Building an Entropy based EOS Table

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Abstract

In traditional EOS routines the electron positron EOS is based on table interpolation of the Helmholtz free energy $F(\rho, T)$ created from a biquintic Hermite polynomial interpolating function.

In this work, we want to create and entropy base interpolating function, $S(\rho, \epsilon_{tot})$ that uses the natural variables used in used by the hydrodynamics solvers.

$$d\epsilon = TdS + \frac{P}{\rho^2}d\rho \tag{1}$$

$$dS = \frac{1}{T}d\epsilon - \frac{P}{T\rho^2}d\rho \tag{2}$$

where $S = S(\rho, \epsilon)$, $T = T(\rho, \epsilon)$, and $P = P(\rho, \epsilon)$.

$$\left.\frac{\partial S}{\partial \epsilon}\right|_{\rho} = \frac{1}{T} \tag{3}$$

$$\left.\frac{\partial S}{\partial \rho}\right|_{\epsilon} = -\frac{P}{T\rho^2} \tag{4}$$

$$\left.\frac{\partial^2 S}{\partial \epsilon^2}\right|_{\rho} = -\frac{1}{T^2}\left.\frac{\partial T}{\partial \epsilon}\right|_{\rho} = -\frac{1}{T^2}\left(\left.\frac{\partial \epsilon}{\partial T}\right|_{\rho}\right)^{-1} \tag{5}$$

$$\left.\frac{\partial^2 S}{\partial \rho^2}\right|_{\epsilon} = \frac{2P}{T\rho^3} - \frac{1}{\rho^2}\left[-\frac{P}{T^2}\left.\frac{\partial T}{\partial \rho}\right|_{\epsilon} + \frac{1}{T}\left.\frac{\partial P}{\partial \rho}\right|_{\epsilon}\right] \tag{6}$$

$$\frac{\partial^2 S}{\partial \epsilon \partial \rho} = -\frac{1}{\rho^2}\left[-\frac{P}{T^2}\left.\frac{\partial T}{\partial \epsilon}\right|_{\rho} + \frac{1}{T}\left.\frac{\partial P}{\partial \epsilon}\right|_{\rho}\right] = \frac{\partial^2 S}{\partial \rho \partial \epsilon} = -\frac{1}{T^2}\left.\frac{\partial T}{\partial \rho}\right|_{\epsilon} = -\frac{1}{T^2}\left.\left(\frac{\partial \rho}{\partial T}\right)^{-1}\right|_{\epsilon} \tag{7}$$

1 Basic Equations

$$P_{tot} = P_{rad} + P_{ion} + P_{ele} + P_{pos} \tag{8}$$

$$\epsilon_{tot} = \epsilon_{rad} + \epsilon_{ion} + \epsilon_{ele} + \epsilon_{pos} \tag{9}$$

$$S_{tot} = S_{rad} + S_{ion} + S_{ele} + S_{pos} \tag{10}$$

1.1 Radiative Terms

$$P_{rad} = \frac{aT^4}{3} = \frac{a(m_e c^2)^4}{3k^4}\beta^4 \tag{11}$$

$$\epsilon_{rad} = \frac{3P_{rad}}{\rho} = \frac{a(m_e c^2)^4}{\rho k^4}\beta^4 \tag{12}$$

$$S^*_{rad} = \frac{P_{rad}/\rho + \epsilon_{rad}}{T} \tag{13}$$

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

1.2 Ion Terms

$$N_{ion} = \frac{N_A \rho}{\bar{A}} \tag{14}$$

$$P_{ion} = \frac{N_A k}{\bar{A}} \rho T = \frac{N_A \rho}{\bar{A}} \beta m_e c^2 \tag{15}$$

$$\epsilon_{ion} = \frac{3}{2} \frac{P_{ion}}{\rho} = \frac{3}{2} \frac{N_A}{\bar{A}} \beta m_e c^2 \tag{16}$$

$$S^*_{ion} = \frac{P_{ion}/\rho + \epsilon_{ion}}{T} + \frac{N_A k}{\bar{A}} log \left[\frac{N_A \rho}{\bar{A}^{5/2}} \left(\frac{N_A h^2}{2\pi kT} \right)^{3/2} \right] = \frac{N_A k}{\bar{A}} \left[\frac{5}{2} - \eta_{ion} \right] \tag{17}$$

where $N_A = 1/1amu$ is used in the Timmes EOS code and h is Planck's constant. Now for the derivatives of S_{ion}

$$\left. \frac{\partial S_{ion}}{\partial \rho} \right|_\epsilon = \frac{N_A k}{\bar{A}} \left. \frac{\partial \eta_{ion}}{\partial \rho} \right|_\epsilon \tag{18}$$

$$\left. \frac{\partial^2 S_{ion}}{\partial \rho^2} \right|_\epsilon = \frac{N_A k}{\bar{A}} \left. \frac{\partial^2 \eta_{ion}}{\partial \rho^2} \right|_\epsilon \tag{19}$$

