DISTLR [Directed Intelligent System for Targeted Lagrangian Relaxation] First Results in KULL

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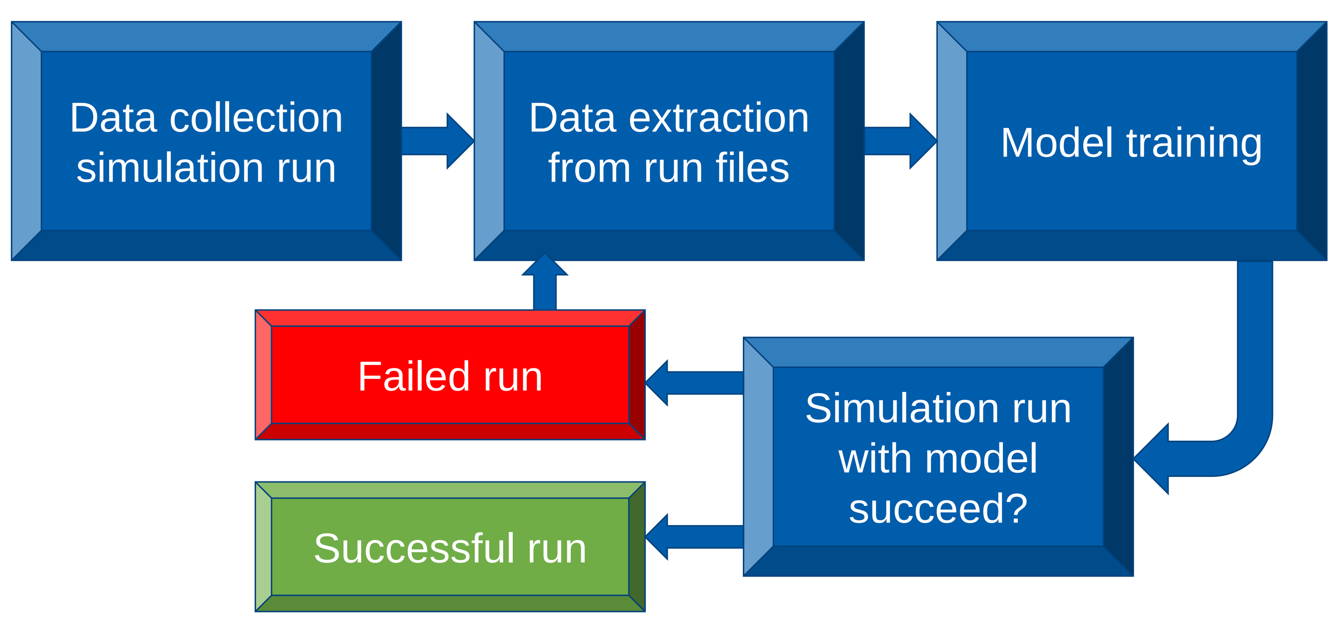
The KULL multi-physics code (like many other HPC simulation codes at LLNL) employs an Arbitrary Lagrangian-Eulerian (ALE) hydrodynamic scheme, in which the mesh moves with the fluid until it becomes distorted, then takes a relaxation and remapping step.

This relaxation is initiated by complex, human-generated rules. DISTLR utilizes supervised learning with Random Forests to automate the process.

