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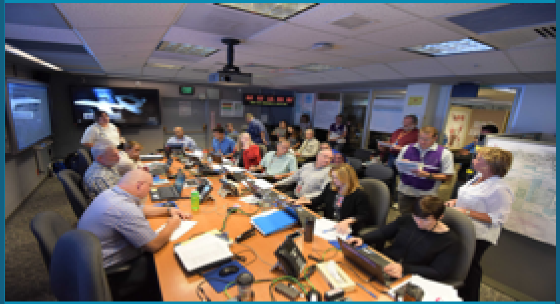
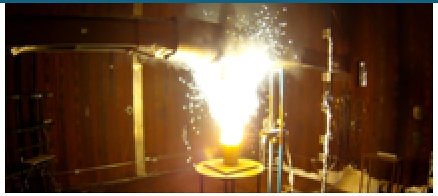
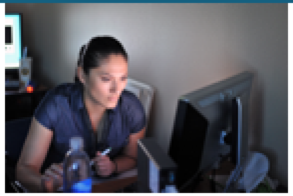
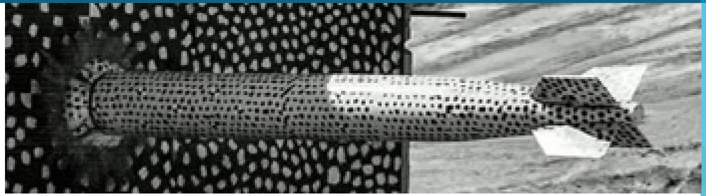
Sandia National Laboratories

# Machine Learning for Accelerating Direct-Simulation Monte-Carlo Collision Operators









Sean T. Miller (1446) and Nathan V. Roberts* (1442)

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U.S. DEPARTMENT OF ENERGY NNSA

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# IDEA SUMMARY

**Motivation:** there are a host of plasma physics problems that are computationally intractable for NNSA, despite being critical to NNSA's missions.

To address this, we are developing algorithmic capabilities for new plasma physics regimes, based on a continuum (Boltzmann) physics model, using

1) Advanced Finite Elements,
2) Machine-Learning-Based Collision Models, and
3) Fluid-Kinetic ("Delta-f") coupling of Boltzmann model and hydrodynamic model

with software that leverages next-generation computing architectures.

$$\partial_t f + \mathbf{v} \cdot \nabla f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = C(f)$$

Boltzmann Equation

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Vlasov Equation — up to 6D

Collision Operator — non-local

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DPG

ML

(this talk)

Boltzmann Equation

# Plasma Physics and the Boltzmann Model

- The unknown in the Boltzmann equation is the distribution *f*, represented in *phase space*.
- Collision operators act on *f* to determine the forcing function for the PDE.
- Since low-velocity and high-velocity particles interact, the collision operator is inherently **nonlocal** in velocity space. This makes it **expensive**. (This also makes it a good candidate for ML.)
- The best approach for approximating Boltzmann depends on the regime:
  - For **high-density** plasmas: use an MHD fluid model.
  - For **low-density** plasmas: use PIC (cost increases with density/collisionality).
  - For cases where these approximations **break down** or are too expensive: use continuum model (FE/FV discretization — our approach).

Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, “A Machine-Learning Approach for Accelerating DSMC Collision Operators.”

# Approximating the Collision Operator: Standard Approaches

- Standard approaches for collision operator: **analytic** and **particle-based models**
- Analytic models: Bhatnagar–Gross–Krook (BGK), Dougherty, Landau, Fokker-Planck, Boltzmann….
  - BGK: cheap but relatively inaccurate
  - Other models are challenging to implement and expensive to evaluate
- Particle-based models: Maxwell-molecule, molecular dynamics, direct-simulation Monte-Carlo (DSMC), …
  - Maxwell-molecule and MD: intractable for more than a few particles
  - DSMC: stochastic approach; can be effective in low- to moderate-collisionality regimes
- We use DSMC as our source of training data
  - Sandia has a history of trusted DSMC implementations (we use EMPIRE-SPIN)

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# Direct-Simulation Monte Carlo (DSMC)

- DSMC: an approach to collision modeling that randomly selects and collides pairs of particles.
  - Collisional probabilities derived from analytical/empirical analysis (e.g., tabular data).
  - Computationally efficient for weak collisionality.
  - Quickly becomes intractable as collisionality is increased.

