# Semi-parametric Modeling of the Equation of State of Dissociating Materials

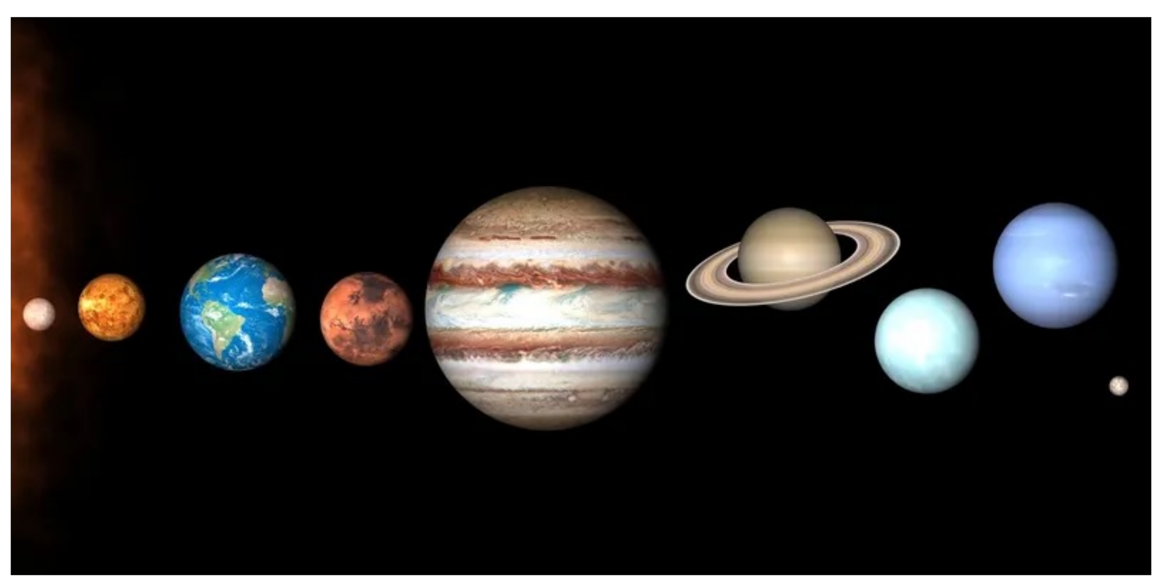
**Jolypich Pek*, Jason Bernstein⁺, Ben Seiyon Lee*, and Philip Myint⁺**

George Mason University* and Lawrence Livermore National Laboratory⁺

## 1. Overview

**Why Do We Need Equation of State (EOS)?**

- Essential for modeling behavior of materials.
- Our interest is in dissociating materials (e.g., $CO_2$) under extreme conditions.
- Applications include planetary science and inertial confinement fusion (ICF).