Leveraging Human Expertise

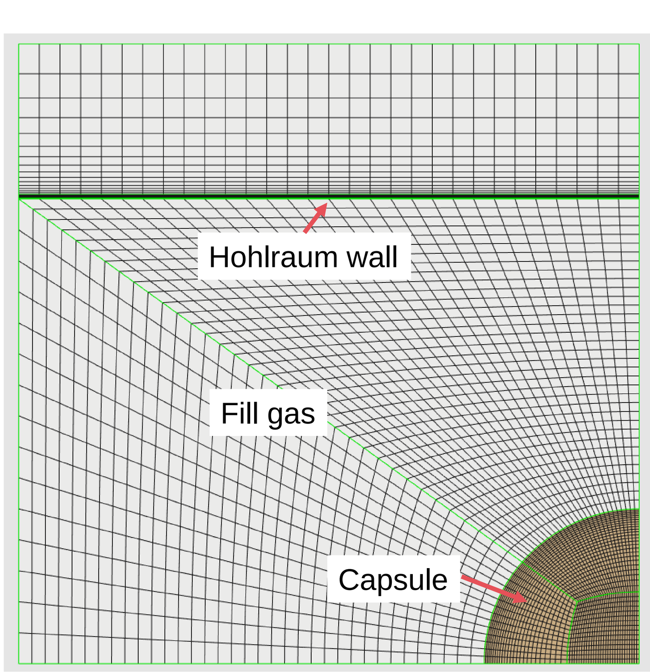
DISTLR 'distills' relaxation techniques honed over the years by design physicists, but aggregates and abstracts them.

- Data are extracted from a simulation employing human-programmed (manual) relaxers
- Features consist of many geometric and physics metrics, including zone shape and nodal velocity
- Labels are the relaxation state determined from manual relaxers



Schematic of DISTLR workflow

A hohlraum-like test problem was developed as a sufficiently complex sandbox in which to test relaxation methods.

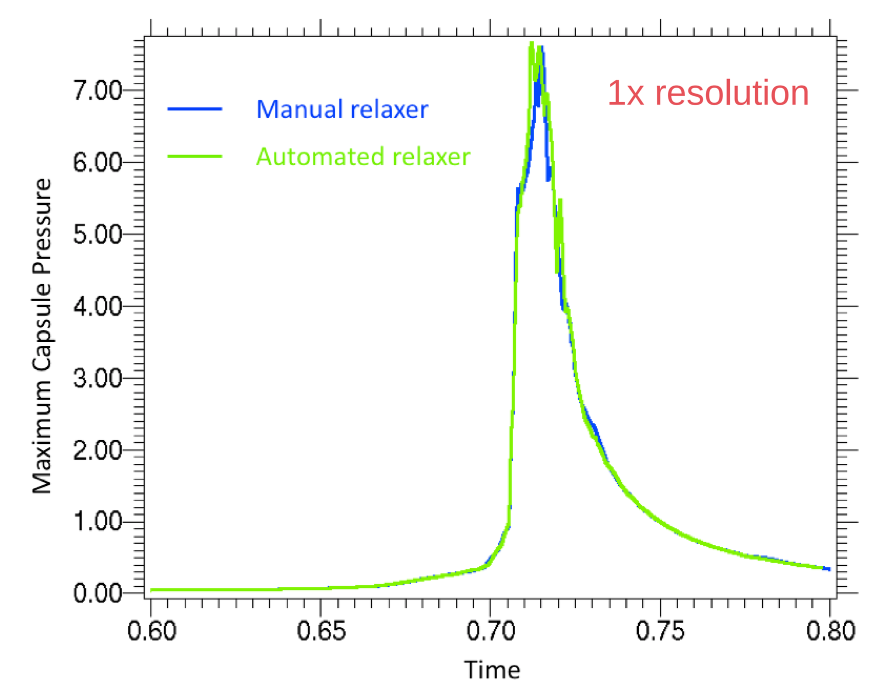


The test problem used for the mesh relaxation study consists of a solid density plastic capsule inside of a gas-filled cylindrical hohlraum. Materials and '1x' resolution mesh shown.

Training at Lower Resolution for Application at Higher Resolution

Initial training for DISTLR utilized data taken from all nodes of the collection, run at 1x resolution (4500 zones), sampled every 100 cycles: approximately 300K data points