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

$$N^*_{ele} = \frac{8\pi\sqrt{2}}{h^3} m_e^3 c^3 \beta^{3/2} \left[F_{1/2}(\eta, \beta) + \beta F_{3/2}(\eta, \beta) \right] \tag{20}$$

$$N_{pos} = \frac{8\pi\sqrt{2}}{h^3} m_e^3 c^3 \beta^{3/2} \left[F_{1/2}(-\eta - 2\beta, \beta) + \beta F_{3/2}(-\eta - 2\beta, \beta) \right] \tag{21}$$

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

$$\beta = kT/(m_e c^2) \tag{22}$$

and the normalized chemical potential energy μ of electrons is

$$\eta = \mu/kT, \tag{23}$$

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

$$F_k(\eta, \beta) = \int_0^\infty \frac{x^k (1 + 0.5\beta x)^{1/2} dx}{\exp(x - \eta) + 1} \tag{24}$$

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 (21).

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

$$N_{ele,matter} = \frac{\bar{Z}}{\bar{A}} N^*_A \rho = \bar{Z} N_{ion}, \tag{25}$$

and charge neutrality requires

$$N_{ele,matter} = N_{ele} - N_{pos} \tag{26}$$

In order to calculate $\frac{\partial^2 S}{\partial \rho \partial \epsilon}$ from (55), the density can be written in terms of the temperature.

$$\rho = \frac{1}{N_A} \frac{\bar{A}}{\bar{Z}} \left[N_{ele} - N_{pos} \right] \tag{27}$$

Solving equation (26) 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 (26) in practice means using a one-dimensional root find method to obtain the root η.

Once η is known from the solution of equation (26), the pressure, specific internal energy, and entropy due to the free electrons and positrons are

$$P^*_{ele} = \frac{16\pi\sqrt{2}}{3h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(\eta,\beta) + \frac{1}{2}\beta F_{5/2}(\eta,\beta) \right] \tag{28}$$

$$P^*_{pos} = \frac{16\pi\sqrt{2}}{3h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(-\eta-2/\beta,\beta) + \frac{1}{2}\beta F_{5/2}(-\eta-2/\beta,\beta) \right] \tag{29}$$

$$\epsilon_{ele} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(\eta,\beta) + \beta F_{5/2}(\eta,\beta) \right] \tag{30}$$

$$\epsilon_{pos} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \beta^{5/2} \left[F_{3/2}(-\eta-2/\beta,\beta) + \beta F_{5/2}(-\eta-2/\beta,\beta) \right] + \frac{2 m_e c^2 N_{pos}}{\rho} \tag{31}$$

$$S_{ele} = \frac{P_{ele}/\rho + \epsilon_{ele}}{T} - \frac{k\eta N_{ele}}{\rho} \tag{32}$$

$$S_{pos} = \frac{P_{pos}/\rho + \epsilon_{pos}}{T} + \frac{k\eta_{pos} N_{pos}}{\rho} \tag{33}$$

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

$$F_k(\eta,\beta) = \int_0^\infty \frac{x^k (1+\beta x/2)^{1/2} dx}{\exp(x-\eta)+1} = \underbrace{\int_0^{S_1} f_1(x=z^2)dx}_{(1)} + \underbrace{\int_{S_1}^{S_2} f_2(x)dx}_{(2)} + \underbrace{\int_{S_2}^{S_3} f_2(x)dx}_{(3)} + \underbrace{\int_{S_3}^{\infty} f_2(x)dx}_{(4)} \tag{34}$$

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

$$f_1(z) = \begin{cases} \frac{2z^{2k+1}\sqrt{1+z^2\beta/2}}{\exp(z^2-\eta)+1}, & \text{if } (z-\eta) < 100; \\ 2z^{2k+1}\sqrt{1+z^2\beta/2}\exp(\eta - z^2), & \text{otherwise}; \end{cases} \tag{35}$$

$$f_2(x) = \begin{cases} \frac{x^k\sqrt{1+x\beta/2}}{\exp(x-\eta)+1}, & \text{if } (x-\eta) < 100; \\ x^k\sqrt{1+x\beta/2}\exp(\eta - x), & \text{otherwise}; \end{cases} \tag{36}$$