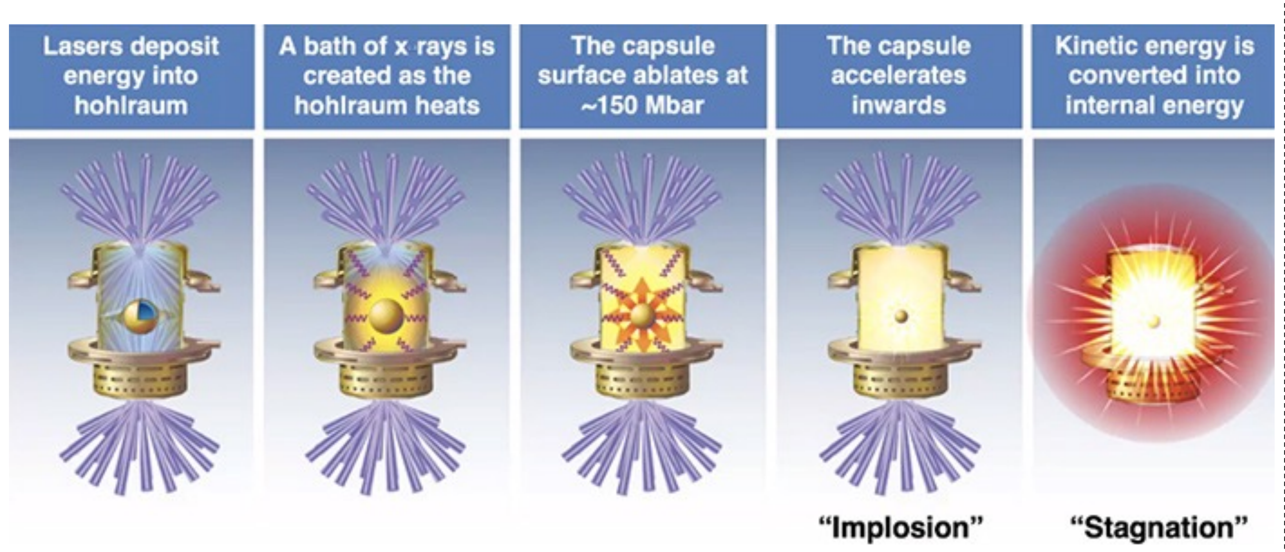



*Figure from [1]*

**Why is Developing EOS Challenging?**

- Need to infer latent molar mass surface from limited theoretical calculations and noisy experimental data.
- Existing EOS models rely on hand-tuned parameters that represent the molar mass surface as a function of temperature and density.

**Our Goal:**

- Automate EOS model development for chemically dissociating systems to improve model accuracy and fit while minimizing computational overhead.

