

Verification of the Hessian calculation in SPEC

J. Loizu

(Dated: February 28, 2018)

This study aims at verifying that the Hessian is calculated correctly in SPEC. To this aim, I start with the simplest possible system where a Hessian can be defined. That is, a slab MRxMHD equilibrium with two relaxed volumes separated by an ideal-interface and unperturbed outer boundaries. In this case, the Hessian is a scalar for which an analytical formula can be derived. Then, the system is extended to a multi-volume equilibrium with toroidal and poloidal symmetry, for which the Hessian is a symmetric, tridiagonal matrix that can also be calculated analytically and thus makes possible exact code verification.

Model

Consider a slab, two-volume MRxMHD equilibrium. That implies a single ideal-interface separating two Taylor states. The boundary geometry is given by a function $R(\theta, \zeta)$ on each of the two sides. Assume the simplest form: $R_0(\theta, \zeta) = 0$ and $R_2(\theta, \zeta) = 1$, where the labels refer to the lower (0) and upper (2) boundaries (see Figure 1). The geometry of the ideal-interface, $R_1(\theta, \zeta)$, is to be calculated. Assume zero pressure and given toroidal and poloidal fluxes, as well as Beltrami parameters, in each volume. Namely, $\{\Psi_{t1}, \Psi_{t2}, \Psi_{p1}, \Psi_{p2}, \mu_1, \mu_2\}$ are given. Here the label “1” refers to the lower volume parameters, and the label “2” refers to the upper volume parameters.

This completely defines the equilibrium problem. Because of the symmetry of the problem, the solution is obviously independent of the two periodic coordinates and only depends on the “radial” coordinate R , which can be parametrized in each volume via a coordinate $s \in [-1, 1]$, such that $R(s) = R_0 + (R_1 - R_0)(1 + s)/2$ in the lower volume and $R(s) = R_1 + (R_2 - R_1)(1 + s)/2$ in the upper volume.

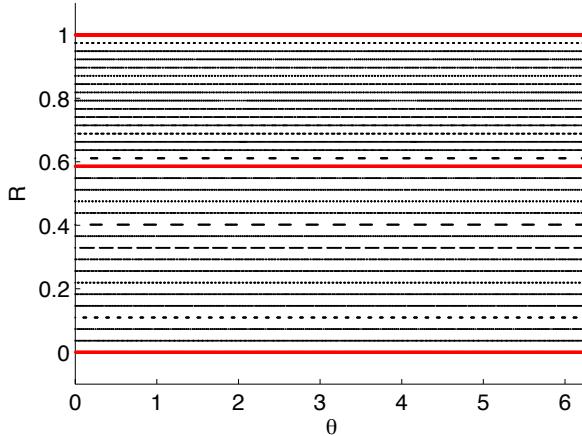


FIG. 1: Poincaré plot for the $N_{vol} = 2$ equilibrium. Red lines indicate lower and upper boundaries, and inner ideal interface.

Analytical prediction

In each volume, the field satisfies $\nabla \times \mathbf{B} = \mu \mathbf{B}$. Given the symmetry of the problem, there is an exact analytical solution, see [Loizu et al, Physics of Plasmas 22, 022501, 2015]. One can write the solution in terms of the fluxes and Beltrami parameters,

$$B_s = 0 \quad (1)$$

$$B_\theta = \frac{\mu}{4\pi} \left(\Psi_t \frac{\sin(\bar{\mu}s)}{\sin(\bar{\mu})} + \Psi_p \frac{\cos(\bar{\mu}s)}{\sin(\bar{\mu})} \right) \quad (2)$$

$$B_\zeta = \frac{\mu}{4\pi} \left(\Psi_t \frac{\cos(\bar{\mu}s)}{\sin(\bar{\mu})} - \Psi_p \frac{\sin(\bar{\mu}s)}{\sin(\bar{\mu})} \right) \quad (3)$$

