Building an Entropy based EOS Table

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Thermodynamic entropy potential where the natural variables are the mean density of the system of particles, ρ, electron fraction, $Y_e - \bar{Z}/\bar{A}$, and $Y = 1/\bar{A}$.

$$dS = \frac{1}{T}dE - \frac{P}{\rho^2 T}d\rho - \frac{\mu_e}{T}dN_e - \sum_i \frac{\mu_i}{T}dN_i \tag{1}$$

$$\frac{\partial S}{\partial E} = \frac{1}{T} \tag{2}$$

$$\frac{\partial S}{\partial \rho} = -\frac{P}{\rho^2 T} = -\frac{\partial S}{\partial E}\frac{P}{\rho^2} \tag{3}$$

$$\frac{\partial S}{\partial N_e} = -\frac{\mu_e}{T} = -\frac{\partial S}{\partial E}\mu_e \tag{4}$$

$$\frac{\partial S}{\partial N_i} = -\frac{\mu_i}{T} = -\frac{\partial S}{\partial E}\mu_i \tag{5}$$

How do we get to this step and is this the correct form of the thermodynamic free entropy potential???

$$dS = \frac{1}{T}dE - \frac{P}{\rho^2 T}d\rho - \frac{\mu_e}{T}dY_e - \frac{\mu_{ion}}{T}dY \tag{6}$$

$$\frac{\partial S}{\partial E} = \frac{1}{T} \tag{7}$$

$$\frac{\partial S}{\partial \rho} = -\frac{P}{\rho^2 T} = -\frac{\partial S}{\partial E}\frac{P}{\rho^2} \tag{8}$$

$$\frac{\partial S}{\partial Y_e} = -\frac{\mu_e}{T} = -\frac{\partial S}{\partial E}\mu_e \tag{9}$$

$$\frac{\partial S}{\partial Y} = -\frac{\mu_{ion}}{T} = -\frac{\partial S}{\partial E}\mu_{ion} \tag{10}$$

In the Timmes EOS, the derivatives $d\bar{Z}$ and $d\bar{A}$ are used so it might be helpful to recast the free entropy potential using these derivatives by using $Y_e = \bar{Z}/\bar{A}$ as

$$dY_e = \frac{\partial Y_e}{\partial \bar{Z}}d\bar{Z} + \frac{\partial Y_e}{\partial \bar{A}}d\bar{A} = \frac{1}{\bar{A}}d\bar{Z} - \frac{Y_e}{\bar{A}}d\bar{A} \tag{11}$$

and

$$dY = \frac{\partial Y}{\partial \bar{Z}}d\bar{Z} + \frac{\partial Y}{\partial \bar{A}}d\bar{A} = -\frac{1}{\bar{A}^2}d\bar{A} \tag{12}$$

As such, the entropy potential is written as

$$dS = \frac{1}{T}dE - \frac{P}{\rho^2 T}d\rho - \frac{\mu_e}{T\bar{A}}d\bar{Z} + \left(\frac{\mu_e Y_e + \mu_{ion}}{T\bar{A}^2}\right)d\bar{A} \tag{13}$$

With these derivatives we can check thermodynamic consistenc

$$\left(\frac{\partial S}{\partial \rho}\right)_E + \left(\frac{\partial S}{\partial E}\right)_\rho \frac{P}{\rho^2} = 0 \tag{14}$$

The Maxwell relation for the free entropy is

$$\left(\frac{\partial P}{\partial E}\right)_\rho = \frac{P}{T}\left(\frac{\partial T}{\partial E}\right)_\rho + \frac{\rho^2}{T}\left(\frac{\partial T}{\partial \rho}\right)_E \tag{15}$$

1 Basic Equations

$$P = P_{rad} + P_{ion} + P_{ele} + P_{pos} + P_{coul} \tag{16}$$

$$E = E_{rad} + E_{ion} + E_{ele} + E_{pos} + E_{coul} \tag{17}$$

$$S = S_{rad} + S_{ion} + S_{ele} + S_{pos} + S_{coul} \tag{18}$$

1.1 Radiative Terms

$$P_{rad} = \frac{aT^4}{3} = \frac{a(m_e c^2)^4}{3k^4}\beta^4 \tag{19}$$

$$E_{rad} = \frac{3P_{rad}}{\rho} = \frac{a(m_e c^2)^4}{\rho k^4}\beta^4 \tag{20}$$

$$S^*_{rad} = \frac{P_{rad}/\rho + E_{rad}}{T} \tag{21}$$

where a is related to the Stephan-Boltzmann constant, $\sigma_B = ac/4$ and c is the speed of light.

1.2 Ion Terms

$$N_{ion} = \frac{N_A \rho}{\bar{A}} \tag{22}$$

$$P_{ion} = \frac{N_A k}{\bar{A}}\rho T = \frac{N_A \rho}{\bar{A}}\beta m_e c^2 \tag{23}$$

$$E_{ion} = \frac{3}{2}\frac{P_{ion}}{\rho} = \frac{3}{2}\frac{N_A}{\bar{A}}\beta m_e c^2 \tag{24}$$

$$S^*_{ion} = \frac{P_{ion}/\rho + E_{ion}}{T} + \frac{N_A k}{\bar{A}} log\left[\frac{N_A \rho}{\bar{A}^{5/2}}\left(\frac{N_A h^2}{2\pi kT}\right)^{3/2}\right] = \frac{N_A k}{\bar{A}}\left[\frac{5}{2} - \eta_{ion}\right] \tag{25}$$

where $N_A = 1/1amu$ is used in the Timmes EOS code and h is Planck's constant.