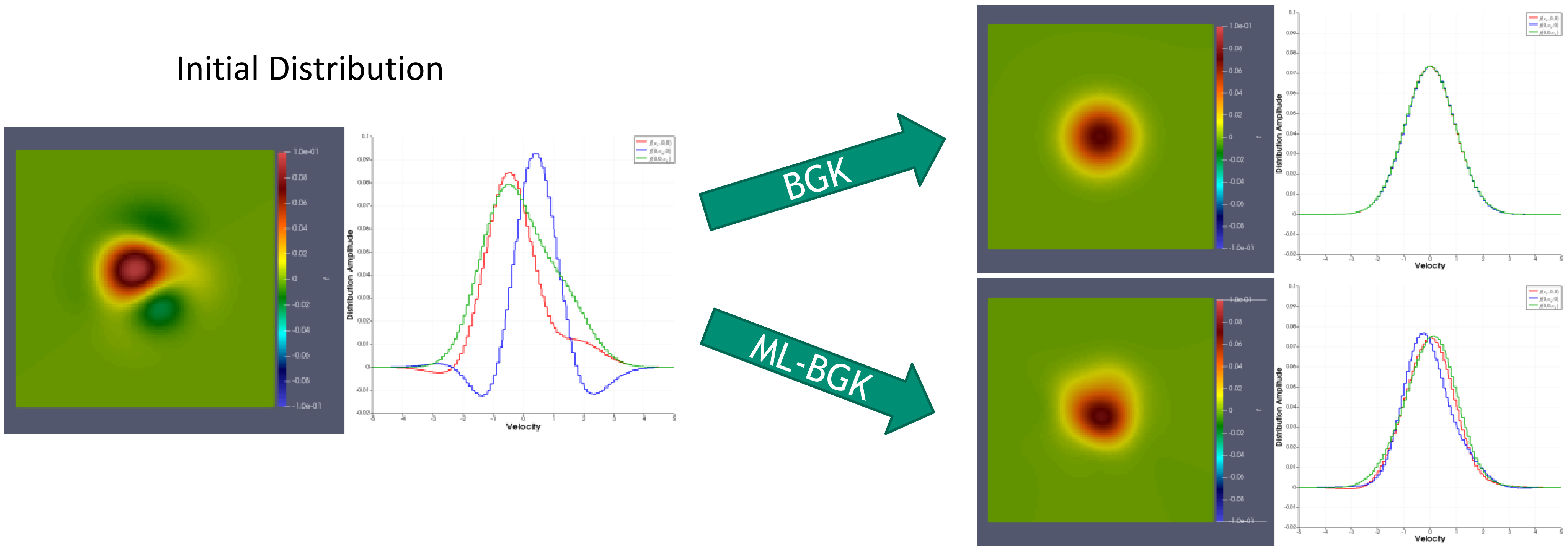
- Main challenge when working with DSMC is accuracy:
  - DSMC relative standard error scales: $\epsilon \propto \frac{1}{\sqrt{N_p N_s}}$
  - $N_p$ : Number of particles
  - $N_s$ : Number of iterations for a given set of initial conditions
  - DSMC runtime scales linearly with $N_p N_s$
  - $\Longrightarrow$ Decreasing error by 50% requires a 4x increase in runtime.

- Can we use machine learning to produce an **efficient** collision operator that maintains DSMC's accuracy?

Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, "A Machine-Learning Approach for Accelerating DSMC Collision Operators."

# Our ML Approach

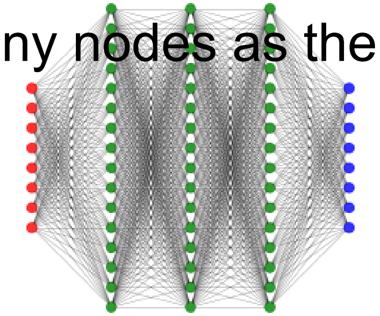
- Initially, we tried learning the DSMC operator directly
  - This led to an operator that did not properly relax to thermal equilibrium:



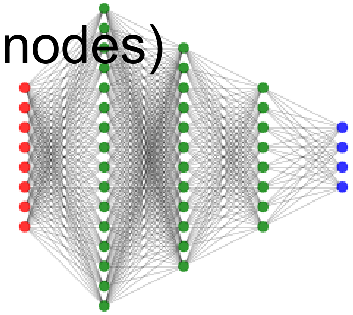

Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, “A Machine-Learning Approach for Accelerating DSMC Collision Operators.”

