Machine Learning Assisted Acceleration of Combustion Simulations

A Probabilistic Neural Network Based Approach

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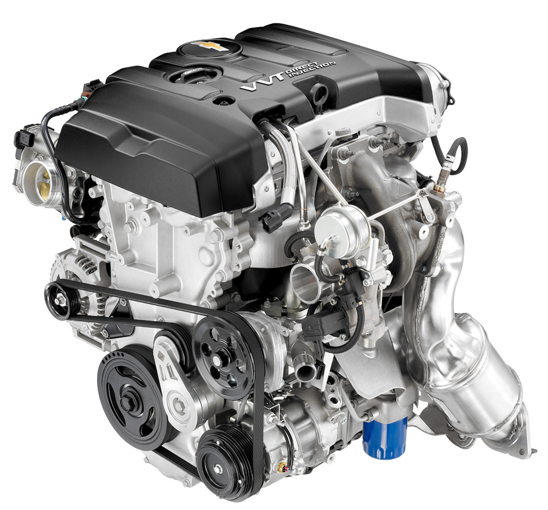
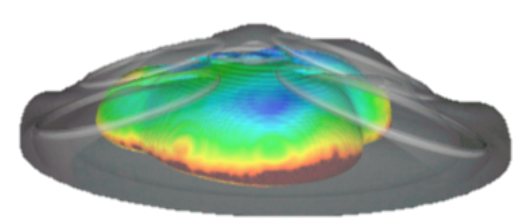
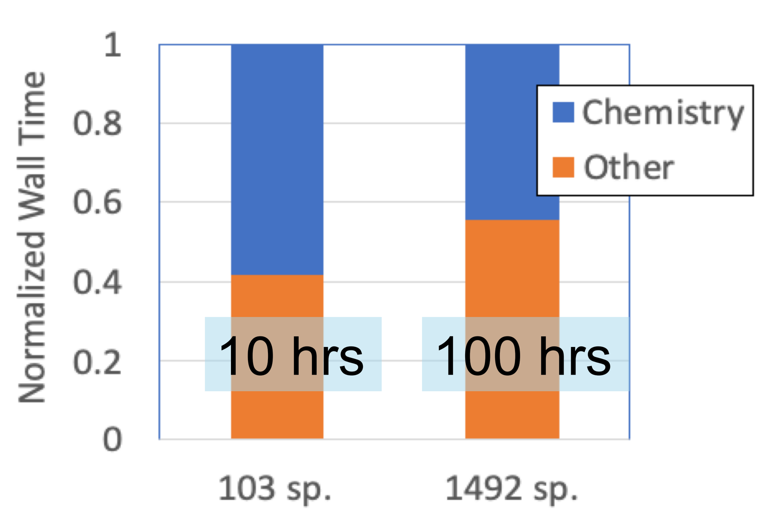
NEED FOR ACCELERATING COMBUSTION SIMULATIONS



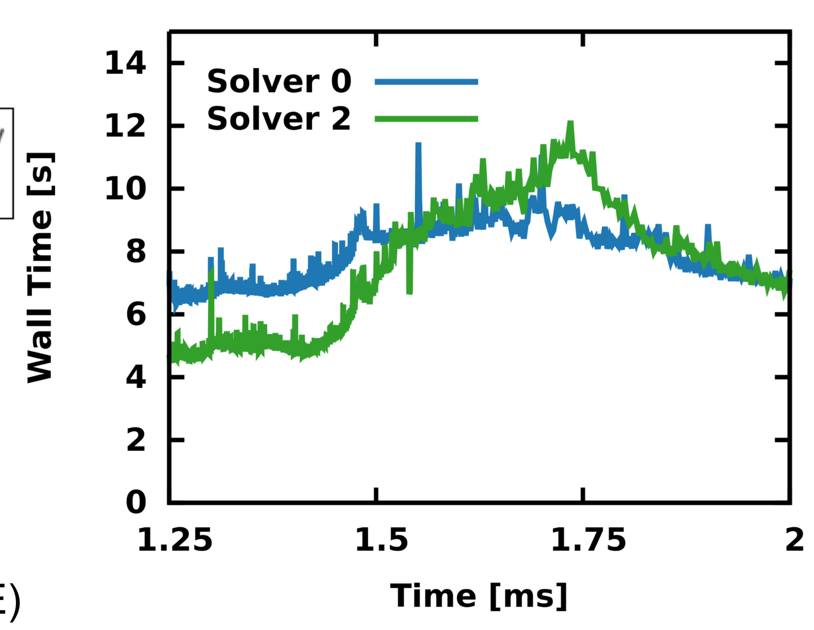


Flame propagation in spark-ignited engine simulation predicted by detailed chemistry