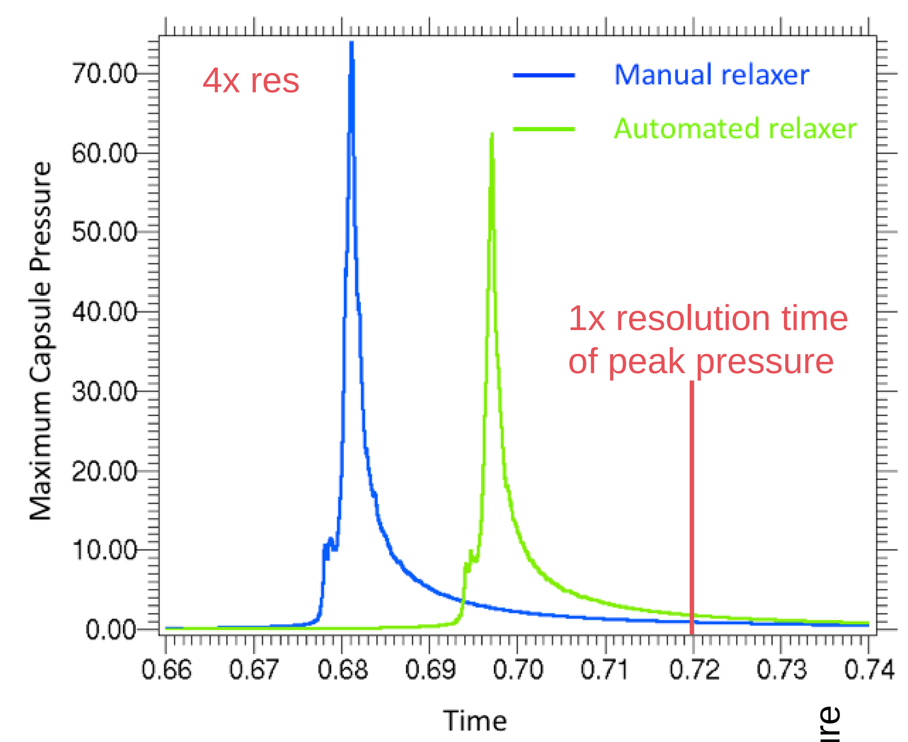
- Random forests trained to mimic separate relaxers, then implemented in inference mode with trained model
- Inference simulation also run at 1x; peak capsule pressures compared



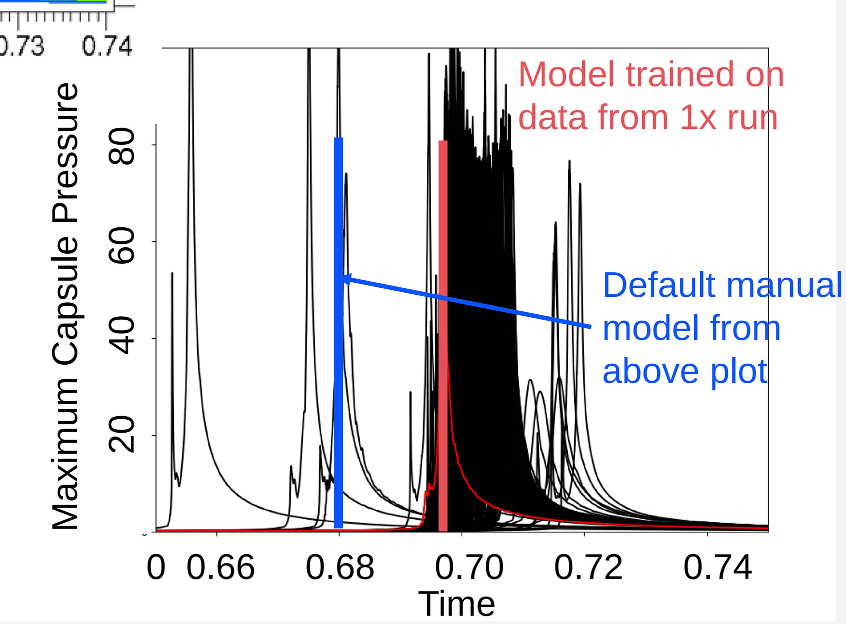
The peak pressure in the test problem capsule was used as a figure of merit to gauge fidelity of run utilizing DISTLR-trained relaxer.

