Consistent Interpolation of the Equation of State in Hydrodynamic Simulations

Michal Zeman, **Pavel Váchal**

Czech Technical University in Prague, Czech Republic

Faculty of Nuclear Sciences and Physical Engineering

Milan Holec

Université de Bordeaux - CNRS - CEA

Centre d'Etudes Lasers Intenses et Applications (CELIA)

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The Objective

Develop a tool for practical evaluation of the Equation of State (EoS) in hydrodynamic simulations based on consistent higher order interpolation of the Helmholtz free energy

Outline of This Presentation

- **The Helmholtz free energy (HFE)**
- **Thermodynamic consistency and other physical requirements on HFE**
- ***Thermodynamic interpolation of HFE***
  vs. *Direct interpolation* of pressure and internal energy
- **The HerEOS tool: Initialization, algorithm, properties**
- **Numerical results, real applications**
- **Practical issues with EoS libraries**

The Euler Equations of Lagrangian Hydrodynamics

$$\frac{\mathrm{d}\,\rho}{\mathrm{d}\,t} = -\rho\,\nabla\cdot\vec{\boldsymbol{v}},$$
$$\rho\,\frac{\mathrm{d}\,\vec{\boldsymbol{v}}}{\mathrm{d}\,t} = -\nabla\,(p_e + p_i) + \nabla\cdot\mu\sigma,$$
$$\rho\,\frac{\mathrm{d}\,\varepsilon_e}{\mathrm{d}\,t} = -p_e\nabla\cdot\vec{\boldsymbol{v}} - \nabla\cdot\vec{\boldsymbol{q}}_H - \nabla\cdot\vec{\boldsymbol{q}}_S,$$
$$\rho\,\frac{\mathrm{d}\,\varepsilon_i}{\mathrm{d}\,t} = (\mu\sigma - p_i\mathbf{I}) : \nabla\vec{\boldsymbol{v}},$$

- **The viscous extension: parabolic terms represented by viscosity μ, symmetrized velocity gradient $\sigma = \frac{1}{2}\,(\nabla\vec{v} + \vec{v}\nabla)$, and electron heat flux $\vec{q}_H$ given by the heat conduction**

$$\rho\,c_{Ve}\,\frac{\mathrm{d}\,T_e}{\mathrm{d}\,t} = -\nabla\cdot\vec{\boldsymbol{q}}_H, \qquad \vec{\boldsymbol{q}}_H = -\kappa_e\nabla T_e.$$

- **The term $-\nabla\cdot\vec{q}_S$ provides a general source of energy, e.g., laser energy deposition.**
- **The Equation of State provides the physical properties of plasma, i.e., the closure**

$$p_e(T_e,\rho), \quad p_i(T_i,\rho), \qquad \varepsilon_e(T_e,\rho), \quad \varepsilon_i(T_i,\rho), \qquad \mu(T_e,T_i,\rho), \qquad c_{Ve}(T_e,\rho), \qquad \kappa_e(T_e,\rho).$$

The Equation of State

- The Equation of State provides the physical properties of plasma, i.e., the closure

$$p_e(T_e,\rho), \quad \varepsilon_e(T_e,\rho), \quad p_i(T_i,\rho), \quad \varepsilon_i(T_i,\rho), \quad \mu(T_e,T_i,\rho)), \quad c_{Ve}(T_e,\rho), \quad \kappa_e(T_e,\rho)$$

- Primary variables of hydrodynamic equations is the set $(\rho,\ \vec{v},\ \varepsilon_e,\ \varepsilon_i)$
  $\Rightarrow$ the inverse evaluations $T_e(\rho,\varepsilon_e)$, $T_i(\rho,\varepsilon_i)$ must also be provided.
- All the thermodynamic quantities can be written as a function of free energy, that is,

$$p_e(f_e(T_e,\rho)), \quad \varepsilon_e(f_e(T_e,\rho)), \quad p_i(f_i(T_i,\rho)), \quad \varepsilon_i(f_i(T_i,\rho)), \quad \mu(f_e(T_e,\rho), f_i(T_i,\rho)), \quad c_{Ve}(f_e(T_e,\rho)),$$

  which makes them inherently dependent $\Rightarrow$ resulting action of EoS is TD consistent.
- We require correct relations to hold between the state variables and their derivatives.
- All variables considered here in their specific form (= per mass) as functions of T and ρ.

The Helmholtz Free Energy (HFE): $f(T, \rho)$

A fundamental thermodynamic quantity, used to express the basic TD quantities in hydro:

- **specific entropy** $s(T, \rho) = -\left(\frac{\partial f}{\partial T}\right)_\rho$,
- **specific internal energy** $\varepsilon(T, \rho) = f + T\,s = f - T\left(\frac{\partial f}{\partial T}\right)_\rho$
- **pressure** $p(T, \rho) = \rho^2 \left(\frac{\partial f}{\partial \rho}\right)_T$.

Useful derived quantities include

- **specific isochoric heat capacity** $c_V(T, \rho) = \left(\frac{\partial \varepsilon}{\partial T}\right)_\rho = T\left(\frac{\partial s}{\partial T}\right)_\rho = -T\frac{\partial^2 f}{\partial T^2}$
- **and the adiabatic speed of sound**

$$c_s(T, \rho) = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\frac{c_P}{c_V}\left(\frac{\partial p}{\partial \rho}\right)_T} = \sqrt{\frac{c_P}{c_V}\frac{\partial}{\partial \rho}\left(\rho^2 \frac{\partial f}{\partial \rho}\right)}$$

$$= \sqrt{2\rho\left(\frac{\partial f}{\partial \rho}\right)_T + \rho^2\left(\frac{\partial^2 f}{\partial \rho^2}\right)_T - \rho^2\left(\frac{\partial^2 f}{\partial T^2}\right)_\rho^{-1}\left(\frac{\partial^2 f}{\partial T \partial \rho}\right)^2}.$$

The Helmholtz Free Energy - "Potentiality"of Quantities

- **The TD quantities originally arise from the HFE differential**

$$\mathrm{d}f = -s\,\mathrm{d}T + \frac{p}{\rho^2}\,\mathrm{d}\rho \qquad \textbf{(1st law of TD)}$$

- **The Helmholtz free energy is a potential, which essentially means that**

$$\frac{\partial^2 f}{\partial T\,\partial \rho} = \frac{\partial^2 f}{\partial \rho\,\partial T}, \qquad \textbf{or, equivalently,} \qquad \frac{\partial p}{\partial T} = -\rho^2\frac{\partial s}{\partial \rho},$$

resp. for pressure and internal energy

$$p - T\frac{\partial p}{\partial T} = \rho^2\frac{\partial \varepsilon}{\partial \rho}.$$

- **NOTE: This also ensures that ε is a potential.**
- **Preserving this property of TD potentials in numerical calculations is important**
- **In practice: Failure to obey all the strict relations $\rightarrow$ inconsistencies in hydro simulation**
  - ◇ **physically incorrect results**

    (e.g.: Non-potential ε $\rightarrow$ work done on the system w/o changing ε $\rightarrow$ violation of TD laws)
  - ◇ **numerical difficulties**
- **We seek to preserve important properties by using a sufficiently high order of interpolation**

Example: The EoS for Monoatomic Ideal Gas

- **pressure** $p(T,\rho) = \frac{N\,k_B\,T}{V(\rho)} = \frac{N\,k_B\,T}{\frac{M}{\rho}} = \frac{N\,k_B\,T\rho}{N\,m_a} = \frac{k_B}{m_a}\,T\,\rho$,
- **specific entropy** $s(T,\rho) = \frac{S}{M} = \frac{k_B}{m_a}\left(\ln\left[\frac{m_a}{\rho}\left(\frac{2\pi\,m_a\,k_B\,T}{h^2}\right)^{\frac{3}{2}}\right] + \frac{5}{2}\right)$,
- **specific internal energy** $\varepsilon(T,\rho) = \frac{U}{M} = \frac{\frac{3}{2}N\,k_B\,T}{N\,m_a} = \frac{3}{2}\frac{k_B}{m_a}T$,
- **specific isochoric heat capacity** $c_V(T,\rho) = \frac{3}{2}\frac{k_B}{m_a}$
- **adiabatic speed of sound** $c_s(T,\rho) = \sqrt{\frac{5}{3}\frac{p}{\rho}} = \sqrt{\frac{5}{3}\frac{k_B\,T}{m_a}}$.