- 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 (25) in the above limit. As such, neglecting any contribution from positrons yields the equation:

$$\frac{\bar{Z}}{\bar{A}} N_A^* \rho = N_{ele} = \frac{2}{h^3}\int_0^{p_F} 4\pi p^2 dp = \frac{8\pi}{3h^3} p_F^3 \to p_F = \left(\frac{\bar{Z}}{\bar{A}} N_A^* \rho \frac{3h^3}{8\pi} \right)^{1/3} \tag{37}$$

The total energy over all possible states is rewritten from (30) as

$$\epsilon_{ele} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \int_0^\infty \frac{(x\beta)^{3/2}(1+0.5x\beta)^{1/2}(1+x\beta)}{\exp(x-\eta)+1} \beta dx \tag{38}$$

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

$$\epsilon_{kin} = mc^2 \left[\left[\left(\frac{p}{mc} \right)^2 + 1 \right]^{1/2} - 1 \right] = \epsilon_p - mc^2 \tag{39}$$

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, $[\exp(x-\eta)+1]^{-1} \to 1$ so the integral may be rewritten as

$$\epsilon_{min} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \int_0^{x_F} (x\beta)^{3/2}(1+0.5x\beta)^{1/2}(1+x\beta)\beta dx \tag{40}$$

We now make the substitution $\theta = x\beta = \epsilon_{kin}/mc^2$. The integral in (40) is then written as

$$\epsilon_{min} = \frac{8\pi\sqrt{2}}{\rho h^3} m_e^4 c^5 \int_0^{\theta_F} (\theta)^{3/2}(1+0.5\theta)^{1/2}(1+\theta)d\theta \tag{41}$$

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

$$g(\theta) = \theta^{3/2}(1+0.5\theta)^{1/2}(1+\theta) \tag{42}$$

$$\lim_{\theta\to 0} g(x) = \theta^{3/2} + 1.25\theta^{5/2} + 0.21875\theta^{7/2} - 0.0234374\theta^{9/2} + \mathcal{O}(\theta^{11/2}) \tag{43}$$

$$\lim_{\theta\to\infty} g(x) = 0.7071107\theta^3 + 1.41421\theta^2 + 0.3535553\theta + \mathcal{O}(\sqrt{1/\theta}) \tag{44}$$

The integrals in these limits can then be computed,

$$\int_0^{\theta_F} \lim_{\theta\to 0} g(x)dx = 0.4\theta_F^{5/2} + 0.3571143\theta_F^{7/2} + 0.04861111\theta_F^{9/2} - 0.004261136\theta_F^{11/2} + \cdots \tag{45}$$

$$\int_0^{\theta_F} \lim_{\theta\to\infty} g(x)dx = 0.176777\theta_F^4 + 0.471403\theta_F^3 + 0.176777\theta_F^2 + \cdots \tag{46}$$

$$\epsilon_{min} = \frac{2}{h}\int_0^{p_F} \left(p^2c^2 + m_e^2c^4\right)^{1/2} 4\pi p^2 dp = \frac{m_e c^2}{\lambda_e^3}\chi(x) = \frac{m_e c^2}{8\pi^2\lambda_e^3}\left[x(1+x^2)^{1/2}(1+2x^2) - \ln\left[x + (1+x^2)^{1/2}\right]\right] \tag{47}$$

Thus an approximation for the minimum energy can be made using the above integrals and the prefactor from (40). These approximations describe the values obtained from Timmes EOS scheme and the current EOS scheme being written.

4 Creating Entropy-based EOS Table

$$\epsilon_3 = \epsilon_{ion} + \epsilon_{ele} + \epsilon_{pos} \tag{48}$$

$$\boxed{S_3 = S_{ion} + S_{ele} + S_{pos}} \tag{49}$$

$$P_3 = P_{ion} + P_{ele} + P_{pos} \tag{50}$$

$$\boxed{\left.\frac{\partial S_3}{\partial \epsilon_3}\right|_\rho = \frac{1}{T}} \tag{51}$$

$$\boxed{\left.\frac{\partial S_3}{\partial \rho}\right|_\epsilon = -\frac{P_3}{T\rho^2}} \tag{52}$$