# Our ML Approach

- Initially, we tried learning the DSMC operator directly
  - This led to an operator that did not properly relax to thermal equilibrium
- Instead, we now learn the *difference* between the more complex, expensive DSMC operator and the cheap-to-evaluate, but inaccurate BGK operator
- We generated 390,000 samples using SPIN (3,000 CPU hours) to use as training data.
- We tried a range of neural network topologies; basic conclusion: we don't need a deep network.
  - In all the results here, we use 2 hidden layers, and a width multiplier of 2 (first hidden layer has twice as many nodes as there are input nodes)



Full Bandwidth
#inputs = #outputs



Truncated
#inputs > #outputs

Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, "A Machine-Learning Approach for Accelerating DSMC Collision Operators."

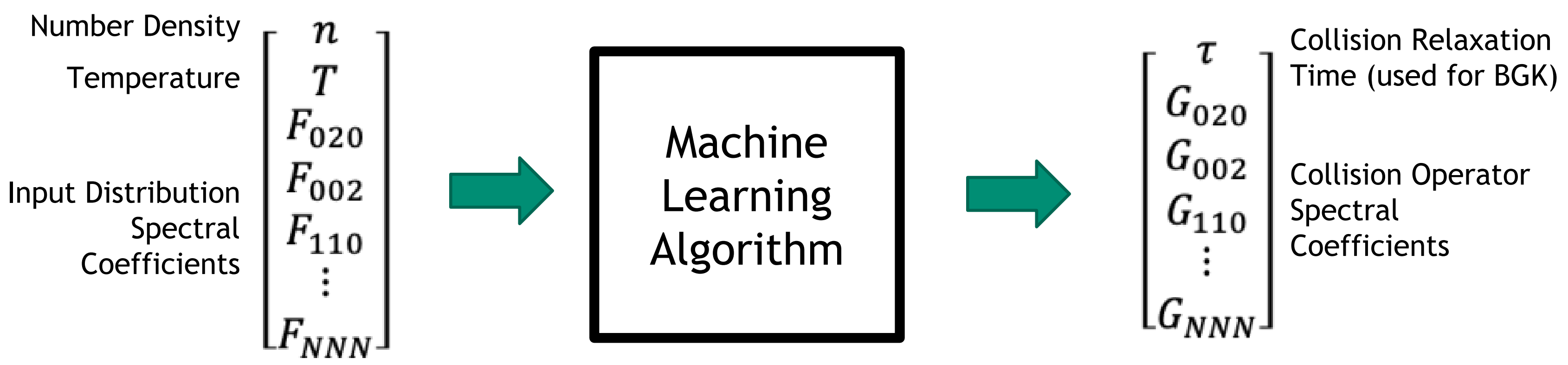
# Representing the Collision Operator

- Inputs and outputs for the machine learning algorithm are expressed in a *spectral* form:

Input Distribution

$$f = f_0 \exp(-\mathbf{w}^2) \sum_{ijk} F_{ijk} H_i(w_x) H_j(w_y) H_k(w_z)$$

Weighting Function ($\exp(-\mathbf{w}^2)$); Normalization Parameter ($f_0$); Spectral Coefficients ($F_{ijk}$); Hermite Polynomials ($H_i$, $H_j$, $H_k$); Scaled Random Velocity Coordinate ($w_z$)




- The spectral representation is designed to enforce the **conservation of mass, momentum, and energy**, as well as **Galilean invariance**.

Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, “A Machine-Learning Approach for Accelerating DSMC Collision Operators.”

# Limitation: Mode Truncation

- High-order modes are ill-represented by our SPIN samples
- The cost of accurately capturing higher modes using stochastic algorithm increases rapidly
- We truncate at modes of order 6: $F_{ijk} : i + j + k \leq 6.$
- This gives 81 inputs to our neural network
    - "Full-Bandwidth" topologies have 80 outputs
    - "Truncated" topologies have 31 outputs (corresponding to modes of order up to 4).
- The modes captured effectively correspond to *moments* of the plasma distribution; we represent moments up to sixth order.