- **All these expressions can be obtained from the specific HFE of monoatomic ideal gas**

$$f(T,\rho) = -\frac{k_B\,T}{m_a}\left(\ln\left[\frac{m_a}{\rho}\left(\frac{2\pi\,m_a\,k_B\,T}{h^2}\right)^{\frac{3}{2}}\right] + 1\right)$$

- **One can easily verify further crucial TD relations, e.g., that HFE the proof that is a potential:**

$$\frac{\partial^2 f}{\partial T\,\partial\rho} = \frac{\partial^2 f}{\partial\rho\,\partial T}, \qquad \textbf{resp.} \qquad p - T\frac{\partial p}{\partial T} = \rho^2\,\frac{\partial\varepsilon}{\partial\rho}.$$

General Physical Requirements on EoS

- **Requirements (obvious or resulting from the TD relations):**
  - **Non-negative fluid pressure and heat capacities:** $p \geq 0$, $c_V \geq 0$, $c_p \geq 0$
  - **Real (non-complex) and non-negative speed of sound:** $c_s \in \mathbb{R}^+$
  - **Non-negative entropy:** $s \geq 0$ (to minimize HFE of the system for maximum entropy)
  - **Internal energy equals to HFE at zero temperature:** $\varepsilon(0, \rho) = f(0, \rho)$.

- **Translating this to Helmholtz free energy f:**
  - f **is monotonically increasing in density** to provide non-negative pressure, $p \geq 0$,
  - f **is monotonically decreasing in temperature,** thus providing non-negative entropy, $s \geq 0$,
  - f **is concave in temperature,** $\frac{\partial^2 f}{\partial T^2} \leq 0$, which ensures that
    - heat capacity is non-negative: $c_V = \frac{\partial \varepsilon}{\partial T} \geq 0$,
    - entropy is monotonically increasing in temperature: $\frac{\partial s}{\partial T} \geq 0$
  - f **satisfies** $\frac{\partial}{\partial \rho}\left(\rho^2 \frac{\partial f}{\partial \rho}\right) \geq 0$, **that is, pressure is monot. increasing in density,** $\frac{\partial p}{\partial \rho} \geq 0$, in order to provide a positive speed of sound: $c_s \in \mathbb{R}^+$

Implementation of EoS - Usual Approach

- **EoS given by discrete values of TD vars (f, p, ε, . . .) on a rectangular grid in the T-ρ space**
- **We want to get the values in a general point (T, ρ).**

- **First choice, most common approach: bilinear *direct interpolation*:**
  - ◇ **Reconstruct each TD variable by linear (dim. split) / bilinear interp. on each bin (T-ρ cell)**
  - ◇ **Direct $\equiv$ interpolation directly applied to discrete data of one given quantity, e.g. p.**
  - ⊕ **Simple, numerically robust**
  - ⊖ **Discontinuous derivatives on bin boundaries $\Rightarrow$ numer. issues, phys. inconsistencies**
  - ◇ **TD quantities particularly difficult** (phase transitions, steep gradients $\Rightarrow$ oscillations.)
  - ◇ **[Kerley et al., 1977]: nice review** motivated by the work with SESAME EoS**, some improvement** thanks to interpolation by rational functions
  - ◇ **TD consistency and physical requirements still largely ignored, for example:**
    - * c_V can be calculated in various ways, equivalent theoretically but not numerically (depending on interp. methods for ε, s, f, on differentiation technique, . . .)
    - * Direct interp. of the discrete values for p and ε does not ensure the existence of HFE satisfying their TD definitions at the same time.

- **From this viewpoint it seems reasonable to apply the *thermodynamic interpolation***
  - $\equiv$ **Interpolate only one state variable, e.g. HFE, and derive the others in a consistent way.**

Consistent & Efficient Interpolation of a General EoS

- **Consistent evaluation of a general EoS based on the Hermite *thermodynamic interpolation* using discrete values of**

$$f, \quad p, \quad \varepsilon, \quad \frac{\partial p}{\partial \rho}, \quad \frac{\partial \varepsilon}{\partial T}, \quad \frac{\partial p}{\partial T}, \quad \frac{\partial \varepsilon}{\partial \rho}$$

  and possibly also higher derivatives, depending on the order of interpolation constructed.

- **Two basic situations: inline EoS and tabulated EoS.**
  - ◇ **Tabulated EoS (given as discrete data):**
    - * **The *TD interpolation* approach provides some additional physical properties, which are usually omitted in hydrodynamic simulations with the bilinear *direct interpolation*.**
    - * **TASK: evaluate the EoS while enforcing physical sanity and the physical consistency inter-relations.**
  - ◇ **Inline EoS library (based on analytical formulas):**
    - * **Interpolation serves mainly to accelerate the evaluation (assuming consistent quant.)**
    - * **However, many of the dependencies ensuring EoS consistency are ignored in existing inline EoS implementations.**
    - * **TASK: substantially accelerate the evaluation of EoS while preserving the same accuracy as with inline calculations, and moreover satisfy all the above physical and thermodynamic constraints.**

Hermite Interpolation

- **Our method is based on the idea from [Swesty & Timmes,1996,2000]: Reconstruct one basic state variable (in our case HFE) by local Hermite-type interpolation of sufficient order.**
- **Hermite interpolation: approximate a general function F by polynomial such, that its values and derivatives up to a certain order at given points agree to those of F.**
  - ◇ **Our use: Reconstruct the HFE on a bin (2D quad in T-ρ space) solely from values and derivatives of HFE at its four corners.** (Hence "local Hermite-type interpolation")
  - ◇ **That is, reconstruct $f(T,\rho)$ from known values and derivatives at discrete points (T,ρ)**
- **To get these discrete input data:**
  - ◇ **HFE directly from the provided EoS library (inline or discrete)**
  - ◇ **Derivatives**
    - ▶ **either from HFE by finite differencing**
    - ▶ **or from p, ε, ... provided by EoS library + corresp. TD relations**

  The latter sounds best, but many consistency issues!
- **Order of interpolation:**
  - ◇ **TD consistency requirements ⇒ at least bicubic interpolation**
    This also provides numerically useful properties (continuous derivatives p and ε).
  - ◇ **[Swesty & Timmes,1996,2000] suggest biquintic** (for further physical and numer. properties)
  - ⊖ **The higher order of interpolation, the more sensitive to the consistency of input data.**
  - ⇒ **With some EoS libraries, one has to**
    - * **use lower order and/or direct interpolation (= give up some TD consistency),**
    - * **or try to automatically detect and correct inconsistencies by pre-processing EoS data**

HerEOS - Part I: Initialization

- ≡ **Creation of interpolation tables (from which the actual interpolation will be constructed):**
  f, f_T, f_ρ, f_{TT}, $f_{\rho\rho}$, $f_{T\rho}$, ... **at given** T-ρ **grid nodes.**
- ▶ **Case 1: Discrete EoS data**
  - ◇ **Simply reuse this grid and load available variables**
    (Typically, the grid is logically rectangular with irregular spacing)
  - ◇ **In most cases, the values of HFE are given.**
  - ◇ **Its derivatives either from the other provided variables (using TD relations) or by FD**
  - ◇ **For higher order interpolations, combine both approches**
  - ◇ **At this point, obvious nonphys. values and inconsistencies can be captured and fixed.**
- ▶ **Case 2: A set of inline functions**
  - ◇ **Construct the** T-ρ **grid as needed (range, spacing, distribution).**
    (Typically a rectangular grid with linear or logarithmic spacing.)
  - ◇ **On it we generate the values of HFE and its derivatives up to the order needed.**
  - ◇ **Derivatives again from derived variables or by finite differencing.**
  - ◇ **Combining these two approaches, we can discover further inconsistencies.**
- • **Done just once as preprocessing step for given EoS and expected** T-ρ **range.**
  - ◇ **Can be stored for reuse with future simulations** $\Rightarrow$ **next time, Part I is skipped.**
  - $\Rightarrow$ **even if costly** (eval. of inline f., sanity checks, consistency repair)**, not a significant burden.**
  - $\Rightarrow$ **even fine** T-ρ **grids can be used** (EoS eval = search of bin + simple interp. formula)