$$\boxed{\left.\frac{\partial^2 S_3}{\partial \epsilon_3^2}\right|_\rho = -\frac{1}{T^2}\left.\frac{\partial T}{\partial \epsilon_3}\right|_\rho = -\frac{1}{T^2}\left(\left.\frac{\partial \epsilon_3}{\partial T}\right|_\rho\right)^{-1}} \tag{53}$$

$$\boxed{\left.\frac{\partial^2 S_3}{\partial \rho^2}\right|_{\epsilon} = \frac{2P_3}{T\rho^3} - \frac{1}{\rho^2}\left[-\frac{P_3}{T^2}\left(\left.\frac{\partial \rho}{\partial T}\right|_{\epsilon}\right)^{-1} + \frac{1}{T}\left.\frac{\partial P_3}{\partial \rho}\right|_{\epsilon}\right]} \tag{54}$$

$$\frac{\partial^2 S_3}{\partial \epsilon_3 \partial \rho} = \frac{P_3}{\rho^2 T^2}\left(\left.\frac{\partial \epsilon_3}{\partial T}\right|_{\rho}\right)^{-1} - \frac{1}{T\rho^2}\left.\frac{\partial P_3}{\partial \epsilon_3}\right|_{\rho} = \frac{P_3}{\rho^2 T^2}\left(\left.\frac{\partial \epsilon_3}{\partial T}\right|_{\rho}\right)^{-1} - \frac{2}{3}\frac{1}{\rho T} \tag{55}$$

$$\boxed{\frac{\partial^2 S_3}{\partial \rho \partial \epsilon_3} = -\frac{1}{T^2}\left.\frac{\partial T}{\partial \rho}\right|_{\epsilon} = -\frac{1}{T^2}\left(\left.\frac{\partial \rho}{\partial T}\right|_{\epsilon}\right)^{-1}} \tag{56}$$

5 Building EOS from Gaussian Process

$$\boxed{T = \left(\left.\frac{\partial S_3}{\partial \epsilon_3}\right|_{\rho}\right)^{-1}} \tag{57}$$

$$\boxed{P_3 = -\rho^2 T\left.\frac{\partial S_3}{\partial \rho}\right|_{\epsilon}} \tag{58}$$

6 Gaussian Process

6.1 Setting up covariance matrix

Here the squared exponential covariance kernel and derivatives are written in terms of $\mathbf{x} = (w, x, y, z)$ and $\mathbf{x}' = (w', x', y', z')$ such that

$$k(\mathbf{x}, \mathbf{x}') = k = \sigma_f^2 \exp\left[-\frac{1}{2}\left[\frac{(w-w')^2}{\ell_1^2} + \frac{(x-x')^2}{\ell_2^2} + \frac{(y-y')^2}{\ell_3^2} + \frac{(x-x')^2}{\ell_4^2}\right]\right] \tag{59}$$

wherethe hyperparameters σ_f is the maximum variance and ℓ_1, ℓ_2, ℓ_3, ℓ_4 are the length scales in the four directions.

$$\nabla_{\mathbf{x}} k = \left[\frac{\partial k}{\partial w}, \frac{\partial k}{\partial x}, \frac{\partial k}{\partial y}, \frac{\partial k}{\partial z}\right] = -\left[\frac{(w-w')}{\ell_1^2}, \frac{(x-x')}{\ell_2^2}, \frac{(y-y')}{\ell_3^2}, \frac{(z-z')}{\ell_4^2}\right] k \tag{60}$$

$$\nabla_{\mathbf{x}'} k = \left[\frac{\partial k}{\partial w'}, \frac{\partial k}{\partial x'}, \frac{\partial k}{\partial y'}, \frac{\partial k}{\partial z'}\right] = \left[\frac{(w-w')}{\ell_1^2}, \frac{(x-x')}{\ell_2^2}, \frac{(y-y')}{\ell_3^2}, \frac{(z-z')}{\ell_4^2}\right] k \tag{61}$$