1.3 Electron-Positron Terms

Both stellar EOS routines in FLASH are based on the formalism of a noninteracting Fermi gas for the electrons and positrons. The number density of free electrons N_{ele} and positrons N_{pos} in this formalism is given by

$$N^*_{ele} = \frac{8\pi\sqrt{2}}{h^3} m_e^3 c^3 \beta^{3/2}\left[F_{1/2}(\eta,\beta) + \beta F_{3/2}(\eta,\beta)\right] \tag{26}$$

$$N_{pos} = \frac{8\pi\sqrt{2}}{h^3} m_e^3 c^3 \beta^{3/2}\left[F_{1/2}(-\eta - 2\beta,\beta) + \beta F_{3/2}(-\eta - 2\beta,\beta)\right] \tag{27}$$

where m_e is the electron rest mass, the relativity parameter β is

$$\beta = kT/(m_e c^2) \tag{28}$$

and the normalized chemical potential energy μ of electrons is

$$\eta = \mu/kT, \tag{29}$$

and $F_k(\eta,\beta)$ is the Fermi-Dirac integral

$$F_k(\eta,\beta) = \int_0^\infty \frac{x^k(1 + 0.5\beta x)^{1/2}dx}{\exp(x - \eta) + 1} \tag{30}$$

The normalized chemical potential η in this formalism has the rest mass energy of the electrons subtracted out. This means that the positron chemical potential must have the rest mass terms appear explicitly, $\eta_{pos} = -\eta - 2/\beta$ as it does in (27).

For complete ionization, the number density of free electrons in the matter is

$$N_{ele,matter} = \frac{\bar{Z}}{\bar{A}} N_A^* \rho = \bar{Z} N_{ion}, \tag{31}$$

and charge neutrality requires

$$N_{ele,matter} = N_{ele} - N_{pos} \tag{32}$$

Solving equation (32) determines the normalized chemical potential η, which was the only unknown. Such a solution fulfills the chemical potentials role as the Lagrange multiplier that was originally introduced to constrain the distribution function to have the correct number of particles. Solving equation (32) in practice means using a one-dimensional root find method to obtain the root η.

Once η is known from the solution of equation (32), the pressure, specific internal energy, and entropy due to the free electrons and positrons are

$$P_{ele}^* = \frac{16\pi\sqrt{2}}{3h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(\eta, \beta) + \frac{1}{2}\beta F_{5/2}(\eta, \beta) \right] \tag{33}$$

$$P_{pos}^* = \frac{16\pi\sqrt{2}}{3h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(-\eta - 2/\beta, \beta) + \frac{1}{2}\beta F_{5/2}(-\eta - 2/\beta, \beta) \right] \tag{34}$$

$$E_{ele} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(\eta, \beta) + \beta F_{5/2}(\eta, \beta) \right] \tag{35}$$

$$E_{pos} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(-\eta - 2/\beta, \beta) + \beta F_{5/2}(-\eta - 2/\beta, \beta) \right] + \frac{2 m_e c^2 N_{pos}}{\rho} \tag{36}$$

$$S_{ele} = \frac{P_{ele}/\rho + E_{ele}}{T} - \frac{k\eta N_{ele}}{\rho} \tag{37}$$

$$S_{pos} = \frac{P_{pos}/\rho + E_{pos}}{T} + \frac{k\eta_{pos} N_{pos}}{\rho} \tag{38}$$

1.4 Coulomb Corrections

The equations for the Coulomb corrections are gathered from the Timmes EOS code and Fryxell et al. [2000]. The electron sphere radius is given by

$$a_{ele} = \left(\frac{1}{\frac{4\pi}{3} \bar{Z} N_{ion}} \right)^{1/3} \tag{39}$$

$$\Gamma_{ele} = \frac{k_q e^2}{a_{ele}} \frac{1}{kT} \tag{40}$$

where, in cgs units, the Coulomb constant, $k_q = 1$. The radius for an ion sphere is

$$a_{ion} = \bar{Z}^{1/3} a_{ele} \tag{41}$$

$$\Gamma = \bar{Z}^{5/3} \Gamma_{ele} = \frac{k_q \bar{Z}^2 e^2}{a_{ion}} \frac{1}{kT} \tag{42}$$

$$f(\Gamma) = \begin{cases} a_1 \Gamma + b_1 \Gamma^{1/4} + c_1 \Gamma^{-1/4} + d_1 & \text{if } \Gamma > 1 \\ -\frac{3^{1/2}}{2} \Gamma^{3/2} + a_2 \Gamma^{b_2} & \text{if } \Gamma \leq 1 \end{cases} \tag{43}$$

$$g(\Gamma) = \begin{cases} a_1 \Gamma + 4 b_1 \Gamma^{1/4} - 4 c_1 \Gamma^{-1/4} + d_1 \ln \Gamma + e_1 & \text{if } \Gamma > 1 \\ -\frac{1}{3^{1/2}} \Gamma^{3/2} + \frac{a_2}{b_2} \Gamma^{b_2} & \text{if } \Gamma \leq 1 \end{cases} \tag{44}$$

where the constants $a_1 = -0.898004$, $b_1 = 0.96786$, $c_1 = 0.220703$, $d_1 = -0.86097$, $e_1 = 2.5269$ are taken from Ogata and Ichimaru [1987]. The remaining constants used are $a_2 = 0.29561$, $b_2 = 1.9885$, and $c_2 = 1/(2\sqrt{3}) = 0.288675$. The c_2 term is necessary in the Timmes EOS because $f(\Gamma \leq 1)/3$ is used and the c_2 is found as the coefficient for the first term in $f(\Gamma \leq 1)$. Incidentally, the two functions are related by, $f = \Gamma dg/d\Gamma$.