HerEOS - Part II: Calculation of Quantities by Interpolation

≡ **Evaluation of EoS in the actual simulation**

- **To get HFE at given (T, ρ):**
  - **find the appropriate bin of the T-ρ grid** (faster if grid rectangular)
  - **compute the interpolation function from the pre-calculated table.**
- **Values of the derived quantities:**
  - ◇ **easily obtained by using corresponding derivatives of the interpolating formula.**
  - ◇ **advantageous to calculate all desired quantities for given (T, ρ) at once.**

Example: Bicubic interpolation on the bin $[T_{i-1}, T_i] \times [\rho_{j-1}, \rho_j]$

- **16 values needed on input (4 per corner of the bin):**
  - $f^{[00]} = f(T_{i-1}, \rho_{j-1})$, $f^{[10]} = f(T_i, \rho_{j-1})$, $f^{[01]} = f(T_{i-1}, \rho_j)$, $f^{[11]} = f(T_i, \rho_j)$,
  - $f_T^{[00]} = \frac{\partial f}{\partial T}(T_{i-1}, \rho_{j-1})$, $f_T^{[10]} = \frac{\partial f}{\partial T}(T_i, \rho_{j-1})$, $f_T^{[01]} = \dots$, $f_T^{[11]} = \dots$,
  - $f_\rho^{[00]} = \frac{\partial f}{\partial \rho}(T_{i-1}, \rho_{j-1})$, $f_\rho^{[10]} = \frac{\partial f}{\partial \rho}(T_i, \rho_{j-1})$, $f_\rho^{[01]} = \dots$, $f_\rho^{[11]} = \dots$,
  - $f_{T\rho}^{[00]} = \frac{\partial^2 f}{\partial \rho\, \partial T}(T_{i-1}, \rho_{j-1})$, $f_{T\rho}^{[10]} = \frac{\partial^2 f}{\partial \rho\, \partial T}(T_i, \rho_{j-1})$, $f_{T\rho}^{[01]} = \dots$, $f_{T\rho}^{[11]} = \dots$.

- **On this interval, scale T and ρ to unit square**

$$t_i(T) = (T - T_{i-1})/\Delta_i^T, \qquad \Delta_i^T = T_i - T_{i-1}, \qquad r_j(\rho) = (\rho - \rho_{j-1})/\Delta_j^\rho, \qquad \Delta_j^\rho = \rho_j - \rho_{j-1}$$

and introduce local auxiliary functions (cubic Hermite base polynomials)

$$\begin{aligned} G_0(t_i(T)) &= t_i - 3\,t_i^2 + 2\,t_i^3, & H_0(r_j(\rho)) &= 1 - 3\,r_j^2 + 2\,r_j^3, \\ G_1(t_i(T)) &= t_i - 2\,t_i^2 + t_i^3, & H_1(r_j(\rho)) &= r_j - 2\,r_j^2 + r_j^3, \\ G_2(t_i(T)) &= -t_i^2 + t_i^3, & H_2(r_j(\rho)) &= -r_j^2 + r_j^3, \\ G_3(t_i(T)) &= 3\,t_i^2 - 2\,t_i^3, & H_3(r_j(\rho)) &= 3\,r_j^2 - 2\,r_j^3. \end{aligned}$$

- **The value of $f(T,\rho)$ will now be approximated by $\tilde{f}_{i,j}(T,\rho)$ as**

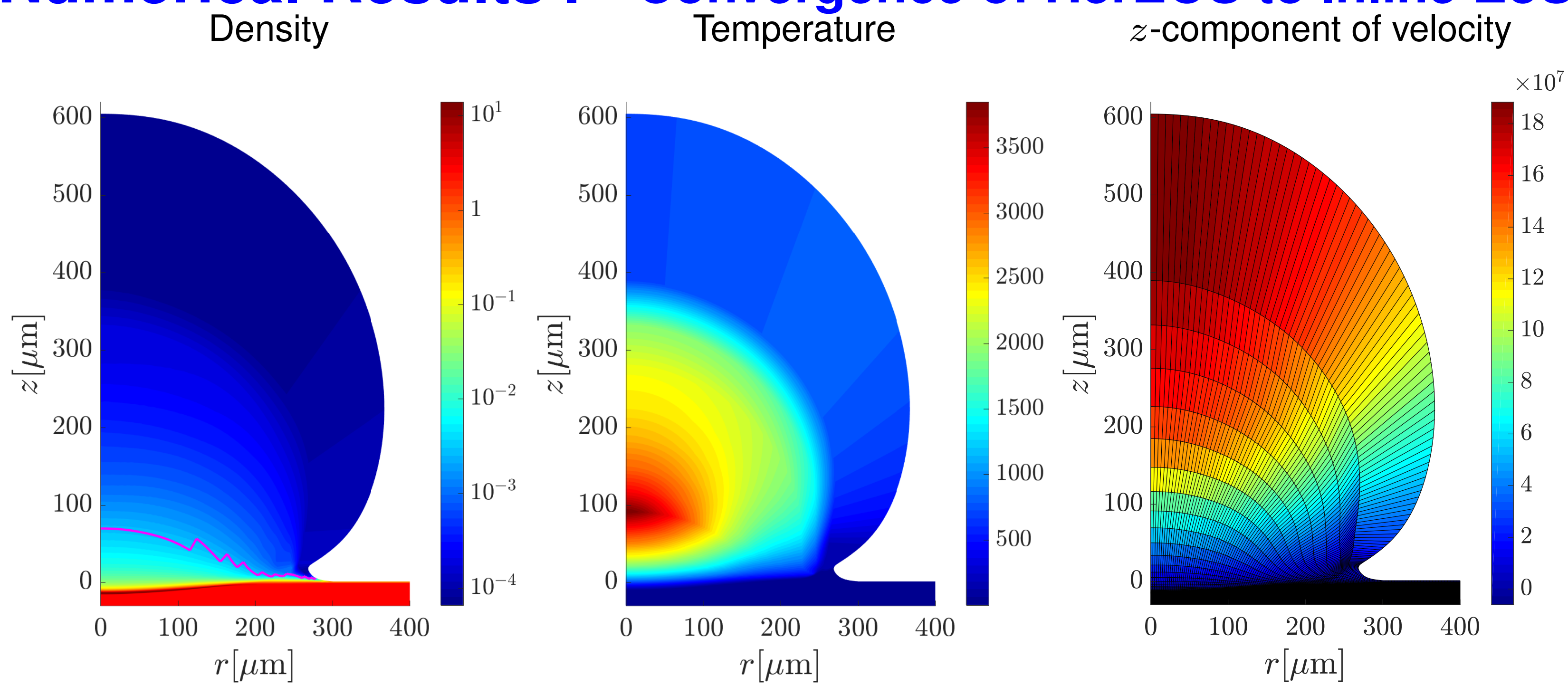
$$\begin{aligned} \tilde{f}_{i,j}(T,\rho) = \;& f^{[00]}\,G_0(T)\,H_0(\rho) + f^{[10]}\,G_3(T)\,H_0(\rho) + f^{[01]}\,G_0(T)\,H_3(\rho) + f^{[11]}\,G_3(T)\,H_3(\rho) \\ & + f_T^{[00]}\,G_1(T)\,H_0(\rho)\,\Delta_i^T + f_T^{[10]}\,G_2(T)\,H_0(\rho)\,\Delta_i^T \\ & + f_T^{[01]}\,G_1(T)\,H_3(\rho)\,\Delta_i^T + f_T^{[11]}\,G_2(T)\,H_3(\rho)\,\Delta_i^T \\ & + f_\rho^{[00]}\,G_0(T)\,H_1(\rho)\,\Delta_j^\rho + f_\rho^{[10]}\,G_3(T)\,H_1(\rho)\,\Delta_j^\rho \\ & + f_\rho^{[01]}\,G_0(T)\,H_2(\rho)\,\Delta_j^\rho + f_\rho^{[11]}\,G_3(T)\,H_2(\rho)\,\Delta_j^\rho \\ & + f_{T\rho}^{[00]}\,G_1(T)\,H_1(\rho)\,\Delta_i^T\,\Delta_j^\rho + f_{T\rho}^{[10]}\,G_2(T)\,H_1(\rho)\,\Delta_i^T\,\Delta_j^\rho \\ & + f_{T\rho}^{[01]}\,G_1(T)\,H_2(\rho)\,\Delta_i^T\,\Delta_j^\rho + f_{T\rho}^{[11]}\,G_2(T)\,H_2(\rho)\,\Delta_i^T\,\Delta_j^\rho. \end{aligned}$$