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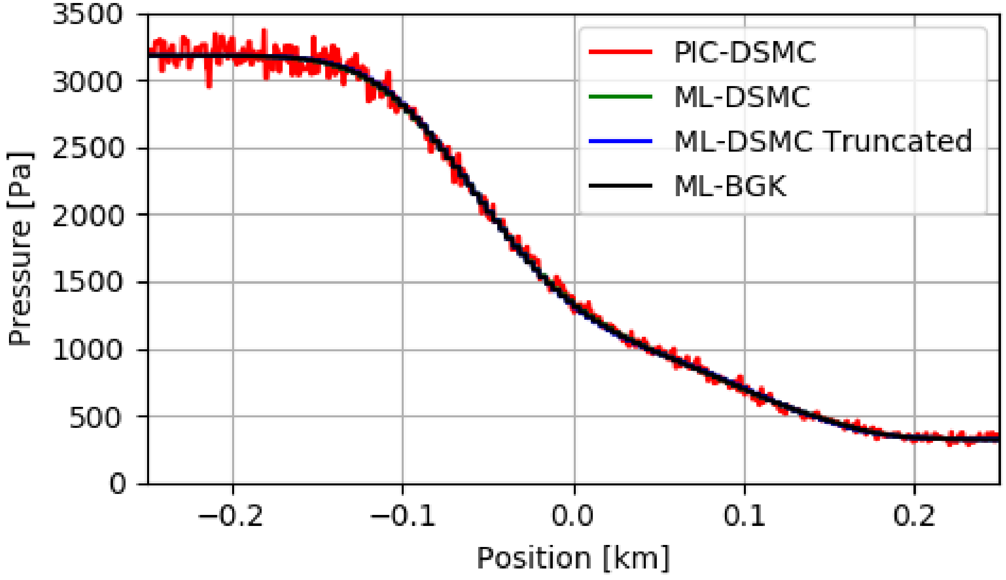
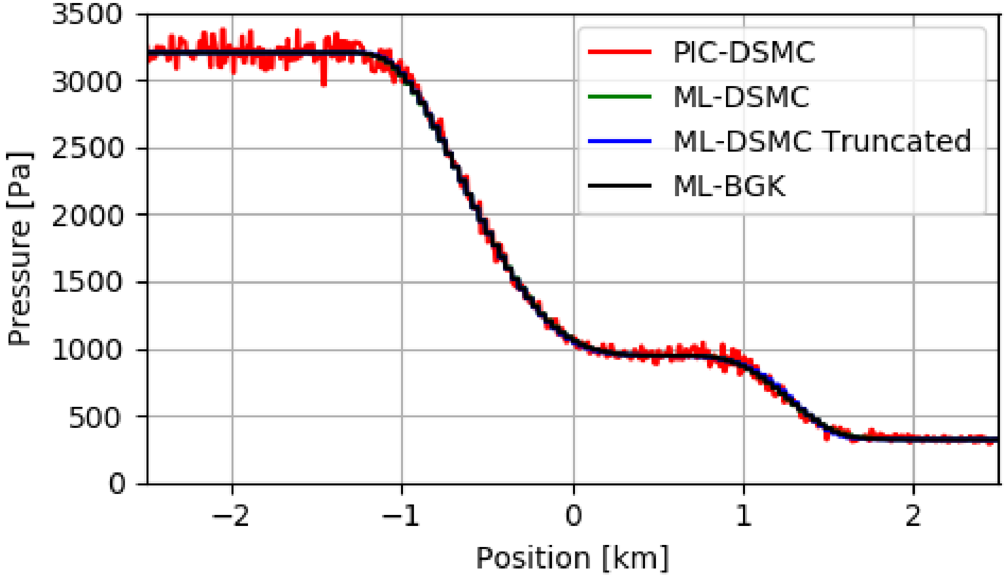
# Numerical Results: Shock Tube Problems

- We show results for two shock tube problems, comparing finite volume code with ML collision operator to EMPIRE PIC + SPIN.