$$E_{coul} = \frac{P_{ion}}{\rho} f(\Gamma) \leq 0 \tag{45}$$

$$P_{coul} = \frac{P_{ion}}{3} f(\Gamma) \leq 0 \tag{46}$$

$$S_{coul} = -\frac{N_A k}{\bar{A}} [g(\Gamma) - f(\Gamma)] = -\frac{P_{ion}}{\rho T} [g(\Gamma) - f(\Gamma)] \leq 0 \tag{47}$$

Note that this form of the Entropy is not the same as Fryxell et al. [2000] which is

$$S_{coul} = \frac{N_A k T}{\bar{A}} \Gamma^2 \frac{dg(\Gamma)}{d\Gamma} = \frac{P_{ion}}{\rho} \Gamma^2 \frac{dg(\Gamma)}{d\Gamma} \tag{48}$$

and it is not clear where this difference comes from and whether there is a typo here. If we attempt to make the Coulomb corrections take a more standard form than

$$S_{coul} = \frac{P'_{coul}/\rho + E'_{coul}}{T} \tag{49}$$

where $E'_{coul} = E_{coul}$ and $P'_{coul} = -P_{ion} g$ using (44).

2 Solving the Fermi-Dirac Integrals

// The Fermi-Dirac integrals are solved following the model of Aparicio 1998 and coded in the Timmes EOS Fortran routine. From the Aparicio 1998 paper, the integral is found to be most accurate when broken into four separate integrals

$$F_k(\eta, \beta) = \int_0^\infty \frac{x^k (1 + \beta x/2)^{1/2} dx}{\exp(x - \eta) + 1} = \underbrace{\int_0^{S_1} f_1(x = z^2) dx}_{(1)} + \underbrace{\int_{S_1}^{S_2} f_2(x) dx}_{(2)} + \underbrace{\int_{S_2}^{S_3} f_2(x) dx}_{(3)} + \underbrace{\int_{S_3}^{\infty} f_2(x) dx}_{(4)} \tag{50}$$

For f_1 and f_2, the integrand of the generalized Fermi-Dirac integrand is rewritten based on two conditions:

$$f_1(z) = \begin{cases} \frac{2z^{2k+1}\sqrt{1+z^2\beta/2}}{\exp(z^2-\eta)+1}, & \text{if } (z - \eta) < 100; \\ 2z^{2k+1}\sqrt{1 + z^2\beta/2}\exp(\eta - z^2), & \text{otherwise;} \end{cases} \tag{51}$$

$$f_2(x) = \begin{cases} \frac{x^k\sqrt{1+x\beta/2}}{\exp(x-\eta)+1}, & \text{if } (x - \eta) < 100; \\ x^k\sqrt{1 + x\beta/2}\exp(\eta - x), & \text{otherwise;} \end{cases} \tag{52}$$

- Integrals (1), (2), and (3) use Gauss-Legendre (G-Le) quadrature for calculating the integrals
- Integral (4) uses Gauss-Laguerre (G-La) quadrature to calculate the integral

3 Calculating the Minimum Energy

A minimum energy for a completley degenerate gas is given in the limit that $T = 0$ and $\eta = \mu/kT \to \infty$ We start by first finding the Fermi momentum, p_F, by solving (31) in the above limit. As such, neglecting any contribution from positrons yields the equation:

$$\frac{\bar{Z}}{\bar{A}} N_A^* \rho = N_{ele} = \frac{2}{h^3} \int_0^{p_F} 4\pi p^2 dp = \frac{8\pi}{3h^3} p_F^3 \to p_F = \left(\frac{\bar{Z}}{\bar{A}} N_A^* \rho \frac{3h^3}{8\pi} \right)^{1/3} \tag{53}$$

The total energy over all possible states is rewritten from (35) as

$$E_{ele} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \int_0^\infty \frac{(x\beta)^{3/2}(1+0.5x\beta)^{1/2}(1+x\beta)}{\exp(x-\eta)+1}\beta dx \tag{54}$$

Recall that in the above equation, $\beta = kT/mc^2$, $\eta = \mu/kT$, and $x = E_{kin}/kT$. With the inclusion of relativistic corrections the kinetic energy is given by

$$E_{kin} = mc^2 \left[\left[\left(\frac{p}{mc} \right)^2 + 1 \right]^{1/2} - 1 \right] = E_p - mc^2 \tag{55}$$

The minimum energy is calculated by integrating the above equation from 0 to x_F where the subscript F denotes the the Fermi energy and associated momentum. In this limit, $[\exp(x-\eta)+1]^{-1} \rightarrow 1$ so the integral may be rewritten as

$$E_{min} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \int_0^{x_F} (x\beta)^{3/2}(1+0.5x\beta)^{1/2}(1+x\beta)\beta dx \tag{56}$$

