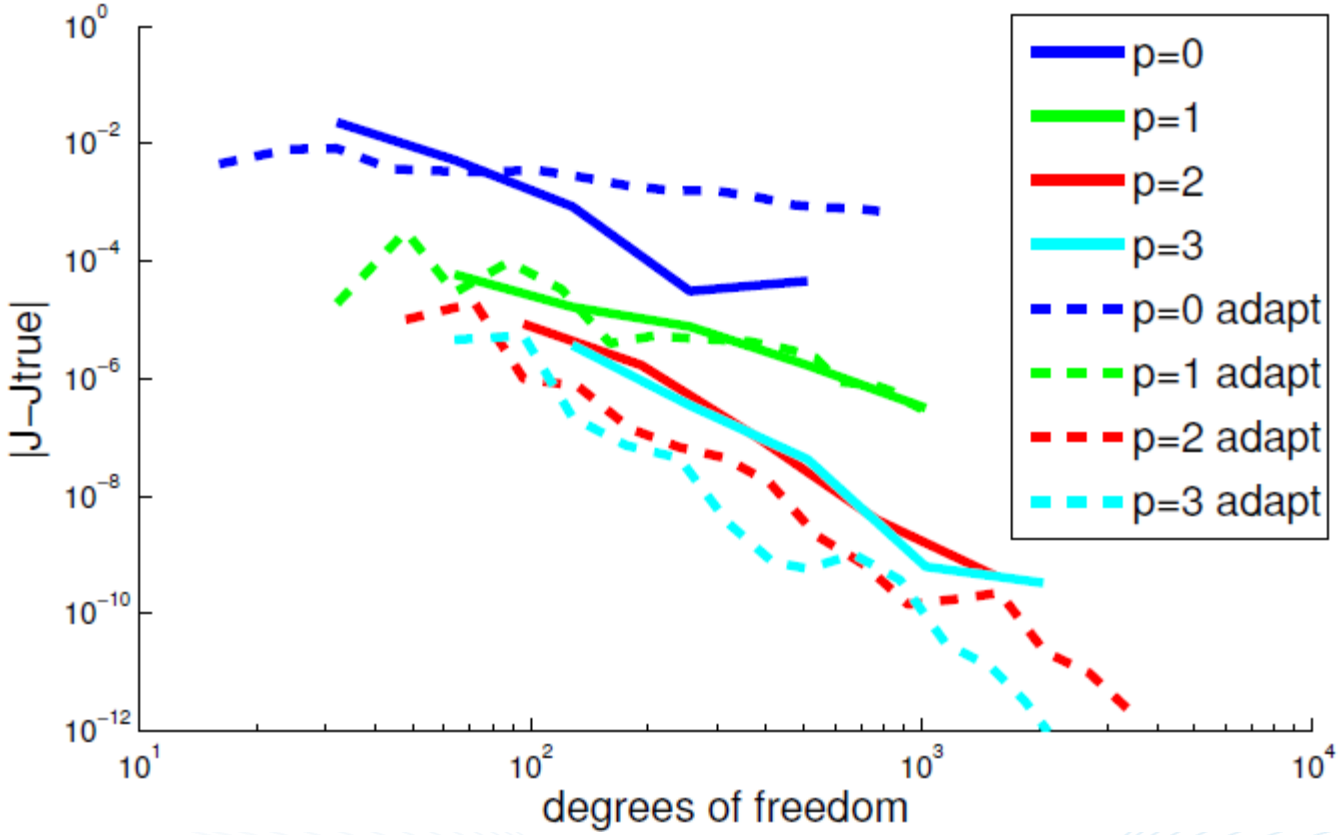
Uniform refinement convergence study for p=2

- J_{true} = exact output
- J = computed output
- J_{corr} = output corrected with error estimate
- ε_{rem} = remaining error estimate (we adapt on this)

Milestone Results: Adaptive Refinement

Strategy

- Error indicator = error estimate localized to elements
- We adapt for a fixed growth of elements per iteration



Convergence of corrected output with adaptive refinement

Milestone Completion

- Completion metric: milestone report
- Currently preparing a journal paper with results for an array of channels

Milestone Discovery and Innovation

- Non-planned results:
  - Roe solver for drift flux functions
  - Adjoint-consistent boundary conditions for 1d channel simulations

Milestone Lessons Learned

- 1D does not showcase adaptive capability that well (not too many choices for refinement)
- An extension to multiple channels helps show the power of adaptivity (some channels do not need to be refined)
- We need to extend our work to two and three dimensions to demonstrate better performance.