- Detailed chemistry is needed to predict ignition and emissions in future engines.
- Chemistry model cost is commonly more than half of the cost of an engine simulation when using detailed chemistry.
- Different chemistry solvers can be faster or slower depending on global and local conditions simulated.



Chemistry solved with Solver 0 (CVODE)



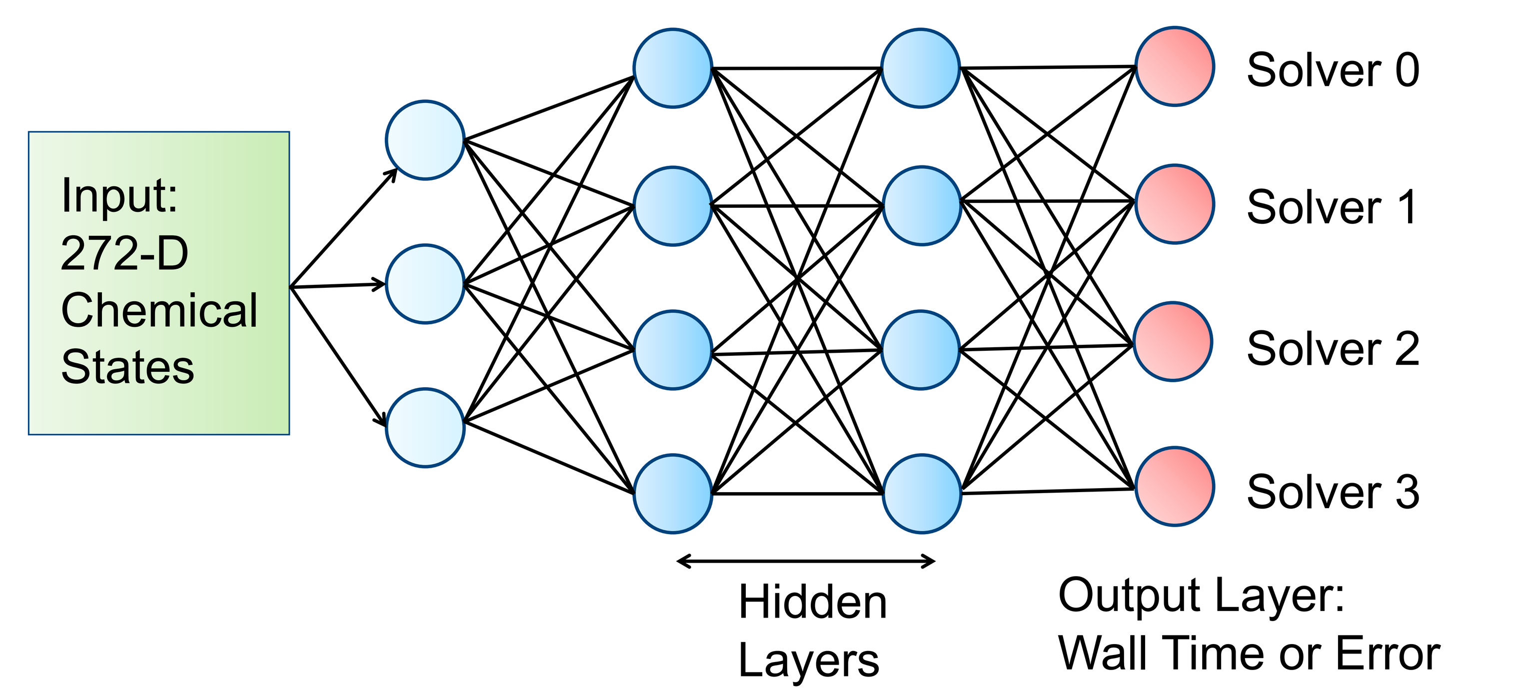
Example data from diesel spray simulation

