Computationally Efficient Prediction of Containment Thermal Hydraulics Using Multi-Scale Simulation

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Co-PIs (NUC university):
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- Igor Bolotnov (North Carolina State University)

Graduate Students:
- Botros Hanna
  - Pursuing PhD; passed Prelim
- Han Bao
  - Pursuing PhD; passed Qualifying
The modeling approaches used in the nuclear industry include system codes and Computational Fluid Dynamics (CFD) codes. CFD codes have the advantage of capturing three dimensional flow behavior, but they are computationally expensive, especially for containment thermal hydraulics. It is infeasible to use CFD for containment thermal-hydraulics.

a. The objective of this project is to learn how to use Coarse Grid simulations in analysis of containment thermal-hydraulics, without loss of essential information. Two projects on this LDRD are pursuing this.


b. Approach:

• Hanna’s work so far: Using coarse-grid and fine-grid simulation results, apply machine learning to develop a model of the correction we need to apply to coarse-grid results.

• Bao’s work so far: Use coarse-grid and fine-grid results to develop an expert system capable of recommending a combination of meshing and X that will yield an optimal result

c. Benefit:

• Using CG-CFD rather than CFD enables us to simulate many time histories, which we need to do in order to adequately explore issue spaces of interest (RISMC-style analysis)
**Simulating Containment Thermal Hydraulics (CTH) using CG-CFD**

A conceptual framework for simulating CTH with CG-CFD. The focus of this work is highlighted in yellow.

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
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<tbody>
<tr>
<td>1-</td>
<td>Coarse grid simulation of each single potential containment phenomena.</td>
</tr>
<tr>
<td>2-</td>
<td>A Library of coarse grid results for each phenomena is created.</td>
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<tr>
<td>3-</td>
<td>Fine grid simulation of each single potential containment phenomena to create correction for each coarse mesh phenomena.</td>
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<td>4-</td>
<td>Coarse grid simulation of the containment scenario.</td>
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<td>5-</td>
<td>Pattern recognition is performed given the library of coarse grid results.</td>
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<tr>
<td>6-</td>
<td>A correction for each coarse grid phenomena is performed.</td>
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<tr>
<td>7-</td>
<td>Because of the interplay between different phenomena, blending functions will be needed.</td>
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</tbody>
</table>

A snapshot of the velocity (in y) profile in a three dimensional quasi steady state turbulent flow in a lid driven cavity. The lid is moving in the X direction. The profile is computed by LES with dynamic Smagorinsky model with fine grid (left) and a coarse grid (right). The fine grid result is mapped to coarse grid (in the middle).
Technical Discussion-2

- Goal 1 of OMIS: Error Estimation of FOM
- Some consideration:
  - Neuron number (1 hidden layer).
  - Evaluation criteria for error estimation:
    1. MSE (mean and variation).
    2. Uncertainty bound.
- 4 different neuron numbers: 5, 10, 20, 50.
- Sample size: 100.

\[ \text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_{\text{real}} - y_{\text{predicted}})^2 \]

<table>
<thead>
<tr>
<th>Neuron Number</th>
<th>Training MSE Mean</th>
<th>Test MSE Mean</th>
<th>STD of Test MSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>8.50E-05</td>
<td>9.61E-05</td>
<td>2.92E-05</td>
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<tr>
<td>10</td>
<td>2.46E-05</td>
<td>7.13E-05</td>
<td>3.55E-05</td>
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<tr>
<td>20</td>
<td>1.41E-05</td>
<td>1.50E-04</td>
<td>8.75E-05</td>
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<tr>
<td>50</td>
<td>1.23E-05</td>
<td>1.29E-04</td>
<td>8.56E-05</td>
</tr>
</tbody>
</table>

Temperature Distribution of Case 4 with Different Meshes

Temperature Distribution of Case 4 with Different Models
Technical Discussion - 3

- **PhD Students Working on This Program:**
  - Botros Hanna, Han Bao
  - *Botros Hanna passed his prelim on June 30 with Bob Youngblood attending as a committee member*

- **Reports:**

- **Papers:**
Conclusion

• This Fiscal Year:
  – Hanna’s work will continue along present lines (discussed in progress report; add turbulent natural convection as a case study)
  – Bao’s work will continue as planned (with additional focus on predictive capability)

• Next Fiscal Year:
  – OMIS (Bao):
    • Improve OMIS framework; Develop and analyze simplified demonstration scenario for CTH (such as gas mixing, stratification and mixing and condensation); Perform OMIS application on the containment experiment (POOLEX/PPOOLEX and PANDA experiment).
  – Coarse-Grained CFD (Hanna):
    • Add another case study (turbulent natural convection); Improve quantification of confidence in the predictions; investigate “well-posedness” of the data-driven model.
    • Hanna will submit and defend his thesis
  – A journal article will be written and submitted