Testing at higher resolution is the first step to understanding the robustness of the model

- Model trained at 1x was then applied to a simulation with twice the resolution in the radial and axial dimensions, for 4x the zone count



Comparison of peak capsule pressure vs. time at 4x resolution. The automated relaxer model is the same one trained on the 1x data, while the manual relaxer relies on ALE parameters that are the same at 1x and 4x.



LHS study at 4x resolution of 600 different sets of ALE parameters for manual relaxation showing variation of peak capsule pressure. Manual and DISTLR results shown for reference.

Accuracy and Performance Optimizations Still Needed

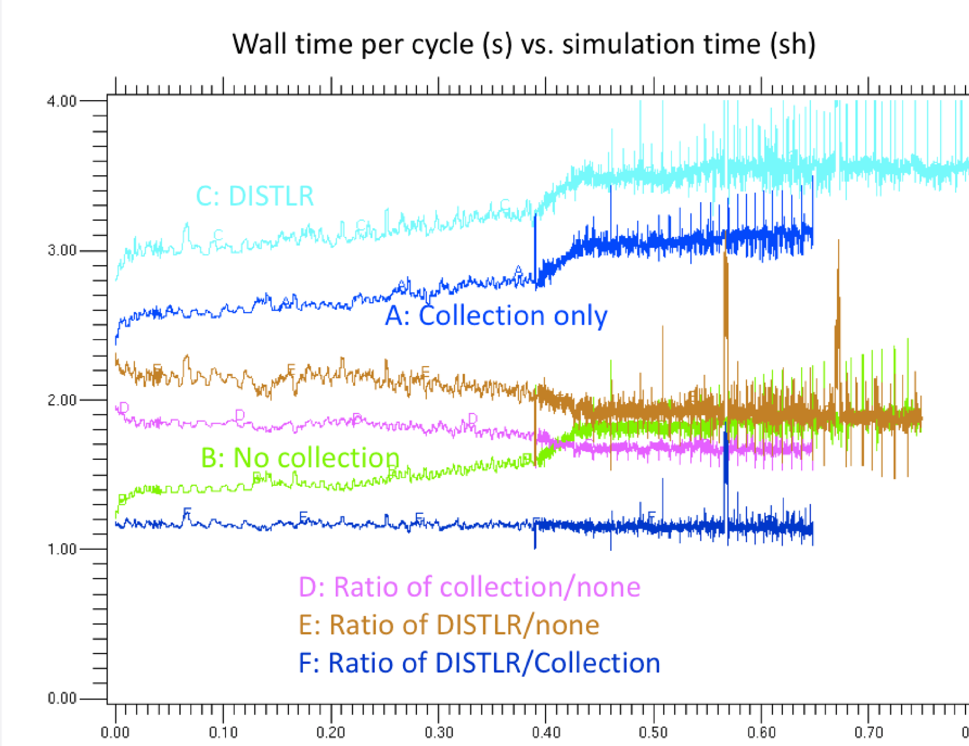
1x resolution

- General relaxer (moving and moderately distorted zones) – 97% accuracy out of 7.5M positives
- Emergency relaxer (severely distorted zones) – 86% accuracy out of 18K positives

4x resolution

- General relaxer – 98.8% accuracy out of 1B positives
- Emergency relaxer – 38.8% accuracy out of 8.25M positives

Accuracy for inference relaxation labels is high at base 1x resolution, but suffers at 4x resolution potentially due to small training set size (general relaxer trained on 82K positive examples, emergency on 384)



Timing data show that data (feature) collection is computationally expensive. The addition of the inference (labeling) step is only a 25% cost on top of collection.

Timing data show that the cost of DISTLR is significant (>2x), no human intervention is required, a major advantage over manual ALE. Efforts to improve performance are currently underway.

Conclusions and Next Steps

DISTLR has been demonstrated to function as a replacement for manual ALE strategies, merging ML work with domain knowledge.

- Can achieve similar physics solutions, even when run at a different resolutions
- Future work will focus on how to improve wallclock performance as well as understanding the impact of false negatives
- Other research areas of importance include how to incorporate new data when the model fails to successfully run a simulation

Machine learning is being employed to leverage domain knowledge and automate tasks in physics simulations

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