GOAL

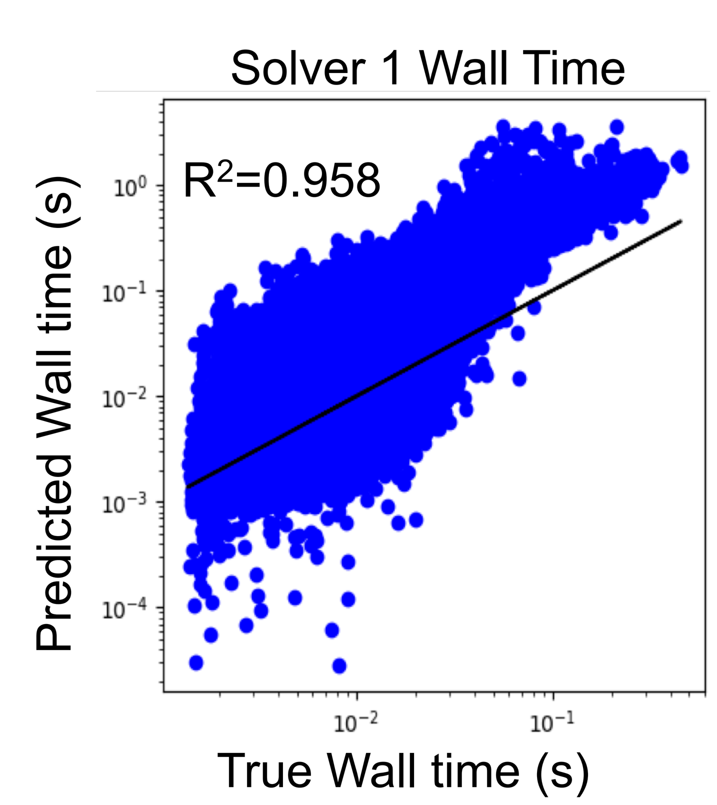
Reduce chemistry model time by > 2x by choosing the fastest chemistry solver under an acceptable error on a cell-by-cell, time-step-by-time-step basis.

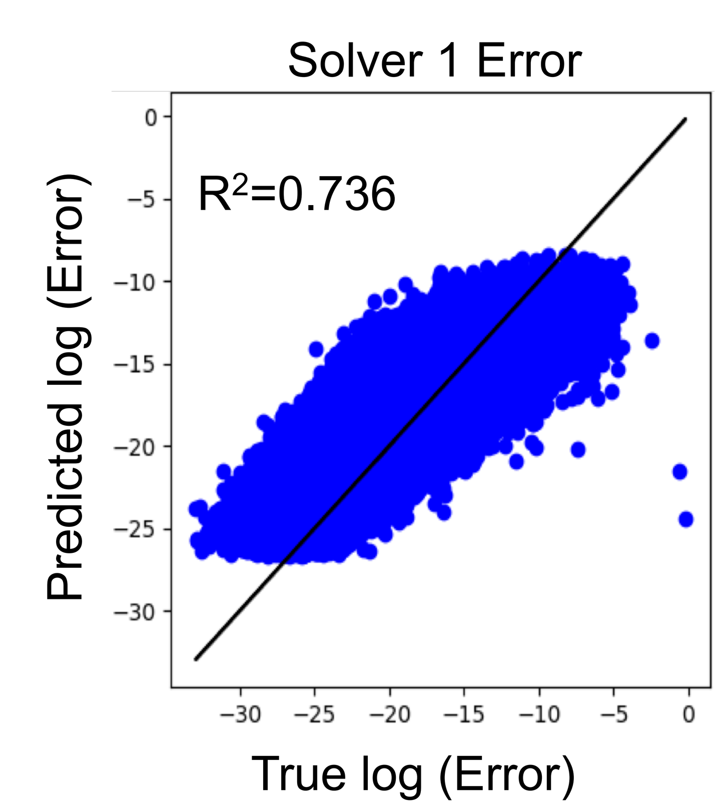
NEURAL NETWORKS FOR PREDICTING CHEMISTRY SOLVERS