where $\bar{\mu} = \mu\Delta/2$ and Δ is the width of each volume, namely $\Delta = R_1 - R_0$ for the lower volume and $\Delta = R_2 - R_1$ for the upper volume. From this solution, we can compute the force imbalance,

$$f = \frac{1}{2}[[B^2]] = \frac{1}{2} \left(B_{upper}^2(s = -1) - B_{lower}^2(s = +1) \right) \quad (4)$$

which gives

$$f = \frac{1}{32\pi^2} \left(\frac{\mu_2^2}{\sin^2(\bar{\mu}_2)} (\Psi_{t2}^2 + \Psi_{p2}^2) - \frac{\mu_1^2}{\sin^2(\bar{\mu}_1)} (\Psi_{t1}^2 + \Psi_{p1}^2) \right). \quad (5)$$

Finally, the Hessian is thus given by:

$$H = \frac{\partial f}{\partial R_1} = \frac{1}{32\pi^2} \left(\mu_1^3 (\Psi_{t1}^2 + \Psi_{p1}^2) \frac{\cos(\bar{\mu}_1)}{\sin^3(\bar{\mu}_1)} + \mu_2^3 (\Psi_{t2}^2 + \Psi_{p2}^2) \frac{\cos(\bar{\mu}_2)}{\sin^3(\bar{\mu}_2)} \right). \quad (6)$$

This is the general expression for the Hessian of this system and depends on the input parameters and the inner interface position R_1 . In the particular case of an equilibrium, $f = 0$, and Eq. (5) provides the value of R_1 at equilibrium. That value can then be inserted in Eq. (6) in order to obtain a prediction for the Hessian at equilibrium.

SPEC calculation

SPEC has been run for this system (using $Lconstraint = 0$ to enforce the fluxes and Beltrami coefficients). The input parameters have been chosen as follows:

$$\Psi_{t1} = 0.6$$

$$\Psi_{t2} = 0.4 \text{ (in the input file the total flux is prescribe here, namely 1)}$$

$$\Psi_{p1} = 0.27$$

$$\Psi_{p2} = -0.2632 \text{ (in the input file the total flux is prescribe here, namely 0.0068)}$$

$$\mu_1 = -1.006$$

$$\mu_2 = -1.032$$

The code is run with $L_{rad} = 8$ and $M_{pol} = N_{tor} = 0$ and converges to $|f| \sim 10^{-16}$. The solutions for the geometry of the inner interface (see Figure 1) and the Hessian as calculated from SPEC are

$$R_{1,spec} = 0.5803498854044925$$

$$H_{spec} = 0.134643681643898$$

which indicates stability of the equilibrium ($H > 0$). Using the same input parameters in Eqs. (5) and (6), we obtain the following analytical predictions:

$$R_{1,theory} = 0.580349885410095$$

$$H_{theory} = 0.134643676139315$$

which is very close to the SPEC values. Given that the force-balance in the SPEC calculation is satisfied to machine precision, the only parameter left that can be tuned to make the SPEC solution converge towards the analytical solution is the radial resolution L_{rad} . For example, for $L_{rad} = 8$, the error in the Beltrami solution is small but finite,

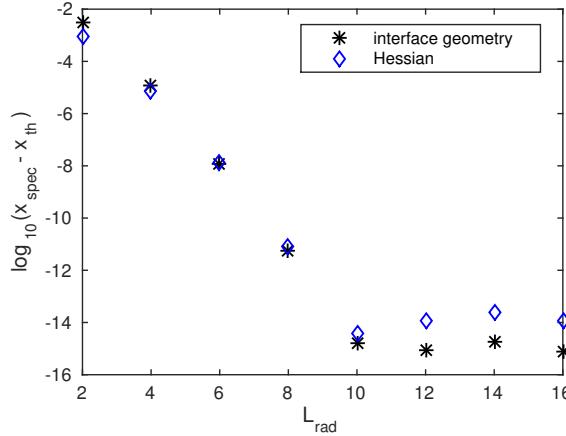


FIG. 2: Distance between SPEC and analytical theory for the $N_{vol} = 2$ equilibrium, as a function of the radial resolution.

and converges towards machine precision with increasing L_{rad} . Thus, we expect that the SPEC solution for R_1 and H will converge towards the analytical solution with increasing L_{rad} . Figure 2 shows that this is the case.