The joint covariance matrix includes the weights for the standard covariance as well as the the gradient and Laplacian terms:

$$\mathbf{K} = \begin{bmatrix}
k & \frac{\partial k}{\partial w'} & \frac{\partial k}{\partial x'} & \frac{\partial k}{\partial y'} & \frac{\partial k}{\partial z'} & \frac{\partial^2 k}{\partial w'^2} & \frac{\partial^2 k}{\partial w' \partial x'} & \cdots & \frac{\partial^2 k}{\partial y' \partial z'} & \frac{\partial^2 k}{\partial z'^2} \\
\frac{\partial k}{\partial w} & \frac{\partial k}{\partial w \partial w'} & \frac{\partial k}{\partial w \partial x'} & \frac{\partial k}{\partial w \partial y'} & \frac{\partial k}{\partial w \partial z'} & \frac{\partial w \partial^2 k}{\partial w \partial w'^2} & \frac{\partial w \partial^2 k}{\partial w \partial w' \partial x'} & \cdots & \frac{\partial^2 k}{\partial y' \partial z'} & \frac{\partial^2 k}{\partial z'^2} \\
\frac{\partial k}{\partial x} & \frac{\partial k}{\partial x \partial w'} & \frac{\partial k}{\partial x \partial x'} & \frac{\partial k}{\partial x \partial y'} & \frac{\partial k}{\partial x \partial z'} & \frac{\partial^2 k}{\partial x \partial w'^2} & \frac{\partial^2 k}{\partial x \partial w' \partial x'} & \cdots & \frac{\partial^2 k}{\partial x \partial y' \partial z'} & \frac{\partial^2 k}{\partial x \partial z'^2} \\
\frac{\partial k}{\partial y} & \frac{\partial^2 k}{\partial y \partial w'} & \frac{\partial^2 k}{\partial y \partial x'} & \frac{\partial^2 k}{\partial y \partial y'} & \frac{\partial^2 k}{\partial y \partial z'} & \frac{\partial^3 k}{\partial y \partial w'^2} & \frac{\partial^3 k}{\partial y \partial w' \partial x'} & \cdots & \frac{\partial^3 k}{\partial y \partial y' \partial z'} & \frac{\partial^3 k}{\partial y \partial z'^2} \\
\frac{\partial k}{\partial z} & \frac{\partial^2 k}{\partial z \partial w'} & \frac{\partial^2 k}{\partial z \partial x'} & \frac{\partial^2 k}{\partial z \partial y'} & \frac{\partial^2 k}{\partial z \partial z'} & \frac{\partial^3 k}{\partial z \partial w'^2} & \frac{\partial^3 k}{\partial z \partial w' \partial x'} & \cdots & \frac{\partial^3 k}{\partial z \partial y' \partial z'} & \frac{\partial^3 k}{\partial z \partial z'^2} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{\partial^2 k}{\partial y \partial z} & \frac{\partial^3 k}{\partial y \partial z \partial w'} & \frac{\partial^3 k}{\partial y \partial z \partial x'} & \frac{\partial^3 k}{\partial y \partial z \partial y'} & \frac{\partial^3 k}{\partial y \partial z \partial z'} & \frac{\partial^4 k}{\partial y \partial z \partial w'^2} & \frac{\partial^4 k}{\partial y \partial z \partial w' \partial x'} & \cdots & \frac{\partial^4 k}{\partial y \partial z \partial y' \partial z'} & \frac{\partial^4 k}{\partial y \partial z \partial z'^2} \\
\frac{\partial^2 k}{\partial z^2} & \frac{\partial^3 k}{\partial z^2 \partial w'} & \frac{\partial^3 k}{\partial z^2 \partial x'} & \frac{\partial^3 k}{\partial z^2 \partial y'} & \frac{\partial^3 k}{\partial z^2 \partial z'} & \frac{\partial^4 k}{\partial z^2 \partial w'^2} & \frac{\partial^4 k}{\partial z^2 \partial w' \partial x'} & \cdots & \frac{\partial^4 k}{\partial z^2 \partial y' \partial z'} & \frac{\partial^4 k}{\partial z^2 \partial z'^2}
\end{bmatrix} + \sigma_n \mathbf{I} \tag{62}$$

6.2 Finding the optimum hyperparameters

We compute the optimum values for the four length scales $[\ell_1, \ell_2, \ell_3, \ell_4]$ 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.

6.3 Computing the posterior

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

$$[\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}](\mathbf{x}^*) = (\bar{\mathbf{k}}^*)^\top \mathbf{K}^{-1} [\mathbf{f}, \nabla \mathbf{f}, \nabla^2 \mathbf{f}]_{1:N}^\top \tag{63}$$

$$\sigma^2(\mathbf{x}^*) = k(\mathbf{x}^*, \mathbf{x}^*) - (\bar{\mathbf{k}}^*)^\top \mathbf{K}^{-1} \bar{\mathbf{k}}^* \tag{64}$$