- Input: CFD chemical state: species concentrations, temperature and pressure (272 dimensions).
- Output: Wall times and solver errors for 4 different solvers.
- Problem: Predict the fastest solver subject to acceptable error.
- Data: 10^6 chemical states sampled from 0- and 1-D combustion systems. Train – Test Split 70% - 30%
- Approach: Supervised learning with deep neural networks to predict wall times and errors as individual regression problems, and choosing the best integrator to minimize wall time within a set error tolerance



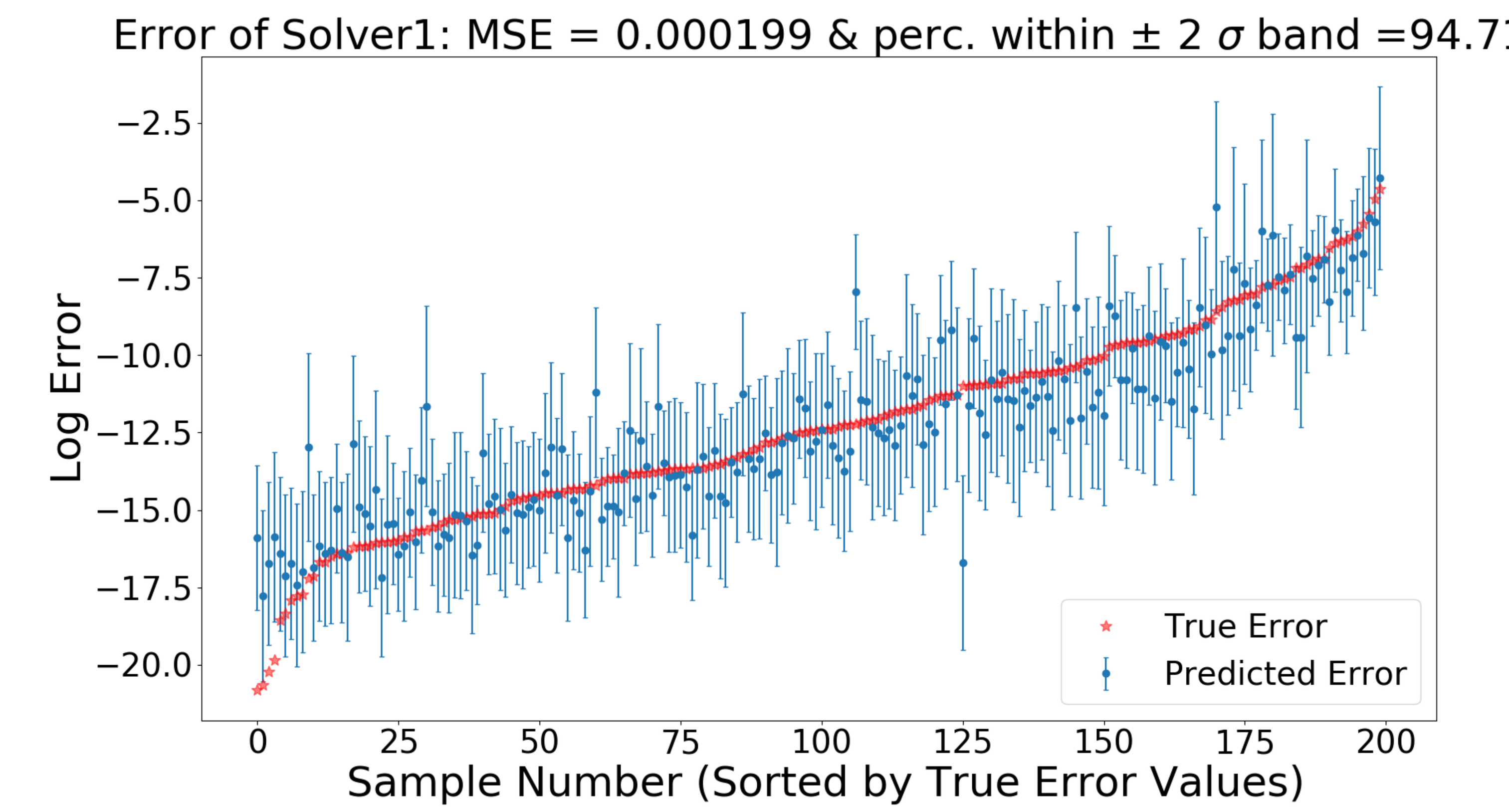
Fully Connected Neural Network predicting wall times and errors as a function of chemical states.



