Center for Exascale-Enabled Scramjet Design

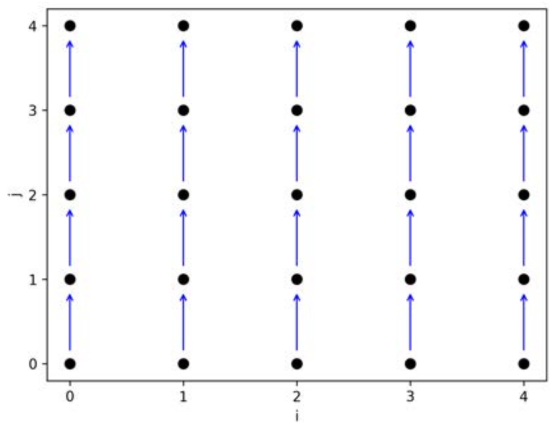
University of Illinois at Urbana-Champaign

Addison Alvey-Blanco: Precise Dependence Analysis in the Context of DG-FEM on GPUs
Isabella Gessman: Scramjet Performance Characterization using Laser Absorption Spectroscopy
Casey Lauer: Red Flags for SciML
German Saltar Rivera: Adjoint-based Training of Embedded Neural-Network Models for Particle-laden Turbulence

Precise Dependence Analysis in the Context of DG-FEM on GPUs

Addison J. Alvey-Blanco (Computer Science, UIUC)

```
for i in range(n):
    for j in range(n):
        # ...
S0:     a[i,j] = a[i,j-1]
        # ...
S1:     b[i,j] = b[i,j-1]
        # ...
```



- Reduce differentiation cost
  - Simplicial element cost: $\mathcal{O}(n^{2d})$
  - Tensor-product element cost: $\mathcal{O}(n^{d+1})$
- Want: further exploitation of the benefits of structures like tensor-product elements
- Need: precise dependency semantics for complex loop tiling strategies

Scramjet Performance Characterization using Laser Absorption Spectroscopy

Isabella Gessman, Tonghun Lee, Greg Elliott

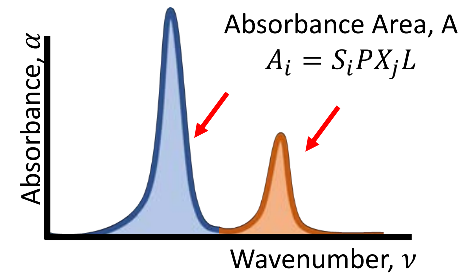
- Tunable Diode Laser Absorption Spectroscopy sensors to characterize facility inflow gas composition and measure combustion products downstream
  - NO concentration, temperature for inflow gas composition in plenum of arc-heater
  - CO, CO_2 concentration measurements for combustion performance characterization

Beer's Law:

$$T_\nu = \left(\frac{I}{I^0}\right)_\nu$$

Absorbance:

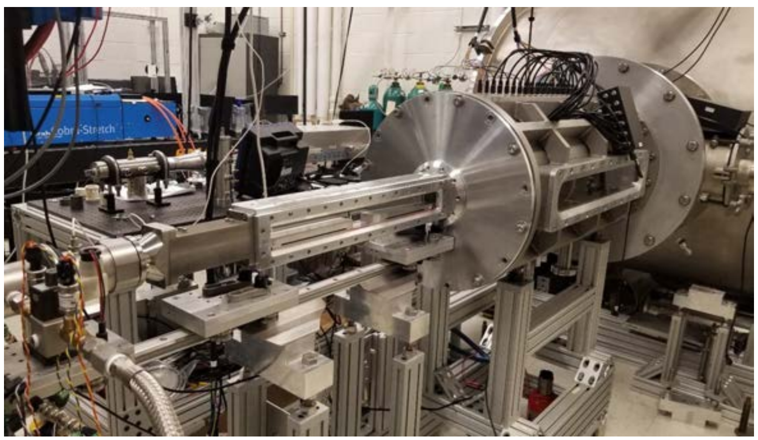
$$\alpha(\nu) = -\ln(T_\nu)$$



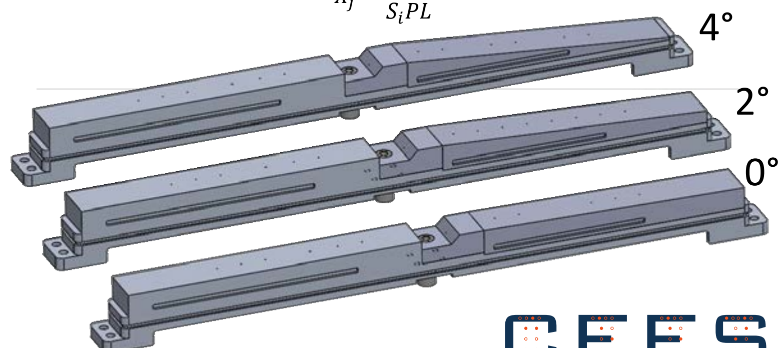
$$S_i(T) = S_i(T_0)\frac{Q(T_0)}{Q(T)}\left(\frac{T_0}{T}\right)exp\left[-\frac{hcE_i''}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]\times\left[1-exp\left(\frac{-hc\nu_{0,i}}{kT}\right)\right]\left[1-exp\left(\frac{-hc\nu_{0,i}}{kT_0}\right)\right]^{-1}$$

$$R = \frac{A_1}{A_2} = \frac{S_1(T)}{S_2(T)} = f(T)$$

$$X_j = \frac{A_i}{S_i P L}$$

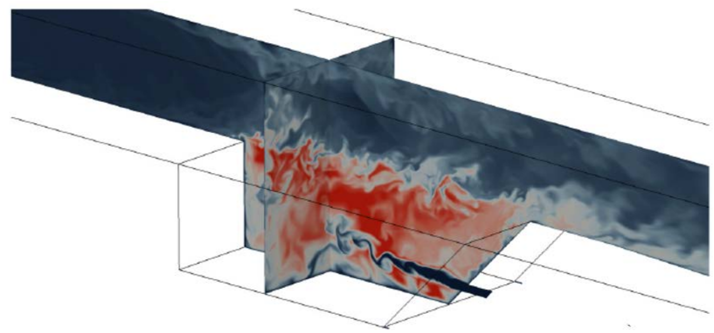


ACT-II Facility



Red Flags for SciML - Casey Lauer

- Machine Learning (ML) surrogate models have been shown to be cheaper replacements for costly calculations, such as chemical kinetics
- Predictive simulations likely too exercise model beyond training
- **Key Concern:** Can we know when an ML model might give importantly wrong results?
- **New Technique**: leave out known physics (e.g., a constraint) in training and use violations of it as a "red flag" signal the predictions are at risk for being wrong
- Initially implementing the ML model in a constrained 0D autoignition system
  - **"Red Flag" Constraint**: atom conservation
  - $\frac{d\boldsymbol{Y}}{dt} = \mathbb{C}\hat{\boldsymbol{s}}$



[Esteban Cisneros]

Adjoint-based Training of Embedded Neural-Network Models for Particle-laden Turbulence

German Saltar Rivera, **Laura Villafañe-Roca**, and **Jonathan Freund**

- A large range of scales makes particle-laden turbulence challenging to simulate
- Embedded ML: a NN term is embedded in the governing equations to account for both unrepresented physics and disretization errors
- Training based on prediction outcome; discrete-exact adjoints provide gradient of PDE + NN to optimize weights
- Current demonstration: particle-laden 2D isotropic turbulence
- See poster for results and future plans!
- Looking for internship Summer 2024