*This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.*

LLNL-POST-2004775

## 2. Equation of State

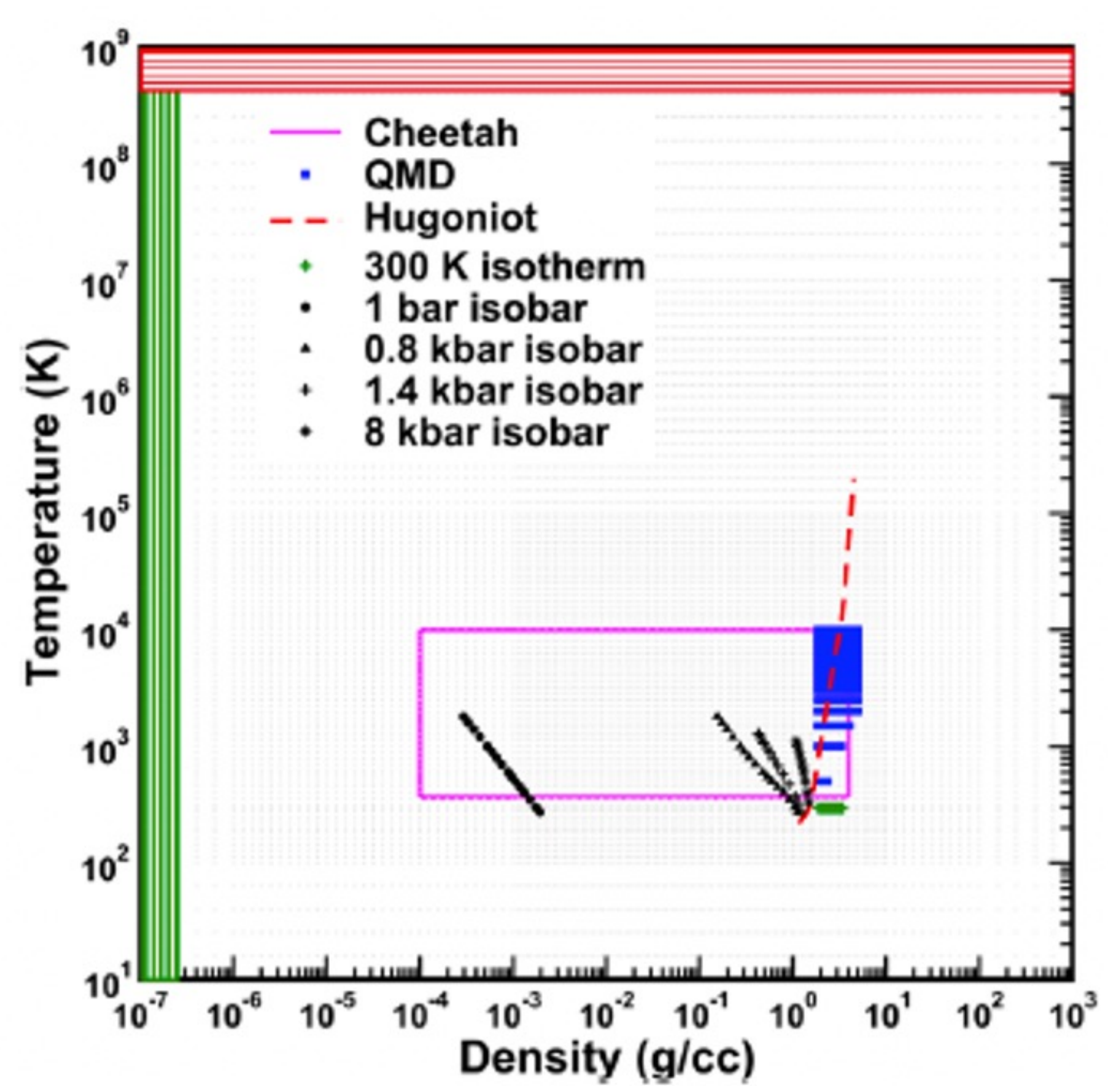
- The EOS model describes the relationship between thermodynamic variables (e.g., pressure, temperature, volume) of materials.
- $F = F(M(T,\rho), T, \rho)$ is our EOS, where $M$ is the molar mass surface.
- Data is on partial derivatives of $F$ such as internal energy