Multi-volume generalization

In general, the Hessian is a matrix of size $N_{gdof} \times N_{gdof}$, where $N_{gdof} = (N_{vol} - 1)\mathcal{N}$ is the number of geometrical degrees of freedom and $\mathcal{N} = N_{tor} + 1 + M_{pol}(2N_{tor} + 1)$ is the total number of Fourier modes. We can make analytical predictions for the Hessian of a multi-volume slab equilibrium if we keep the symmetry of the system, namely $N_{tor} = M_{pol} = 0$, which implies $\mathcal{N} = 1$ and thus $N_{gdof} = N_{vol} - 1$.

The geometrical degrees of freedom can be ordered as $\{R_l, l = 1 \dots N_{gdof}\}$, with the “lower” and “upper” boundaries, $R_0 = 0$ and $R_{N_{vol}} = 1$, given as input. The force imbalance on each of the interfaces, f_l , satisfies Eq. (5) with appropriate indexing,

$$f_l = \frac{1}{32\pi^2} \left(\frac{\mu_{l+1}^2}{\sin^2(\bar{\mu}_{l+1})} (\Psi_{t,l+1}^2 + \Psi_{p,l+1}^2) - \frac{\mu_l^2}{\sin^2(\bar{\mu}_l)} (\Psi_{t,l}^2 + \Psi_{p,l}^2) \right), \quad (7)$$

where $\bar{\mu}_l = \mu_l \Delta_l / 2$ and $\Delta_l = R_l - R_{l-1}$. The Hessian is now given by

$$H_{lk} = \frac{\partial f_l}{\partial R_k} = \frac{1}{32\pi^2} \times \begin{cases} \mu_l^3 (\Psi_{t,l}^2 + \Psi_{p,l}^2) \frac{\cos(\bar{\mu}_l)}{\sin^3(\bar{\mu}_l)} + \mu_{l+1}^3 (\Psi_{t,l+1}^2 + \Psi_{p,l+1}^2) \frac{\cos(\bar{\mu}_{l+1})}{\sin^3(\bar{\mu}_{l+1})} & \text{for } k = l \\ -\mu_l^3 (\Psi_{t,l}^2 + \Psi_{p,l}^2) \frac{\cos(\bar{\mu}_l)}{\sin^3(\bar{\mu}_l)} & \text{for } k = l - 1 \\ -\mu_{l+1}^3 (\Psi_{t,l+1}^2 + \Psi_{p,l+1}^2) \frac{\cos(\bar{\mu}_{l+1})}{\sin^3(\bar{\mu}_{l+1})} & \text{for } k = l + 1 \\ 0 & \text{otherwise} \end{cases}$$

and therefore is expected to be symmetric, tridiagonal matrix.

SPEC calculation

SPEC has been run with $N_{vol} = 5$ and $L_{constraint} = 0$. The input parameters have been chosen as follows:

$$\begin{aligned} \Psi_{t,l} &= \{0.2, 0.2, 0.2, 0.2, 0.2\} \\ \Psi_{p,l} &= \{0.255, 0.159, 0, -0.159, -0.255\} \\ \mu_l &= \{-0.189, -0.256, -1.44, -0.256, -0.189\} \end{aligned} \quad (8)$$

The code is run with $L_{rad} = 8$ and $M_{pol} = N_{tor} = 0$ and converges to $|f| \sim 10^{-16}$. The resulting equilibrium geometry is shown in Fig. 3. For these parameters, the prediction for the Hessian is shown in Fig. 4 and the Hessian

as calculated by SPEC is shown in Fig. 5. The coefficients of H are in very good agreement and the Hessian is indeed *symmetric* and *tridiagonal*. Figure 6 shows how the Hessian matrix coefficients obtained from SPEC converge towards the analytical coefficients as L_{rad} is increased, with an error quickly reaching machine precision.