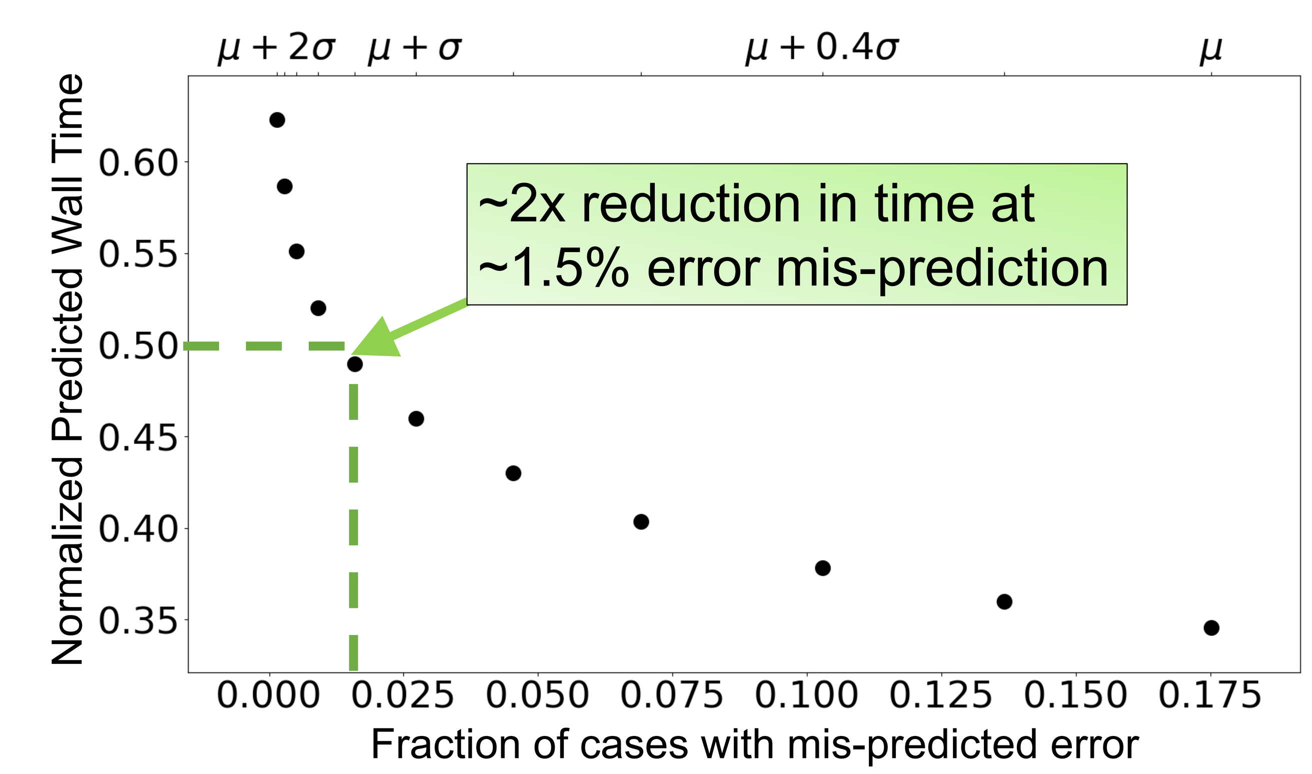


- Lower R^2 for error prediction: Significant % of the variability in the errors cannot be explained by the variability of the chemical states.
- Need for quantifying the variabilities ⇒ Modeling uncertainties!

Probabilistic Layers: Distribution over weights $p(w|\mathcal{D})$



Probabilistic network enables estimating uncertainties of predictions



- Mis-predicted error cases have true error > threshold but predicted error < threshold.
- Error (**μ + σ**) cutoff provides more conservative choice of solver.
- Variance information enables trade-off choice between shortest wall time and minimizing error mis-predictions

CONCLUSIONS

- Neural networks can be utilized to build scalable models for predicting the best chemistry solver for combustion simulations
- Modeling uncertainty in the prediction model provides extra decision making information
- This tool will result in significant time savings for expensive high fidelity combustion simulations.

Data-driven learning with uncertainties predicts chemistry solver timing and error performance.

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