HerEOS Code - Selected Properties

- **For now works with (includes or uses) several EoS, namely**
  - **ideal polytropic gas,**
  - **QEOS [More et al., 1988],**
  - **MPQeos [Kemp & Meyer-ter-Vehn, 1998],**
  - **FEOS [Faik, 2012, 2018],**
  - **BADGER [Heltemes & Moses, 2012],**
  - **SESAME [Lyon, Johnson et al., 1992].**

  Incorporation of further EoS is straightforward.
- **Particular regime** (interp. order, ways to calculate derivatives) **can be combined for each EoS**
- **General interfaces for C/C++ and Fortran $\Rightarrow$ easy linking to various codes, e.g.**
  - **PALE [Liska et al., 2008, 2011] - 2D ALE hydro + plasma code**
  - **PETE [Holec, 2016] - Lagrangian code, nonlocal transport, high-order curvilinear MFEM**
- **Currently used for comparing various EoS within the same code (seldom done before)**
- **Sanity checks: fast convergence of interp. results to inline values, TD bicubic & biquintic**
- **Speed-up:**
  - **General inline EoS libraries: with TD interp. much faster than with direct inline calc.**
  - **Evaluation of “realistic” EoS usually among the most expensive parts.**
  - **Using denser EoS data interpolation tables** (higher T-ρ resol.) **does not cost much more.**
  - **Higher order *TD interp.* only slightly more expensive than bilin. *direct interp.* & provides more state variables $\Rightarrow$ more complex models w/o additional (incompatible) methods.**

Numerical Results I - Convergence of HerEOS to Inline EoS



- **Laser-target interaction simulated by code PALE in r-z regime**
- $40\,\mu\mathrm{m}$ **thick Al foil irradiated by a normally incident** $100\,\mathrm{J}$ **Nd laser pulse (**$\lambda = 1053\,\mathrm{nm}$**) Gaussian in time and space (**$t_{\mathrm{FWHM}} = 300\,\mathrm{ps}$**, focal spot radius** $r_f = 100\,\mu\mathrm{m}$**).**
- **To start with: very sparse computational mesh (**130×140 **cells)**
- **Situation at** $100\,\mathrm{ps}$ **after maximum intensity of the laser**

Numerical Results I - Convergence of HerEOS to Inline EoS

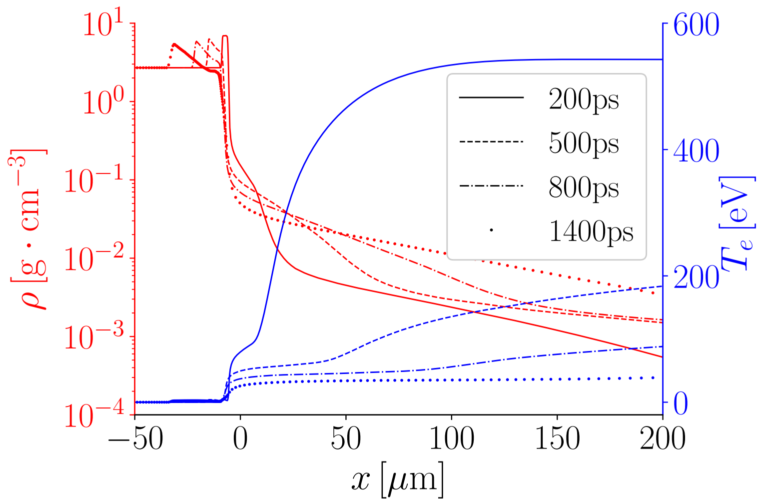
- **To check convergence of *thermodynamic interpolation* to the solution with inline EoS.** (Convergence w.r.t. size of the interp. tables / resolution of T-ρ grid)
- **Ideal gas EoS, $\gamma = 5/3$.** (Too simple, but we need consistent data and enough derivatives)
- **Relative discrepancies at the location of maximum density:**

Number of T-ρ bins	Bicubic ρ	Bicubic p	Bicubic T	Bicubic u_z	Biquintic ρ	Biquintic p	Biquintic T	Biquintic u_z
20×20	1.10e-2	7.71e-2	8.90e-2	3.59e-2	9.87e-3	1.71e-2	7.34e-3	4.41e-3
80×80	1.92e-3	3.44e-2	3.24e-2	2.36e-2	1.01e-5	2.23e-5	1.21e-5	6.83e-6
320×320	8.50e-6	2.02e-5	1.18e-5	4.13e-6	1.29e-6	2.49e-6	1.12e-6	7.11e-7

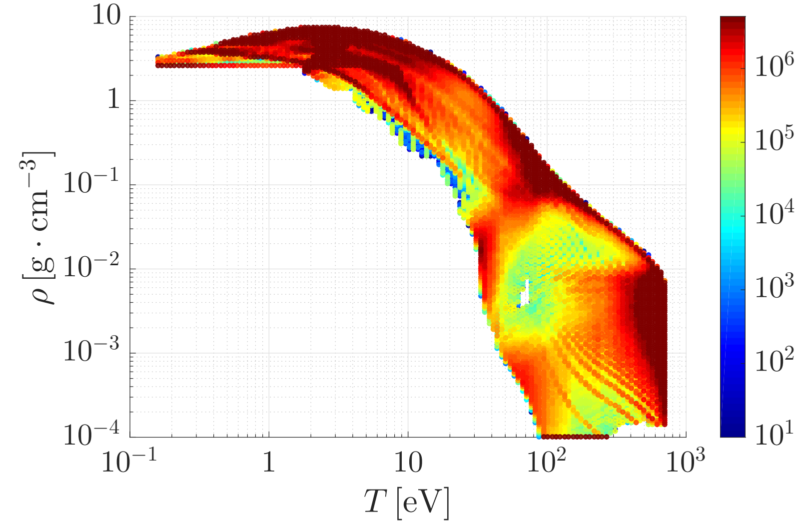
- **Interpolation-based solution is close to the inline-based solution already with very sparse T-ρ grids (low resolution of interp. tables) and quickly converges**
- **This is the case for biquintic as well as bicubic *thermodynamic interpolation*.**