Weakly Collisional Regime
(shock not visible)




Moderately Collisional Regime
(shock formation clear)

- Here, the ML-BGK is a "pure" BGK operator; only the collision frequency is machine-learned.
- All three models appear to agree well with the PIC+SPIN results.

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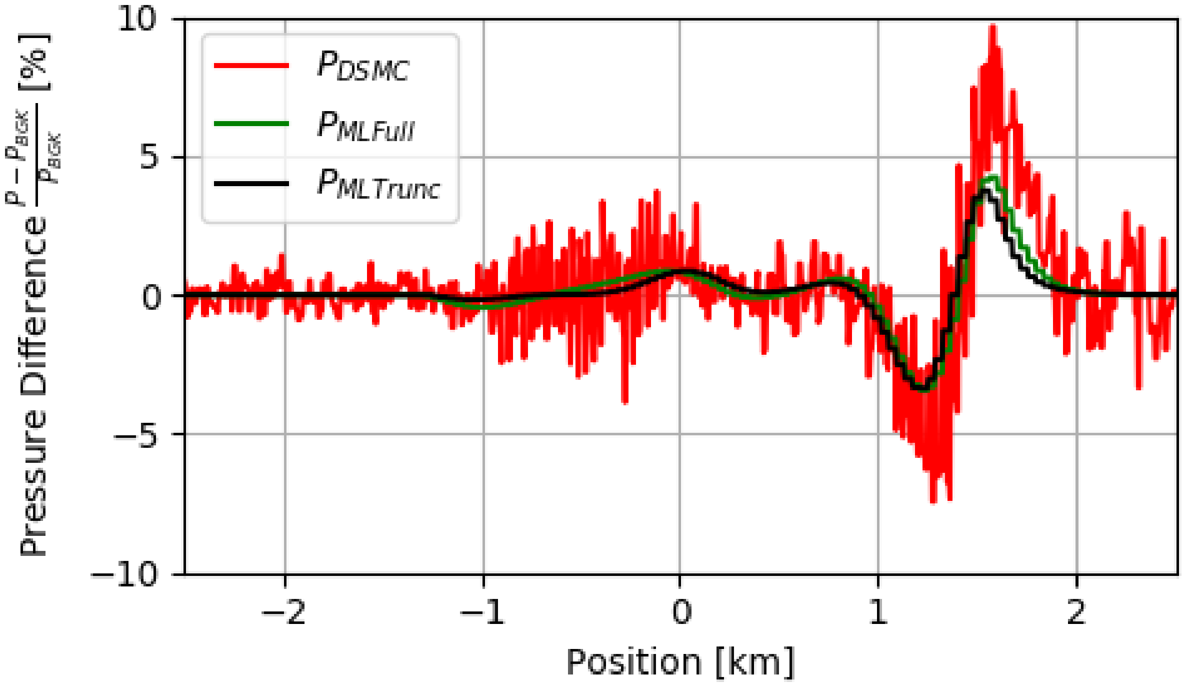
# Numerical Results: Shock Tube Problems

- Digging a bit deeper on the moderately collisional results, we subtract off the pressure value when using the BGK operator alone.




- We see that we capture the difference between BGK and DSMC quite well with either the full or the truncated ne The ML results effectively smooth out the noise, and otherwise represent the DSMC operator quite accurately.
- In this regime, evaluating the ML operator is about **100x faster** than the corresponding SPIN evaluation.

Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, "A Machine-Learning Approach for Accelerating DSMC Collision Operators."

# Conclusions

- For appropriately defined collisional regimes, we can indeed produce an ML collision operator that reflects SPIN's behavior, with substantial reduction in computational cost.

- Careful design of the ML operator is vital:
  - We learn the **difference** between BGK and DSMC
  - We enforce key physical properties (**conservation, Galilean invariance**) through the modal representation of the operator.

- See Sean's talk from MLDL 2020 for some further details on the technical approach.

- Also see our paper (now available on request to Sandians; will be submitted to R&A in the next couple of weeks):

  Sean T. Miller, Nathan V. Roberts, and Eric C. Cyr, "A Machine-Learning Approach for Accelerating DSMC Collision Operators." To be submitted soon (target: *Journal of Plasma Physics*).