We now make the substitution $\theta = x\beta = E_{kin}/mc^2$. The integral in (56) is then written as

$$E_{min} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \int_0^{\theta_F} (\theta)^{3/2}(1+0.5\theta)^{1/2}(1+\theta)d\theta \tag{57}$$

NOTE: I have not been able to find an analytic solution to the above integral but I could determine it numerically. However we can take a look at some limiting cases for the integrand

$$g(\theta) = \theta^{3/2}(1+0.5\theta)^{1/2}(1+\theta) \tag{58}$$

$$\lim_{\theta\rightarrow 0} g(x) = \theta^{3/2} + 1.25\theta^{5/2} + 0.21875\theta^{7/2} - 0.0234374\theta^{9/2} + \mathcal{O}(\theta^{11/2}) \tag{59}$$

$$\lim_{\theta\rightarrow\infty} g(x) = 0.707107\theta^3 + 1.41421\theta^2 + 0.353553\theta + \mathcal{O}(\sqrt{1/\theta}) \tag{60}$$

The integrals in these limits can then be computed,

$$\int_0^{\theta_F} \lim_{\theta\rightarrow 0} g(x)dx = 0.4\theta_F^{5/2} + 0.357143\theta_F^{7/2} + 0.0486111\theta_F^{9/2} - 0.004261136\theta_F^{11/2} + \cdots \tag{61}$$

$$\int_0^{\theta_F} \lim_{\theta\rightarrow\infty} g(x)dx = 0.176777\theta_F^4 + 0.471403\theta_F^3 + 0.176777\theta_F^2 + \cdots \tag{62}$$

$$E_{min} = \frac{2}{h}\int_0^{p_F} \left(p^2c^2 + m_e^2c^4\right)^{1/2} 4\pi p^2 dp = \frac{m_e c^2}{\lambda_e^3}\chi(x) = \frac{m_e c^2}{8\pi^2\lambda_e^3}\left[x(1+x^2)^{1/2}(1+2x^2) - \ln\left[x + (1+x^2)^{1/2}\right]\right] \tag{63}$$

Thus an approximation for the minimum energy can be made using the above integrals and the prefactor from (56). These approximations describe the values obtained from Timmes EOS scheme and the current EOS scheme being written.

4 Using the Entropy-based EOS Table

The new EOS table contains values for the entropy and entropy derivatives with respect to energy, E, density, ρ, Ye, and Y.

$$T = \left(\frac{\partial S}{\partial E}\right)^{-1} \tag{64}$$

$$\frac{\partial T}{\partial E} = -T^2 \frac{\partial^2 S}{\partial E^2} \tag{65}$$

$$\frac{\partial T}{\partial \rho} = -T^2 \frac{\partial^2 S}{\partial \rho \partial E} \tag{66}$$

$$P = -\rho^2 T \frac{\partial S}{\partial \rho} \tag{67}$$

$$\frac{\partial P}{\partial E} = \frac{P}{T}\frac{\partial T}{\partial E} - \rho^2 T \frac{\partial^2 S}{\partial E \partial \rho} \tag{68}$$

$$\frac{\partial P}{\partial \rho} = -\rho^2 T \frac{\partial^2 S}{\partial \rho^2} + \frac{T}{\rho}\frac{P}{T} + \frac{P}{T}\frac{\partial T}{\partial \rho} \tag{69}$$

5 Gaussian Process

In order to generate an interpolation of enetropy and its derivatives by gaussian process, we begin by assuming there exists a large four-dimensional lattice. For this section, the four dimensions are energy denoted by w, density denoted by x, Ye denoted by y, and $1/\bar{A}$ denoted by z. We assume that a single four dimensional cell or hypercube in this lattice is composed of N vertices or points where the entropy, its four first derivatives, and ten second derivatives are saved. The smallest hypercube has $N = 16$ points and we will assume below that we are interpolating somewhere inside a single hypercube, $c = 1$.

5.1 Setting up covariance matrix

Interpolation by gaussian process begins by building the covariance matrix. For this work we use a squared exponential covariance kernel, $\mathbf{k}$, that is constructed using a set of N points described by a four variable vector $\mathbf{x}_i = (w_i, x_i, y_i, z_i)$ and $\mathbf{x}_j = (w_j, x_j, y_j, z_j)$ where $i, j = 1 - N$. An $N \times N$ matrix, $\mathbf{k}$ is generate with each element given by

$$k(\mathbf{x}_i, \mathbf{x}_j) = k_{ij} = \sigma_f^2 \exp\left[-\frac{1}{2}\left[\frac{(w_i - w_j)^2}{\ell_{w,c}^2} + \frac{(x_i - x_j)^2}{\ell_{x,c}^2} + \frac{(y_i - y_j)^2}{\ell_{y,c}^2} + \frac{(z_i - z_j)^2}{\ell_{z,c}^2}\right]\right] \tag{70}$$

where the hyperparameters $\sigma_f = 1$ is the maximum variance and $\ell_{w,c}$, $\ell_{x,c}$, $\ell_{y,c}$, $\ell_{z,c}$ are the length scales in the four directions that are specific to each cell, c, and not to the points. Note that k_{ij} has a maximum value of 1 when $i = j$ for instance or when the length scales are very large. The minimum value is zero, as in when, for fixed length scales, the distance between points at i and j are very large for instance.