$$\mathrm{E} = -T^2 \left(\frac{\partial(F/T)}{\partial T}\right)_V$$

and pressure

$$\mathrm{P} = -\left(\frac{\partial F}{\partial \rho}\right)_T$$

- The $CO_2$ data shown in the figure below is compiled by Wu et al (2019) from multiple theoretical models, simulations, and experimental sources.




- **Method:** We employ a semi-parametric interpolation approach that integrates these diverse data sources to bridge gaps in the EOS.

## 3. Statistical Methodology

**Latent Surface Modeling:**

- We model the latent molar mass $M(T,\rho)$ using semi parametric approach.
- Regularization techniques applied to aid basis selection and prevent overfitting.

**Gaussian Radial Basis Functions**

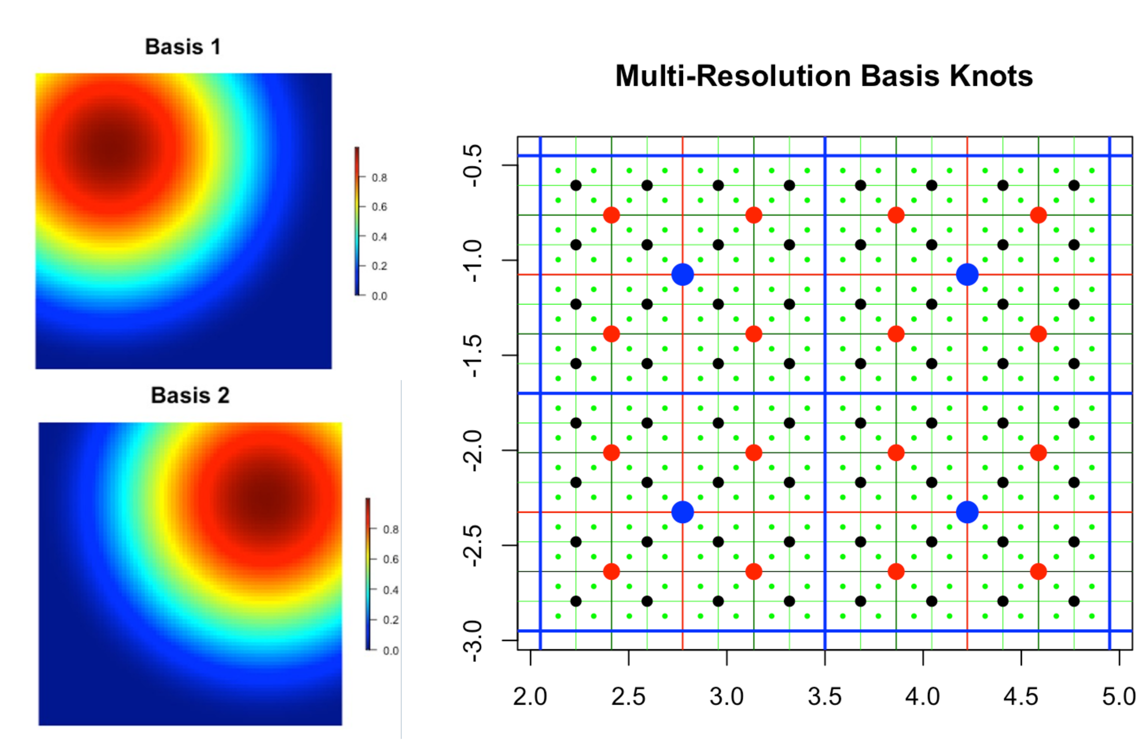
- Spline model is $M(T,\rho) = \Phi\delta$, where $\Phi(T,\rho)$are basis functions.

$$\Phi_k(s) = \exp(-\ell \|s - u_k\|^2)$$

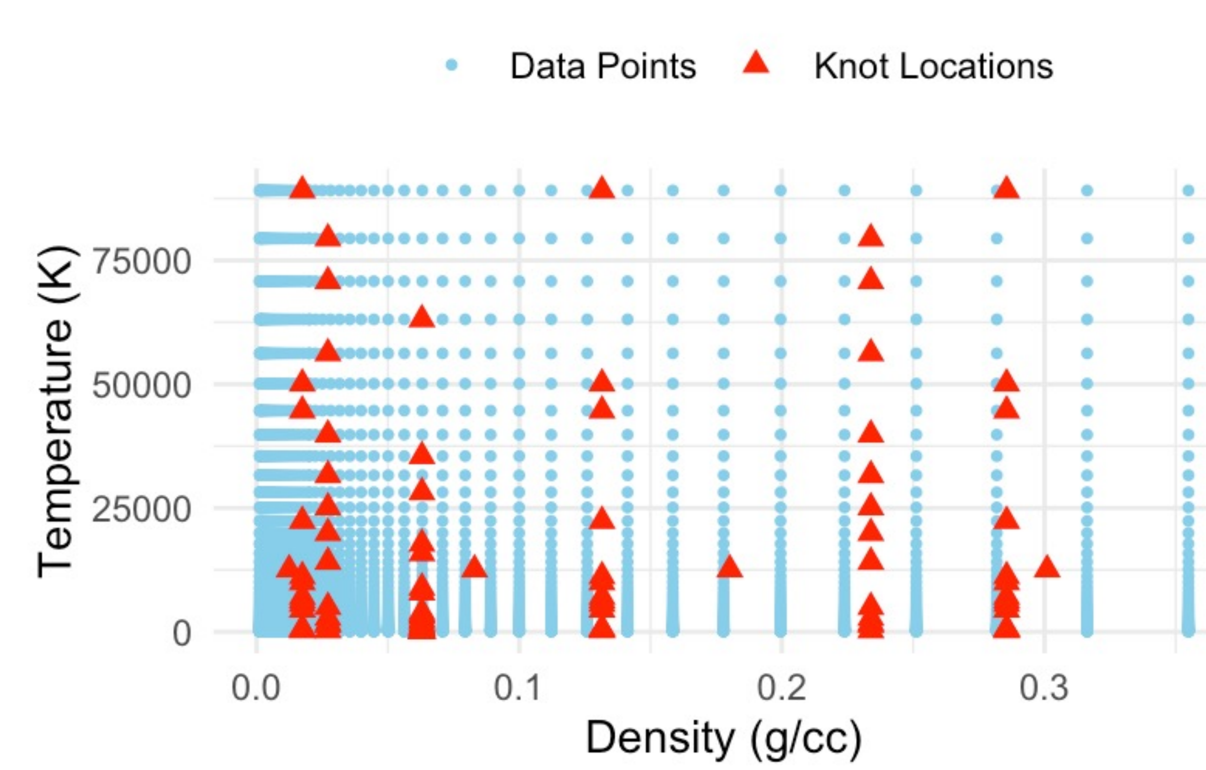
- Here $u_k$ is a knot location and $\ell$ is the length scale.
- We want to estimate the basis coefficients $\delta$.