Numerical Results II - LULI Prepulse

ρ and T profiles at certain times



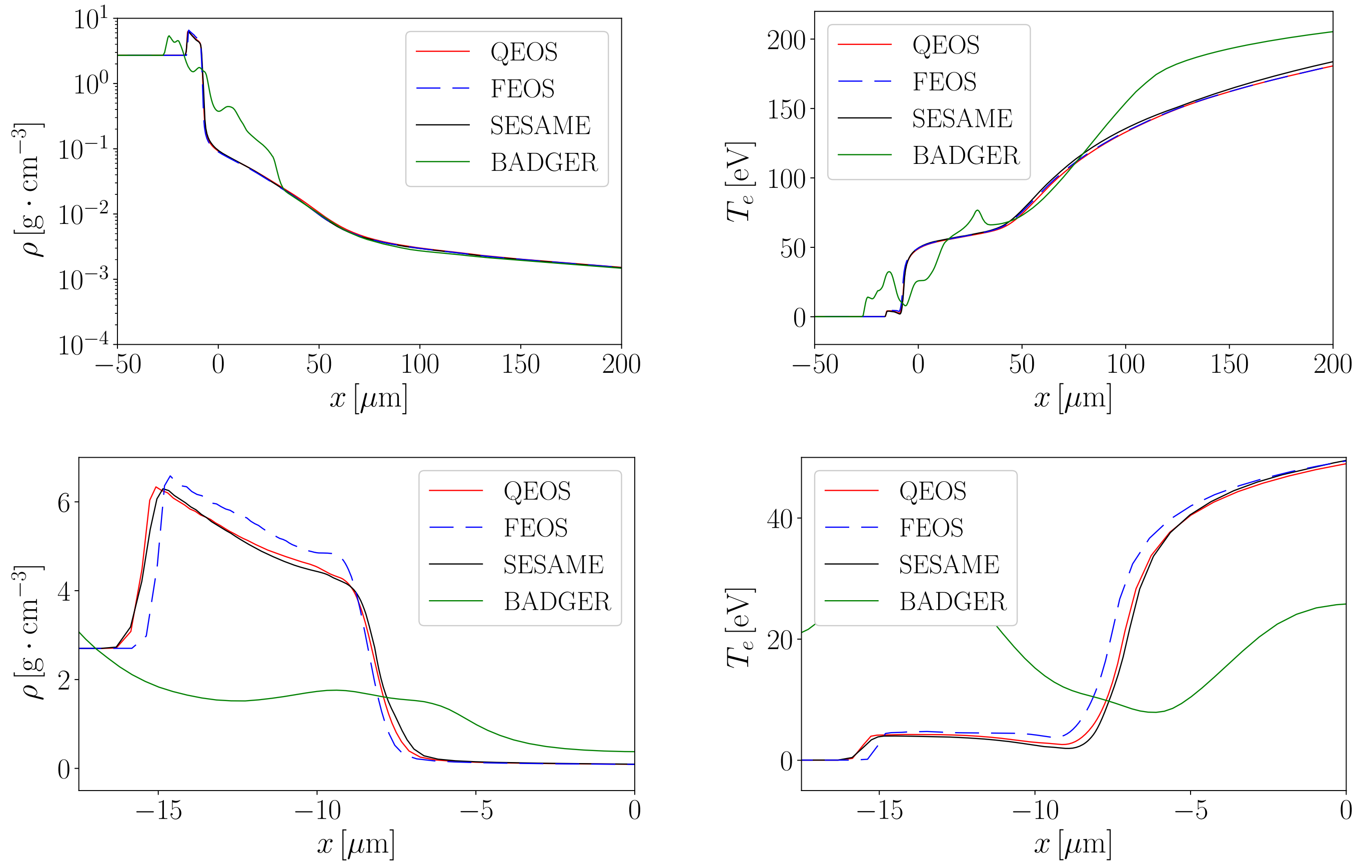
(T-ρ) region of interest & No. of calls



- **To demonstrate the effect of various EoS and assess the efficiency of HerEOS**
- **Like [Fajardo et al., 2001], simulated an experiment for the pre-pulse of $100\,\mathrm{TW}$ LULI laser.**
- **Al target irradiated by a normally incident $600\,\mathrm{ps}$ long (FWHM) laser pulse Gaussian in time as well as space, with peak intensity $I_{\max} = 5{\times}10^{13}\,\mathrm{W}\cdot\mathrm{cm}^{-2}$.**
- **Code PETE run in 1D with $I_{\max}$** (that is, with intensity as on the laser beam axis in the 2D case) **up to final time $1400\,\mathrm{ps}$ after the laser intensity maximum.**
- **Postprocessed data compared to measured values of partial ionization [Fajardo et al., 2001].**

Numerical Results II - LULI Prepulse

① **Comparison of EoS: ρ (left) and T (right), $500\ \mathrm{ps}$ after the laser intensity maximum**

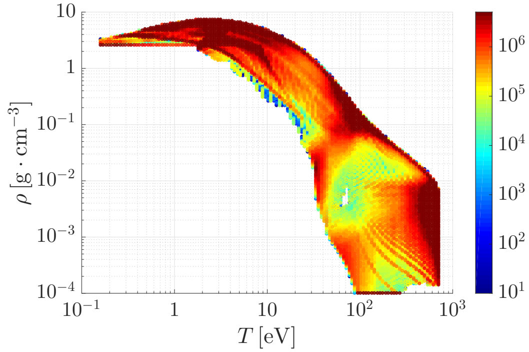


- **All tested EoS behave similarly, except for BADGER** (wave splits into two: irrelevant)
- **Very good correspondence between QEOS and SESAME results.**

Numerical Results II - LULI Prepulse

② Assessment of the efficiency of HerEOS

- **Focus only on the part performing the actual evaluation of EoS:**



"Net time": each bin (rectangular cell) of the region of T-ρ space visited throughout the simulation times the number of visits (color map)

- **Inline FEOS calls replaced by bicubic *TD interpolation* of HFE $\rightarrow$ net time reduced by 23%**
- **Inline FEOS calls replaced by bilinear *direct interp.* of p and ε $\rightarrow$ net time reduced by 60%**
- **As expected, an even better improvement can be obtained for more complicated EoS and for simulations using more derived variables.** (FEOS is still cheap compared to other EoS.)

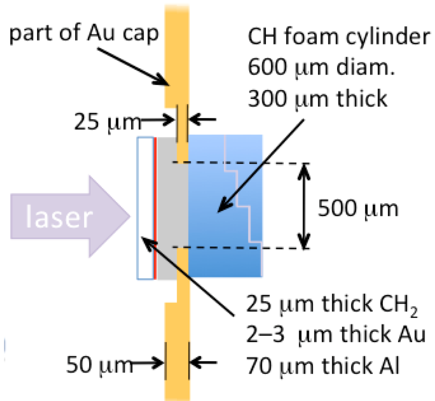
  In our case: replacing inline BADGER by interpolation of BADGER-generated discrete data

  $\rightarrow$ **cost reduced by 97% (bicubic *thermodynamic interpolation*), resp.**

  $\rightarrow$ **cost reduced by 99% (bilinear *direct interpolation*)!**

Numerical Results III - Shock Velocity in Foam at OMEGA

- **Experiment OMEGA, University of Rochester [Falk, Holec et al., 2017, 2018, . . .]**
- **Hydro shock in a polystyrene foam $\rightarrow$ warm dense matter conditions $\rightarrow$ analysis of EoS.**



- **Multi-layer target consisting of**
  - $25\,\mu\text{m}$ **plastic (CH) ablator**
  - 2–$3\,\mu\text{m}$ **Au coating** to shield X-ray radiation
  - $70\,\mu\text{m}$ **Al pusher**
  - $300\,\mu\text{m}$ **of C_8H_8 polystyrene foam ($\rho = 0.14\,\text{g} \cdot \text{cm}^{-3}$)**
- **15 laser beams overlapped $\rightarrow$ planar *square* drive,** $7 \times 10^{14}\,\text{W} \cdot \text{cm}^{-2}$**, duration** $2\,\text{ns}$**,** $\lambda = 351\,\text{nm}$

- **The laser-driven shock gradually propagates through target layers into the foam, where the actual shock velocity is measured experimentally.**
- **TD conditions in the shock wave traveling through the C_8H_8 foam studied with a number of diagnostics developed for the platform including VISAR, SOP and XRTS**
- **Shock velocity measured by an interferometer VISAR system by detecting shock break-out times across four $40\,\mu\text{m}$ steps manufactured on the back side of the target.**
- **Shock break-out times also measured independently by the SOP system**

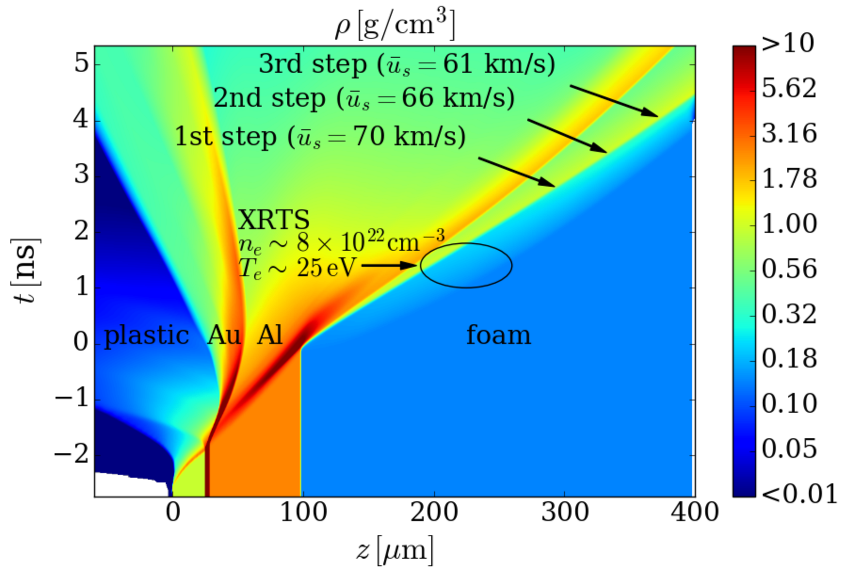
Numerical Results III - Shock Velocity in Foam at OMEGA

- **Measured shock velocities at break-out:** $57.8{\pm}3.8$, $64.0{\pm}4.9$, **resp.** $67.5{\pm}5.0\,\mathrm{km\cdot s^{-1}}$
- **Density colormap from the simulation:**

  ◇ Arrows in the foam layer: positions of steps on the back of target

  ◇ Simulated shock **velocities in very good agreement** with exper. measurements.