The first derivatives can be constructed as follows

$$\left[\frac{\partial \mathbf{k}}{\partial w_i}, \frac{\partial \mathbf{k}}{\partial x_i}, \frac{\partial \mathbf{k}}{\partial y_i}, \frac{\partial \mathbf{k}}{\partial z_i}\right] = -\left[\frac{(w_i - w_j)}{\ell_{w,c}^2}, \frac{(x_i - x_j)}{\ell_{x,c}^2}, \frac{(y_i - y_j)}{\ell_{y,c}^2}, \frac{(z_i - z_j)}{\ell_{z,c}^2}\right]\mathbf{k} \tag{71}$$

$$\left[\frac{\partial \mathbf{k}}{\partial w_j}, \frac{\partial \mathbf{k}}{\partial x_j}, \frac{\partial \mathbf{k}}{\partial y_j}, \frac{\partial \mathbf{k}}{\partial z_j}\right] = \left[\frac{(w_i - w_j)}{\ell_{w,c}^2}, \frac{(x_i - x_j)}{\ell_{x,c}^2}, \frac{(y_i - y_j)}{\ell_{y,c}^2}, \frac{(z_i - z_j)}{\ell_{z,c}^2}\right]\mathbf{k} \tag{72}$$

$$\left[\frac{\partial^2 \mathbf{k}}{\partial w_i^2}, \frac{\partial^2 \mathbf{k}}{\partial x_i^2}, \frac{\partial^2 \mathbf{k}}{\partial y_i^2}, \frac{\partial^2 \mathbf{k}}{\partial z_i^2}\right] = \left[\left(\frac{(w_i - w_j)^2}{\ell_{w,c}^4} - \frac{1}{\ell_{w,c}^2}\right), \left(\frac{(x_i - x_j)^2}{\ell_{x,c}^4} - \frac{1}{\ell_{x,c}^2}\right), \left(\frac{(y_i - y_j)^2}{\ell_{y,c}^4} - \frac{1}{\ell_{y,c}^2}\right), \left(\frac{(z_i - z_j)^2}{\ell_{z,c}^4} - \frac{1}{\ell_{z,c}^2}\right)\right]\mathbf{k} \tag{73}$$

Note that

$$\left[\frac{\partial^2 \mathbf{k}}{\partial w_i^2}, \frac{\partial^2 \mathbf{k}}{\partial x_i^2}, \frac{\partial^2 \mathbf{k}}{\partial y_i^2}, \frac{\partial^2 \mathbf{k}}{\partial z_i^2}\right] = \left[\frac{\partial^2 \mathbf{k}}{\partial w_j^2}, \frac{\partial^2 \mathbf{k}}{\partial x_j^2}, \frac{\partial^2 \mathbf{k}}{\partial y_j^2}, \frac{\partial^2 \mathbf{k}}{\partial z_j^2}\right] \tag{74}$$

Here are some mixed partial examples

$$\frac{\partial^2 \mathbf{k}}{\partial w_i \partial x_i} = \frac{\partial^2 \mathbf{k}}{\partial w_j \partial x_j} = \left(\frac{(w_i - w_j)}{\ell_{w,c}^2}\right)\left(\frac{(x_i - x_j)}{\ell_{x,c}^2}\right)\mathbf{k} \tag{75}$$

$$\frac{\partial^2 \mathbf{k}}{\partial w_i \partial x_j} = \frac{\partial^2 \mathbf{k}}{\partial w_j \partial x_i} = -\left(\frac{(w_i - w_j)}{\ell_{w,c}^2}\right)\left(\frac{(x_i - x_j)}{\ell_{x,c}^2}\right)\mathbf{k} \tag{76}$$

The other derivatives are found in a similar way. The joint covariance matrix includes the weights for the standard covariance as well as the the gradient and Laplacian terms:

$$\mathbf{K} = \begin{bmatrix} \mathbf{k} & \frac{\partial \mathbf{k}}{\partial w_j} & \frac{\partial \mathbf{k}}{\partial x_j} & \frac{\partial \mathbf{k}}{\partial y_j} & \frac{\partial \mathbf{k}}{\partial z_j} & \frac{\partial^2 \mathbf{k}}{\partial w_j^2} & \frac{\partial^2 \mathbf{k}}{\partial w_j \partial x_j} & \cdots & \frac{\partial^2 \mathbf{k}}{\partial y_j \partial z_j} & \frac{\partial^2 \mathbf{k}}{\partial z_j^2} \\ \frac{\partial \mathbf{k}}{\partial w_i} & \frac{\partial^2 \mathbf{k}}{\partial w_i \partial w_j} & \frac{\partial^2 \mathbf{k}}{\partial w_i \partial x_j} & \frac{\partial^2 \mathbf{k}}{\partial w_i \partial y_j} & \frac{\partial^2 \mathbf{k}}{\partial w_i \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial w_i \partial w_j^2} & \frac{\partial^3 \mathbf{k}}{\partial w_i \partial w_j \partial x_j} & \cdots & \frac{\partial^3 \mathbf{k}}{\partial w_i \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial w_i \partial z_j^2} \\ \frac{\partial \mathbf{k}}{\partial x_i} & \frac{\partial^2 \mathbf{k}}{\partial x_i \partial w_j} & \frac{\partial^2 \mathbf{k}}{\partial x_i \partial x_j} & \frac{\partial^2 \mathbf{k}}{\partial x_i \partial y_j} & \frac{\partial^2 \mathbf{k}}{\partial x_i \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial x_i \partial w_j^2} & \frac{\partial^3 \mathbf{k}}{\partial x_i \partial w_j \partial x_j} & \cdots & \frac{\partial^3 \mathbf{k}}{\partial x_i \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial x_i \partial z_j^2} \\ \frac{\partial \mathbf{k}}{\partial y_i} & \frac{\partial^2 \mathbf{k}}{\partial y_i \partial w_j} & \frac{\partial^2 \mathbf{k}}{\partial y_i \partial x_j} & \frac{\partial^2 \mathbf{k}}{\partial y_i \partial y_j} & \frac{\partial^2 \mathbf{k}}{\partial y_i \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial w_j^2} & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial w_j \partial x'} & \cdots & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial z_j^2} \\ \frac{\partial \mathbf{k}}{\partial z_i} & \frac{\partial^2 \mathbf{k}}{\partial z_i \partial w_j} & \frac{\partial^2 \mathbf{k}}{\partial z_i \partial x_j} & \frac{\partial^2 \mathbf{k}}{\partial z_i \partial y_j} & \frac{\partial^2 \mathbf{k}}{\partial z_i \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial z_i \partial w_j^2} & \frac{\partial^3 \mathbf{k}}{\partial z_i \partial w_j \partial x_j} & \cdots & \frac{\partial^3 \mathbf{k}}{\partial z_i \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}}{\partial z_i \partial z_j^2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial^2 \mathbf{k}}{\partial y_i \partial z_i} & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial z_i \partial w_j} & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial z_i \partial x_j} & \frac{\partial^3 k}{\partial y_i \partial z_i \partial y_j} & \frac{\partial^3 \mathbf{k}}{\partial y_i \partial z_i \partial z_j} & \frac{\partial^4 \mathbf{k}}{\partial y_i \partial z_i \partial w_j^2} & \frac{\partial^4 \mathbf{k}}{\partial y_i \partial z_i \partial w_j \partial x_j} & \cdots & \frac{\partial^4 \mathbf{k}}{\partial y_i \partial z_i \partial y_j \partial z_j} & \frac{\partial^4 \mathbf{k}}{\partial y_i \partial z_i \partial z_j^2} \\ \frac{\partial^2 \mathbf{k}}{\partial z_i^2} & \frac{\partial^3 \mathbf{k}}{\partial z_i^2 \partial w_j} & \frac{\partial^3 \mathbf{k}}{\partial z_i^2 \partial x_j} & \frac{\partial^3 \mathbf{k}}{\partial z_i^2 \partial y_j} & \frac{\partial^3 \mathbf{k}}{\partial z_i^2 \partial z_j} & \frac{\partial^4 \mathbf{k}}{\partial z_i^2 \partial w_j^2} & \frac{\partial^4 \mathbf{k}}{\partial z_i^2 \partial w_j \partial x_j} & \cdots & \frac{\partial^4 \mathbf{k}}{\partial z_i^2 \partial y_j \partial z_j} & \frac{\partial^4 \mathbf{k}}{\partial z_i^2 \partial z_j^2} \end{bmatrix} + \sigma_n \mathbf{I} \tag{77}$$

To be clear, the joint covariance is composed of the known or training points. The largest, $\mathbf{K}$ will be is $15N \times 15N$ if all derivatives are included. The point for interpolation is given by $\mathbf{x}^* = (w^*, x^*, y^*, z^*)$. A covariance matrix, $\mathbf{k}^*$ can be made between the training points and the interpolating variables, each element is definfed by

$$k(\mathbf{x}^*, \mathbf{x}_j) = k_j^* = \sigma_f^2 \exp\left[-\frac{1}{2}\left[\frac{(w^* - w_j)^2}{\ell_{w,c}^2} + \frac{(x^* - x_j)^2}{\ell_{x,c}^2} + \frac{(y^* - y_j)^2}{\ell_{y,c}^2} + \frac{(z^* - z_j)^2}{\ell_{z,c}^2}\right]\right] \tag{78}$$

By using a single interpolating point, $\mathbf{k}^*$ is a $1 \times N$ vector. The following are several examples of the partial derivatives.

$$\left[\frac{\partial \mathbf{k}^*}{\partial w^*}, \frac{\partial \mathbf{k}^*}{\partial x^*}, \frac{\partial \mathbf{k}^*}{\partial y^*}, \frac{\partial \mathbf{k}^*}{\partial z^*}\right] = -\left[\frac{(w^* - w_j)}{\ell_{w,c}^2}, \frac{(x^* - x_j)}{\ell_{x,c}^2}, \frac{(y^* - y_j)}{\ell_{y,c}^2}, \frac{(z^* - z_j)}{\ell_{z,c}^2}\right]\mathbf{k} \tag{79}$$

$$\left[\frac{\partial \mathbf{k}^*}{\partial w_j}, \frac{\partial \mathbf{k}^*}{\partial x_j}, \frac{\partial \mathbf{k}^*}{\partial y_j}, \frac{\partial \mathbf{k}^*}{\partial z_j}\right] = \left[\frac{(w^* - w_j)}{\ell_{w,c}^2}, \frac{(x^* - x_j)}{\ell_{x,c}^2}, \frac{(y^* - y_j)}{\ell_{y,c}^2}, \frac{(z^* - z_j)}{\ell_{z,c}^2}\right]\mathbf{k}^* \tag{80}$$