**Knot Placement Algorithm:**

- **Multi-Resolution:** Radial Basis Functions placed at varying resolution to capture global and local variations in the data.

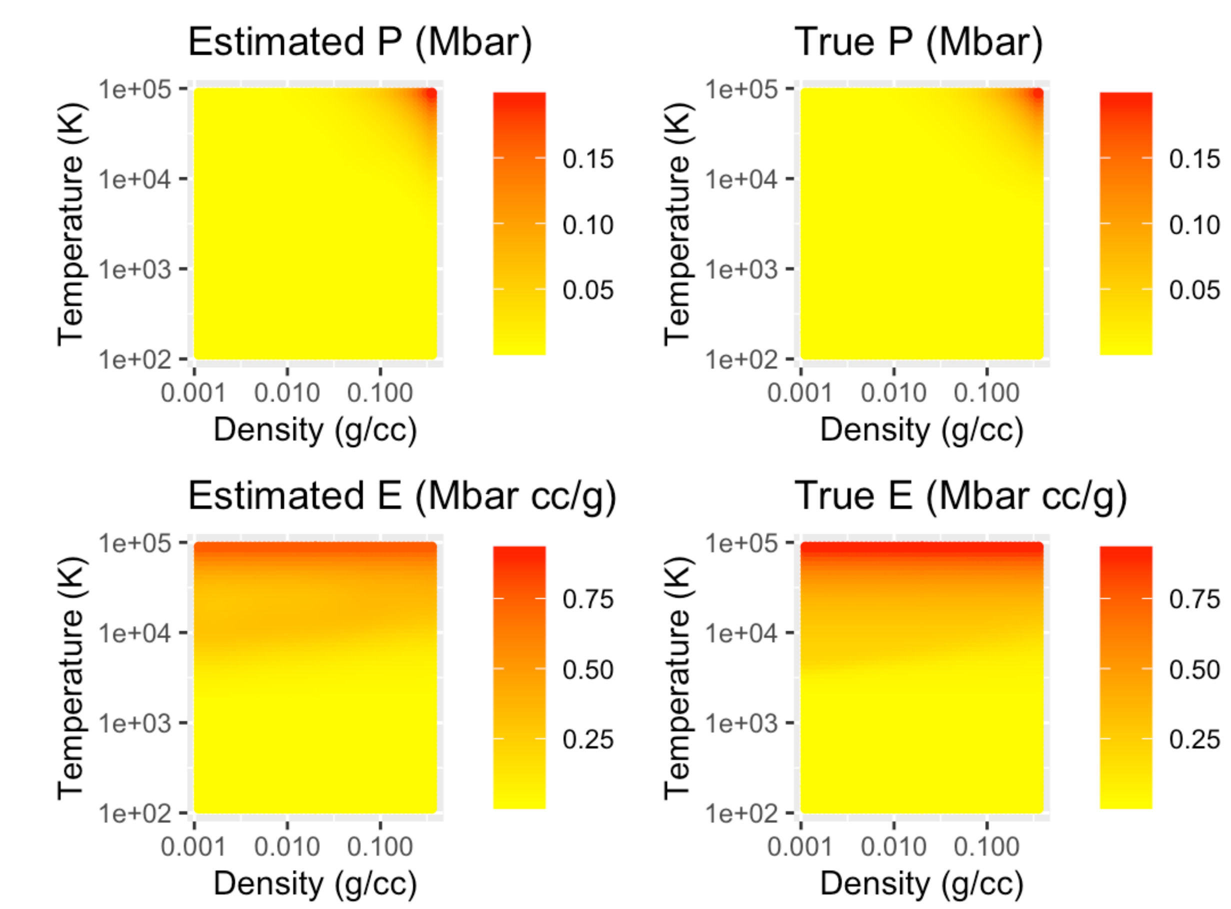



- **Adaptive K-Means Clustering:** dynamically place knots in regions where the data are dense.

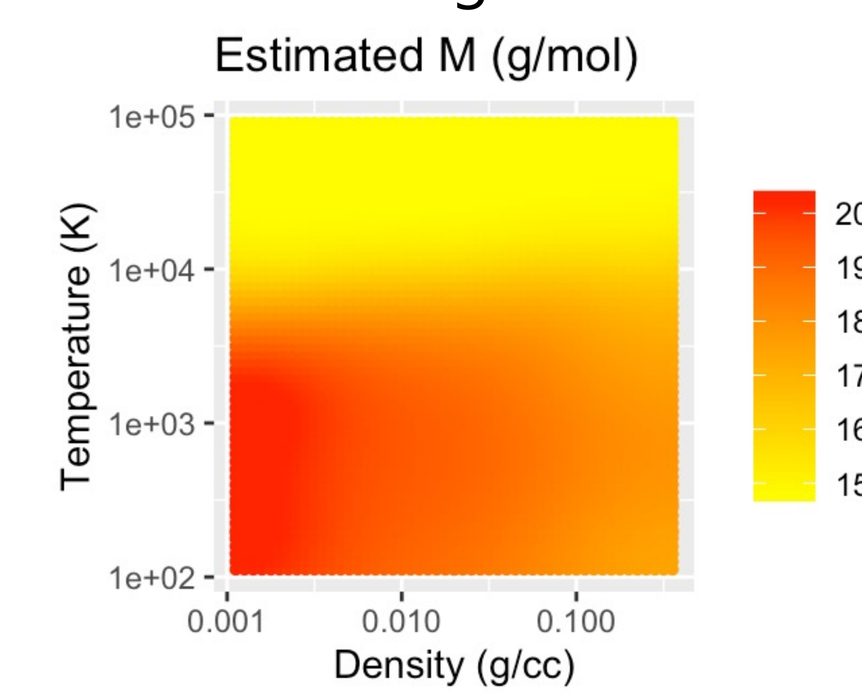



## 4. Results

- Multiple optimization algorithm were applied to minimize the mean squared error (MSE) for predictions of E and P.
- Estimated energy and pressure surfaces align well particularly at higher $T$ and $\rho$.




- Molar mass surface plot shows smooth transition across regions




## 5. Future Work

- Explore alternative basis functions and regularization methods to improve interpolation accuracy and robustness.

**References:**

[1] Osolin, C. (2023, February 23). *Star Power: Blazing the path to fusion ignition*. National Ignition Facility & Photon Science. https://lasers.llnl.gov/news/star-power-blazing-the-path-to-ignition

[2] Wu, C. J., Young, D. A., Sterne, P. A., & Myint, P. C. (2019c). Equation of state for a chemically dissociative, polyatomic system: Carbon dioxide. The Journal of Chemical Physics, 151(22). https://doi.org/10.1063/1.5128127