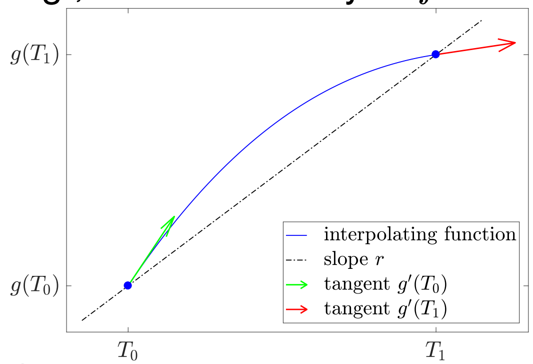
  ◇ **Hugoniot jump condition** analysis: simulated shock velocity **in excellent agreement** with SESAME TD jump conditions at every moment of propagation

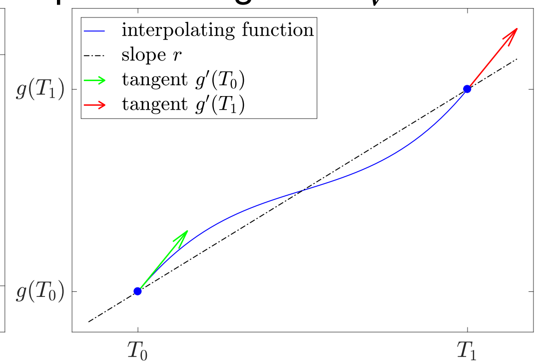


- **Sign of a finite preheat** due to nonlocal electron transport **seen in simulation and experiment**
- **Values of T and ρ extremely sensitive to the EoS model**
  $\Rightarrow$ **proper EoS (here SESAME) is absolutely essential for the hydrodynamic simulation**
- **SESAME tables suffer from serious inconsistency in provided TD quantities (esp. HFE),**
  $\Rightarrow$ **consistent *TD interpolation* of HFE replaced by bilinear *direct interpolation* of p and ε**

Issues with EoS Libraries - Monotonicity, Convexity

- **Practical issues arising with popular EoS libraries (inline as well as discrete)**
- **Even simple tests reveal violations of TD consistency and physical relevance requirements**
  - ◇ e.g., check concavity of f in T to prevent negative c_V.





For a bicubic function:
check if
$$\big(g'(T_0)-r\big)\big(g'(T_1)-r\big) \leq 0,$$
where
$$r = \frac{g(T_1)-g(T_0)}{T_1-T_0}.$$

  - ◇ **Situation gets more complicated**
    - * **with higher-order *thermodynamic interpolations***
    - * **when ρ and p are also taken into account**
- **Same techniques detect places in discrete EoS where values of derived variables (p, ε, . . .) are inconsistent with discrete values of actual HFE and consequently its derivatives**
- **Such inconsistencies thus generate spurious oscillations of the interpolating function**

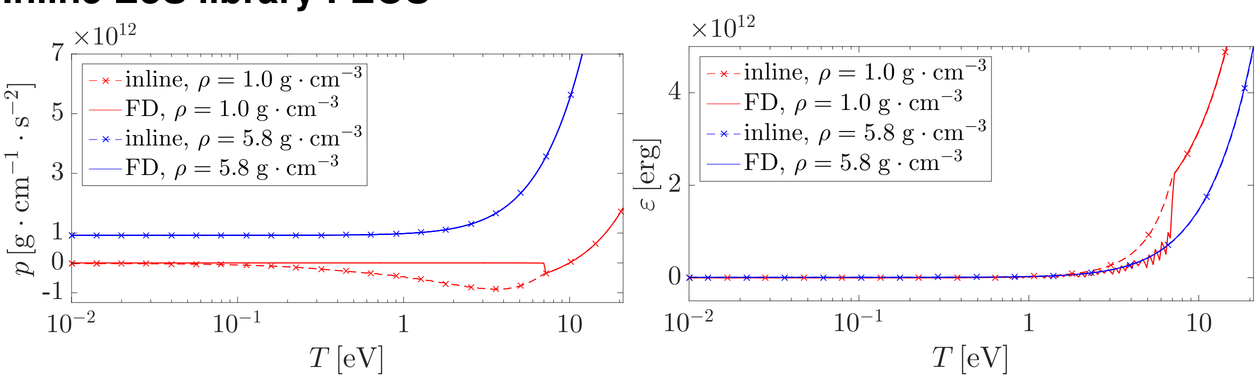
Issues with EoS Libraries - Inconsistent Variables

- **EoS library must obey TD and physical requirements for**
  - **physically relevant results**
  - **stability of the simulation.**
- **HFE usually not explicitly used by codes, but holds the key to consistent EoS calculations**
- **Idea: check the consistency of the HFE values by integrating over its differential as**

$$f(\rho_1, T_1) - f(\rho_0, T_0) = \int_{\rho_0}^{\rho_1} \frac{\partial f}{\partial \rho}\, \mathrm{d}\rho + \int_{T_0}^{T_1} \frac{\partial f}{\partial T}\, \mathrm{d}T = \int_{\rho_0}^{\rho_1} \frac{p}{\rho^2}\, \mathrm{d}\rho - \int_{T_0}^{T_1} s\, \mathrm{d}T,$$

(where p and s are provided by the EoS) **with the value of HFE provided by the EoS.**

- **Or: Compare derivatives of HFE**
  - **calculated from p and ε provided by the EoS**
  - **obtained by applying finite diff. on HFE provided by EoS**
- **Inconsistency found in many EoS libraries, both inline and discrete!**
- **Inline EoS library FEOS**



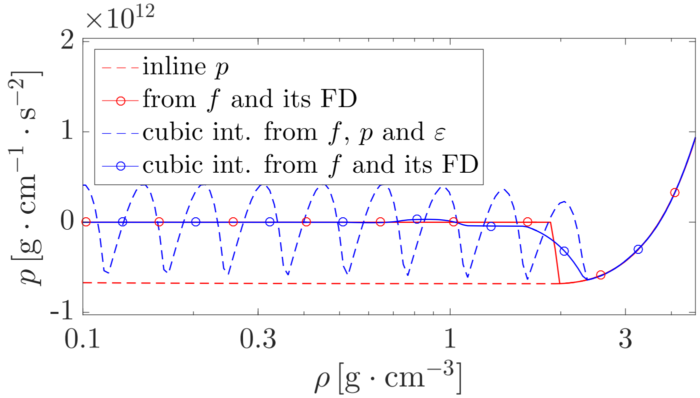
◇ Direct inline call: negative p

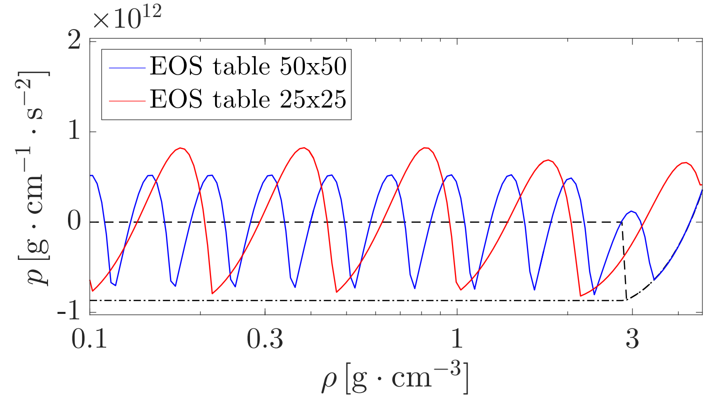
◇ TD interpolation: p almost OK, but ε oscillates

◇ Discrep. due to separate postprocess of p and ε? ◇ No interp. so far, just inline EoS and FD!