$$\left[\frac{\partial^2 \mathbf{k}^*}{\partial w^{*2}}, \frac{\partial^2 \mathbf{k}^*}{\partial x^{*2}}, \frac{\partial^2 \mathbf{k}^*}{\partial y^{*2}}, \frac{\partial^2 \mathbf{k}^*}{\partial z^{*2}}\right] = \left[\left(\frac{(w^* - w_j)^2}{\ell_{w,c}^4} - \frac{1}{\ell_{w,c}^2}\right), \left(\frac{(x^* - x_j)^2}{\ell_{x,c}^4} - \frac{1}{\ell_{x,c}^2}\right), \left(\frac{(y^* - y_j)^2}{\ell_{y,c}^4} - \frac{1}{\ell_{y,c}^2}\right), \left(\frac{(z^* - z_j)^2}{\ell_{z,c}^4} - \frac{1}{\ell_{z,c}^2}\right)\right]\mathbf{k}^* \tag{81}$$

$$\left[\frac{\partial^2 \mathbf{k}^*}{\partial w^{*2}}, \frac{\partial^2 \mathbf{k}^*}{\partial x^{*2}}, \frac{\partial^2 \mathbf{k}^*}{\partial y^{*2}}, \frac{\partial^2 \mathbf{k}^*}{\partial z^{*2}}\right] = \left[\frac{\partial^2 \mathbf{k}^*}{\partial w_j^2}, \frac{\partial^2 \mathbf{k}^*}{\partial x_j^2}, \frac{\partial^2 \mathbf{k}^*}{\partial y_j^2}, \frac{\partial^2 \mathbf{k}^*}{\partial z_j^2}\right] \tag{82}$$

$$\frac{\partial^2 \mathbf{k}^*}{\partial w^* \partial x^*} = \frac{\partial^2 \mathbf{k}^*}{\partial w_j \partial x_j} = \left(\frac{(w^* - w_j)}{\ell_{w,c}^2}\right)\left(\frac{(x^* - x_j)}{\ell_{x,c}^2}\right)\mathbf{k}* \tag{83}$$

$$\frac{\partial^2 \mathbf{k}^*}{\partial w^* \partial x_j} = \frac{\partial^2 \mathbf{k}^*}{\partial w_j \partial x^*} = -\left(\frac{(w^* - w_j)}{\ell_{w,c}^2}\right)\left(\frac{(x^* - x_j)}{\ell_{x,c}^2}\right)\mathbf{k}^* \tag{84}$$

The full matrix is then given by

$$
\mathbf{K}^* = \begin{bmatrix}
\mathbf{k}^* & \frac{\partial \mathbf{k}^*}{\partial w_j} & \frac{\partial \mathbf{k}^*}{\partial x_j} & \frac{\partial \mathbf{k}^*}{\partial y_j} & \frac{\partial \mathbf{k}^*}{\partial z_j} & \frac{\partial^2 \mathbf{k}^*}{\partial w_j^2} & \frac{\partial^2 \mathbf{k}^*}{\partial w_j \partial x_j} & \cdots & \frac{\partial^2 \mathbf{k}^*}{\partial y_j \partial z_j} & \frac{\partial^2 \mathbf{k}^*}{\partial z_j^2} \\
\frac{\partial \mathbf{k}^*}{\partial w^*} & \frac{\partial^2 \mathbf{k}^*}{\partial w^* \partial w_j} & \frac{\partial^2 \mathbf{k}^*}{\partial w * \partial x_j} & \frac{\partial^2 \mathbf{k}^*}{\partial w^* \partial y_j} & \frac{\partial^2 \mathbf{k}^*}{\partial w^* \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial w^* \partial w_j^2} & \frac{\partial^3 \mathbf{k}^*}{\partial w^* \partial w_j \partial x_j} & \cdots & \frac{\partial^3 \mathbf{k}^*}{\partial w^* \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial w^* \partial z_j^2} \\
\frac{\partial \mathbf{k}^*}{\partial x^*} & \frac{\partial^2 \mathbf{k}^*}{\partial x^* \partial w_j} & \frac{\partial^2 \mathbf{k}^*}{\partial x^* \partial x_j} & \frac{\partial^2 \mathbf{k}^*}{\partial x^* \partial y_j} & \frac{\partial^2 \mathbf{k}^*}{\partial x^* \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial x^* \partial w_j^2} & \frac{\partial^3 \mathbf{k}^*}{\partial x^* \partial w_j \partial x_j} & \cdots & \frac{\partial^3 \mathbf{k}^*}{\partial x^* \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial x^* \partial z_j^2} \\
\frac{\partial \mathbf{k}^*}{\partial y^*} & \frac{\partial^2 \mathbf{k}^*}{\partial y^* \partial w_j} & \frac{\partial^2 \mathbf{k}^*}{\partial y^* \partial x_j} & \frac{\partial^2 \mathbf{k}^*}{\partial y^* \partial y_j} & \frac{\partial^2 \mathbf{k}^*}{\partial y^* \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial y^* \partial w_j^2} & \frac{\partial^3 \mathbf{k}^*}{\partial y^* \partial w_j \partial x'} & \cdots & \frac{\partial^3 \mathbf{k}^*}{\partial y^* \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial y^* \partial z_j^2} \\
\frac{\partial \mathbf{k}^*}{\partial z^*} & \frac{\partial^2 \mathbf{k}^*}{\partial z^* \partial w_j} & \frac{\partial^2 \mathbf{k}^*}{\partial z^* \partial x_j} & \frac{\partial^2 \mathbf{k}^*}{\partial z^* \partial y_j} & \frac{\partial^2 \mathbf{k}^*}{\partial z^* \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial z^* \partial w_j^2} & \frac{\partial^3 \mathbf{k}^*}{\partial z^* \partial w_j \partial x_j} & \cdots & \frac{\partial^3 \mathbf{k}^*}{\partial z^* \partial y_j \partial z_j} & \frac{\partial^3 \mathbf{k}^*}{\partial z^* \partial z_j^2} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{\partial^2 \mathbf{k}^*}{\partial y^* \partial z^*} & \frac{\partial^3 \mathbf{k}^*}{\partial y^* \partial z^* \partial w_j} & \frac{\partial^3 \mathbf{k}^*}{\partial y^* \partial z^* \partial x_j} & \frac{\partial^3 k^*}{\partial y^* \partial z^* \partial y_j} & \frac{\partial^3 \mathbf{k}}{\partial y^* \partial z^* \partial z_j} & \frac{\partial^4 \mathbf{k}^*}{\partial y^* \partial z^* \partial w_j^2} & \frac{\partial^4 \mathbf{k}^*}{\partial y^* \partial z^* \partial w_j \partial x_j} & \cdots & \frac{\partial^4 \mathbf{k}^*}{\partial y^* \partial z^* \partial y_j \partial z_j} & \frac{\partial^4 \mathbf{k}^*}{\partial y^* \partial z^* \partial z_j^2} \\
\frac{\partial^2 \mathbf{k}^*}{\partial z^{*2}} & \frac{\partial^3 \mathbf{k}^*}{\partial z^{*2} \partial w_j} & \frac{\partial^3 \mathbf{k}^*}{\partial z^{*2} \partial x_j} & \frac{\partial^3 \mathbf{k}^*}{\partial z^{*2} \partial y_j} & \frac{\partial^3 \mathbf{k}^*}{\partial z^{*2} \partial z_j} & \frac{\partial^4 \mathbf{k}^*}{\partial z_i^2 \partial w_j^2} & \frac{\partial^4 \mathbf{k}^*}{\partial z^{*2} \partial w_j \partial x_j} & \cdots & \frac{\partial^4 \mathbf{k}^*}{\partial z^{2*} \partial y_j \partial z_j} & \frac{\partial^4 \mathbf{k}^*}{\partial z^{*2} \partial z_j^2}
\end{bmatrix} \tag{85}
$$