Issues with EoS Libraries - Inconsistent Variables

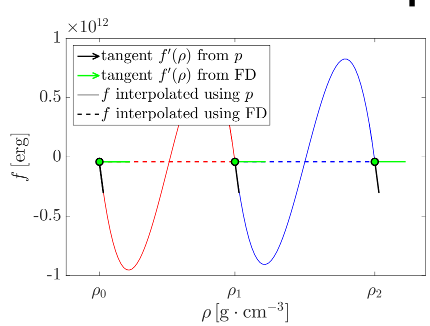
- **Employing bicubic *TD interpolation* on such inconsistent data produces oscillations:**

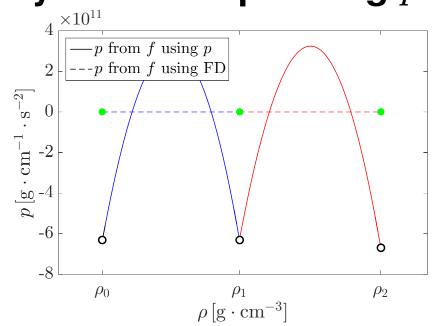




  - ◇ Blue dashed: Inline values of f constant, but inline values of $p \sim \frac{\partial f}{\partial \rho}$ negative $\Rightarrow$ oscillations
  - ◇ Depending on the density of (T, ρ) grid (spacing of EoS data)! - see right Fig.
  - ◇ Blue solid: Using FD helps a bit, but we lose information (not use EoS pressure).

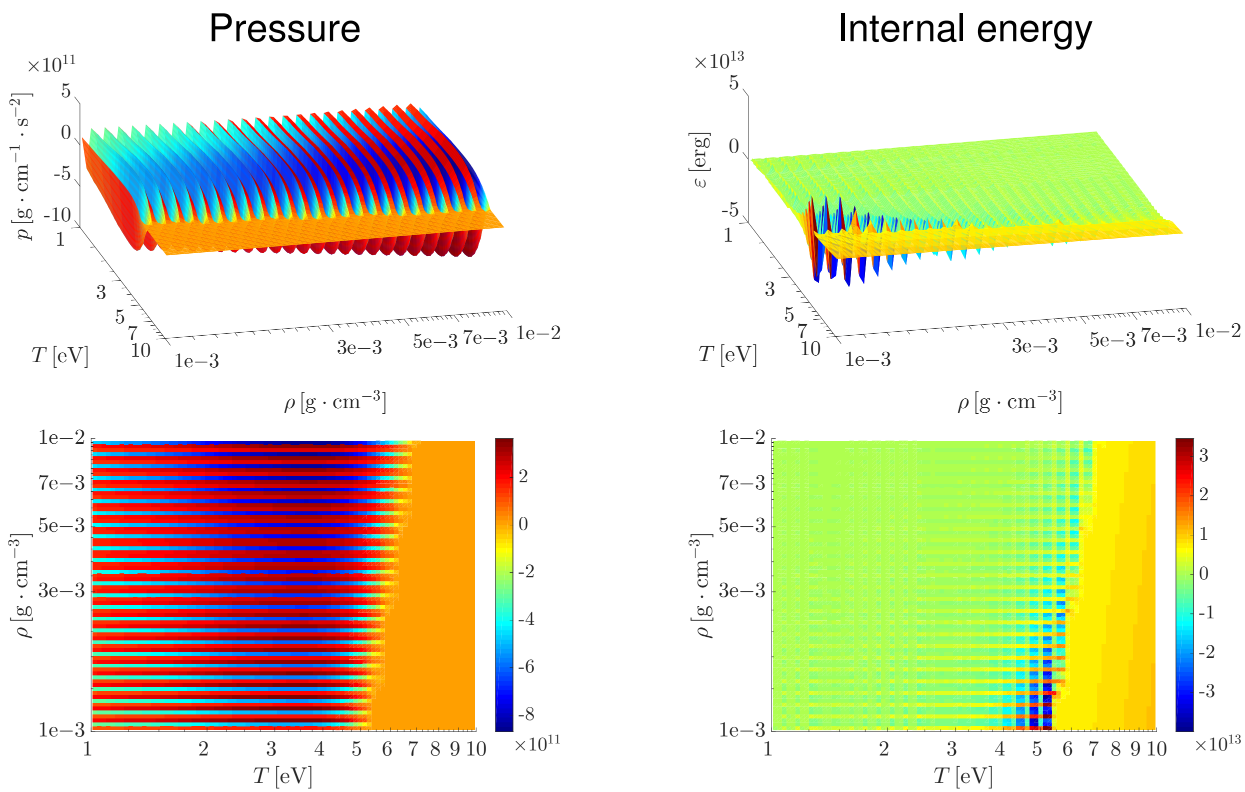
- **Detail of the interpolation of HFE and consequently on corresponding** p





Issues with EoS Libraries - Inconsistent Variables

FEOS for electrons, Al, bicubic *TD interpolation* of f from inline EoS vals of f, p, ε



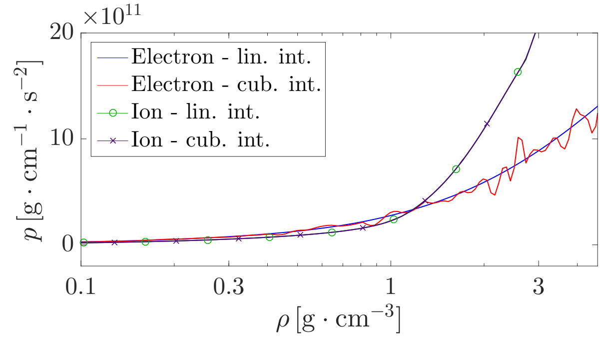
- ◇ Spurious oscillations appear on a wide region of (T, ρ) space, inherent to both p and ε.
- ◇ Regions with $\frac{\partial p}{\partial \rho} < 0 \Rightarrow$ complex speed of sound $\rightarrow$ fails if not treated

- **Unfortunately, using FD to get p and ε does not prevent all the oscillations!**

Issues with EoS Libraries - Inconsistent Variables

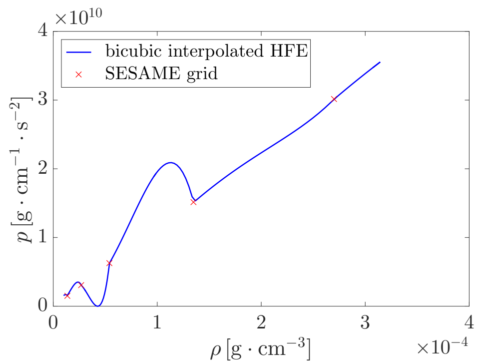
Discrete EoS:

- **SESAME, pressure for electrons and ions,** bicubic *TD interpolation* (red, purple) vs. bilinear *direct interpolation* (blue, green)

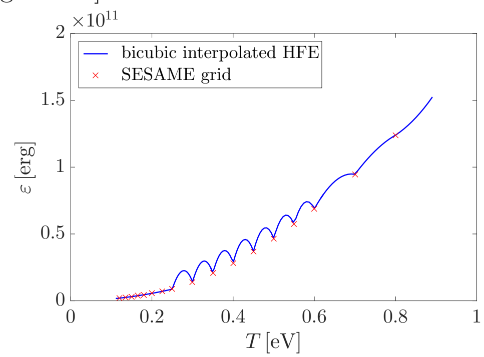


- **SESAME for electrons in Aluminum:**

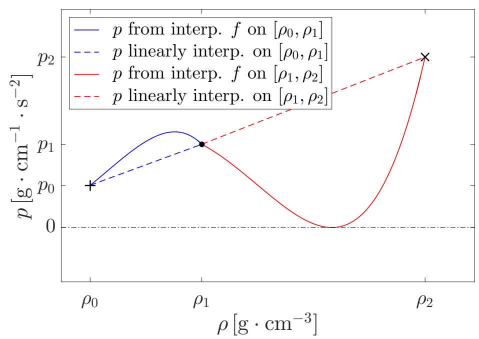
Pressure at $T = 250\,\mathrm{eV}$



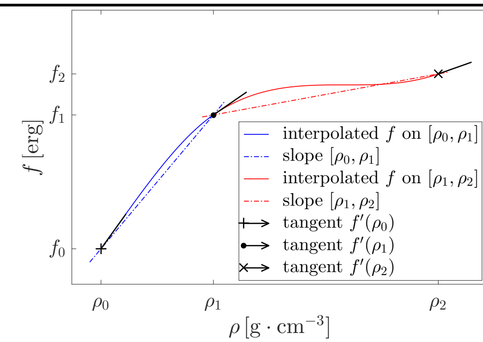
Internal energy at $\rho = 6e\text{-}5\,\mathrm{g/cm}^3$