The size of $\mathbf{K}^*$ is $15 \times 15N$ if first and second derivatives are included.

5.2 Finding the optimum hyperparameters

We compute the optimum values for the four length scales $[\ell_{w,c}, \ell_{w,c}, \ell_{y,c}, \ell_{z,c}]$ by minimizing the log marginal likelihood function determined trhought the following steps

1. $L = \text{cholesky}(\mathbf{K})$: The cholesky decomposition is done using numpy in python, np.linalg.cholesky(K)
2. $\alpha = L^\top \setminus (L \setminus [\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}])$: This factor is found using scipy in python, scipy.linalg.cho_factor(K,f)
3. $\log p([\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}]|x) = -0.5 \left([\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}]^\top \alpha + 2 \sum_i \log L_{ii} + n/2 \log(2\pi) \right)$: log marginal likelihood function where n is the size of the matrix

In order to find the length scales that minimize the log marginal likelihood function, a Nelder-Mead method in python is used.

5.3 Computing the posterior

Given a new set of variables, $\mathbf{x}^*$, the posterior or interpolated value, $\mathbf{f}^* \approx f(\mathbf{x}^*)$, can be determined and its posterior mean and covariance is given by

$$
[\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}](\mathbf{x}^*) = \mathbf{K}^* \mathbf{K}^{-1} [\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}]^\top \tag{86}
$$

$$
\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - (\bar{\mathbf{k}}^*)^\top \mathbf{K}^{-1} \bar{\mathbf{k}}^* \tag{87}
$$

So if we are only considering interpolating for entropy, S and the first two derivatives for energy, E, and density ρ then

$$
\left[S^*, \frac{\partial S^*}{\partial E}, \frac{\partial S^*}{\partial \rho} \right] = \mathbf{K^*}_{3 \times 3N} \mathbf{K}^{-1}_{3N \times 3N} \left[S_{1 \dots N}, \frac{\partial S}{\partial E}_{1 \dots N}, \frac{\partial S}{\partial \rho}_{1 \dots N} \right]^\top \tag{88}
$$

where, for this problem, $\mathbf{K^*}_{3 \times 3N}$ is a $3 \times 3N$ matrix and $\mathbf{K}^{-1}$ is a $3N \times 3N$ matrix.

References

B. Fryxell, K. Olson, P. Ricker, F. Timmes, M. Zingale, D. Lamb, P. MacNeice, R. Rosner, J. W. Truran, and H. Tufo. Flash: An adaptive mesh hydrodynamics code for modeling astrophysical thermonuclear flashes. *Astrophys. J. Supp. Series*, 131:273, 2000.

Shuji Ogata and Setsuo Ichimaru. Critical examination of n dependence in the monte carlo calculations for a classical one-component plasma. *Phys. Rev. A*, 36:5451–5454, Dec 1987. doi: 10.1103/PhysRevA.36.5451. URL https://link.aps.org/doi/10.1103/PhysRevA.36.5451.