↑ Pressure, ↑
↑ zoom of ↑



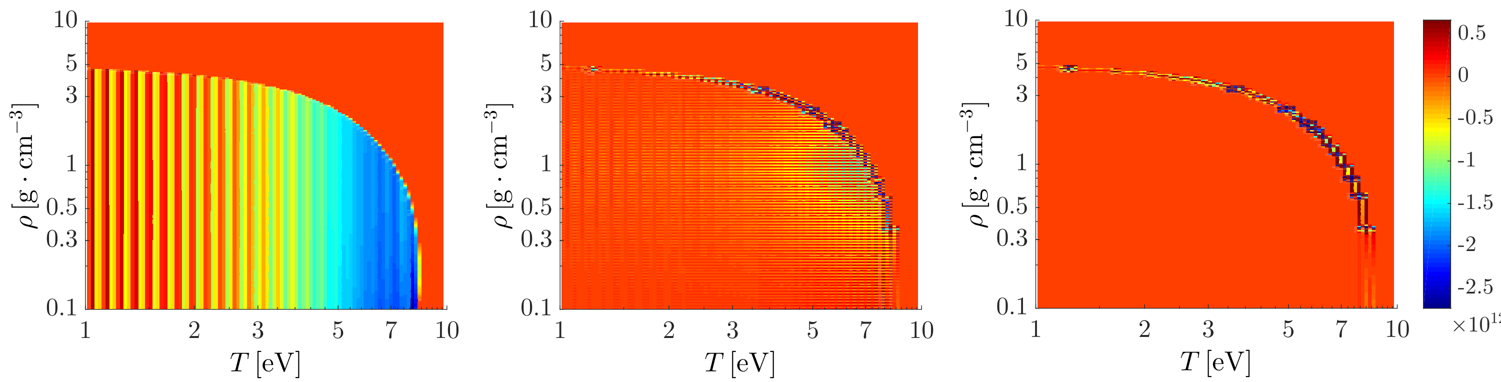
⟵ ⟵ ⟵
HFE corresp. to
⟵ ⟵ ⟵



Issues with EoS Libraries - HFE Not Being a Potential

- **Requirement** $\frac{\partial^2 f}{\partial T\,\partial \rho} = \frac{\partial^2 f}{\partial \rho\,\partial T}$ **can be written as** $p - T\frac{\partial p}{\partial T} = \rho^2\,\frac{\partial \varepsilon}{\partial \rho}$
- **Must hold for any EoS (inline or discrete) at any** (T, ρ) **and can be checked explicitly by FD**
- $\geq$ **Bicubic *TD interp.*** on consistent data **satisfies by definition, *direct interp.* of** p **and** ε **do not**
- **FEOS: Discrepancy** $\mathrm{Err}^{\mathrm{pot}} = p - T\frac{\partial p}{\partial T} - \rho^2\,\frac{\partial \varepsilon}{\partial \rho}$.

Inline HFE values and . . . **inline** p and ε (default for FEOS users) **(left)**
. . . p and ε from **bicubic *TD interpolation*** of HFE **(middle)**
. . . p and ε from **finite differencing** of inline HFE **(right)**

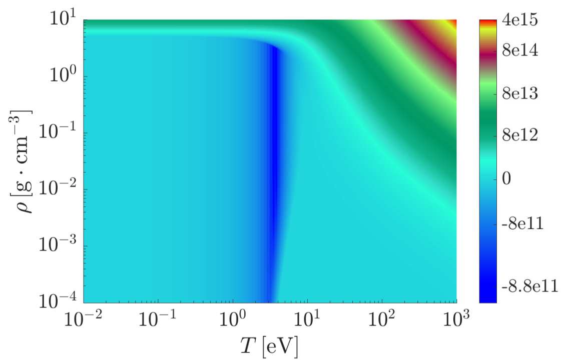


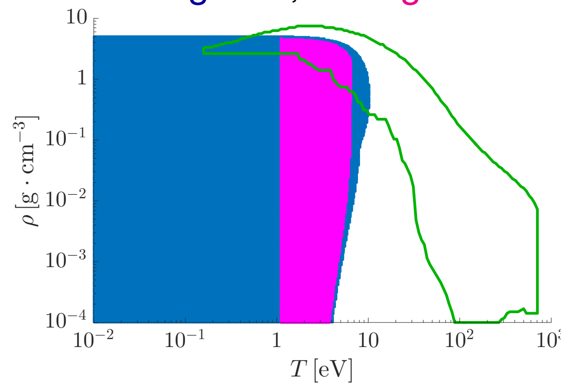
NOTE: Typical pressure in the region $\approx 10^{12}\ \mathrm{g/cm/s^2}$

- **Similar (but less serious) violation of "potentiality" is observed in the discrete SESAME EoS**
- **Suggests to use higher order *TD interpolation* + recover consistency in inconsistent data**

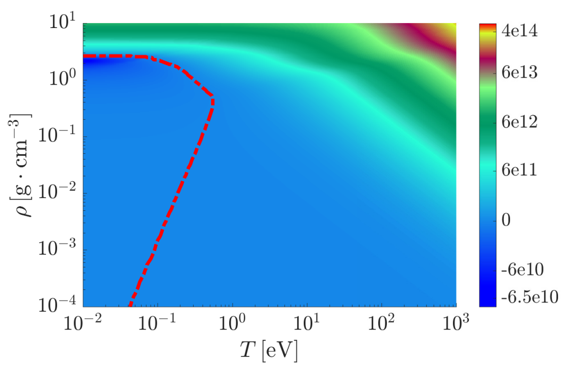
Issues with EoS Libraries - Physical Irrelevance

- **Multiple models combined on the T-ρ domain $\Rightarrow$**
  - **numerical artifacts on transitions**
  - **misuse of model outside validity range**
- **Negative electron pressure given by inline FEOS:** Blue: negative, Magenta: very negative

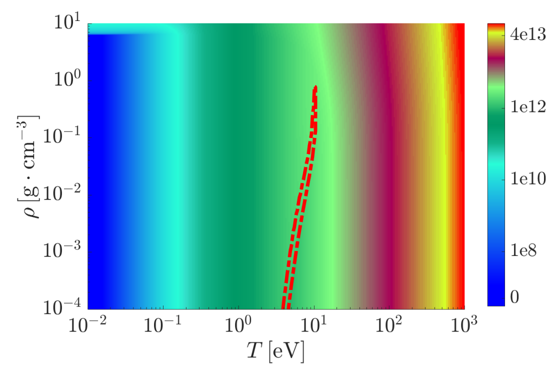




- **SESAME, ion pressure for Aluminum**
  (negative values of pressure)



- **FEOS, ion internal energy for CH**
  (non-monot. ε at phase transition $\Rightarrow c_V < 0$)



Lesson Learned

- **Sometimes data provided by library (inline FEOS, discrete SESAME) are too inconsistent**
  $\Rightarrow$ **constructed *TD interpolation* of HFE too oscillatory**
    $\Rightarrow$ **give up some consistency and use classical bilinear *direct interpolation* of p and ε.**

Summary

- **HerEOS: a library for the evaluation of general EoS by Hermite-type interpolation**
- **Provides some very desirable TD properties**
- **Tested with various inline (analytical) and tabulated EoS**
- **Applied in two-temperature hydrodynamic simulations of laser heated plasma**
- **Tested and used in several multi-D hydro codes in Fortran and C++, Python planned**
- **Significant reduction of computational cost achieved and further reduction expected**
- **For EoS libraries providing inconsistent data, fallback to classical bilin. *direct interpolation***

Future Work

- **Alternative approximation techniques such as surface fitting** (suggested by J. Grove)
- **Detection and automatic correction of obvious flaws in source EoS data** (machine learning)
- HFE often inconsistent with p and ε $\Rightarrow$ **Automatic construction of HFE / its values from p, ε**

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