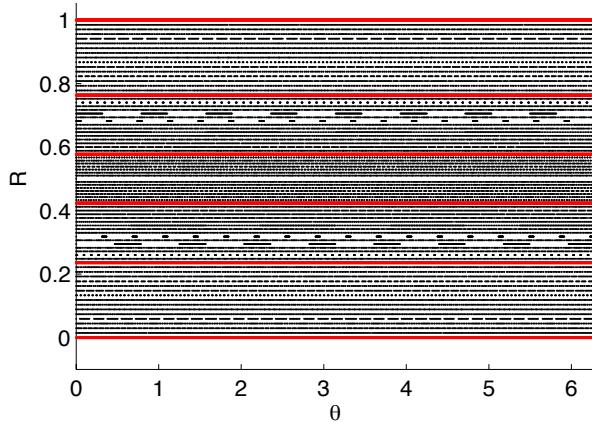


FIG. 3: Poincaré plot for the $N_{vol} = 5$ equilibrium. Red lines indicate lower and upper boundaries, and inner ideal interfaces.

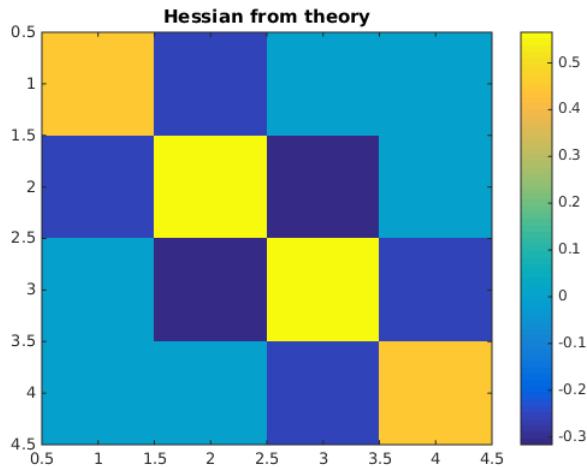


FIG. 4: Coefficients of the 4×4 Hessian matrix from the theory.

Extension of the Hessian to include $m > 0$ perturbations

Consider now the possibility of $m = 1$ perturbations in both the field and interface geometry. For simplicity, we keep the boundary unperturbed. The Hessian is now a matrix of size $N_{gdof} \times N_{gdof}$, where $N_{gdof} = (N_{vol} - 1)\mathcal{N}$ is the number of geometrical degrees of freedom and $\mathcal{N} = N_{tor} + 1 + M_{pol}(2N_{tor} + 1) = 2$ is the total number of Fourier modes. For example, if $N_{vol} = 5$, then the Hessian is a 8×8 matrix.

The geometrical degrees of freedom can be labeled as $\{R_{l,m} ; l = 0 \dots N_{vol} ; m = 0, 1\}$, with the “lower” and “upper” boundary geometries given as input, $R_{0,0} = R_{0,1} = 0$ and $R_{N_{vol},0} = 1$, $R_{N_{vol},1} = 0$.

The force-imbalance on each of the interfaces, $l = 1 \dots N_{vol} - 1$, is

$$f_l = \frac{1}{2}[[B^2]]_l^{l+1} = f_l(\{R_{l,m}\}) = \sum_m f_{l,m}(\{R_{l,m}\}) \cos(m\theta) \quad (9)$$

and an equilibrium must satisfy $f_{l,m} = 0$ for all l, m (so in principle N_{gdof} equations). The task is now to calculate

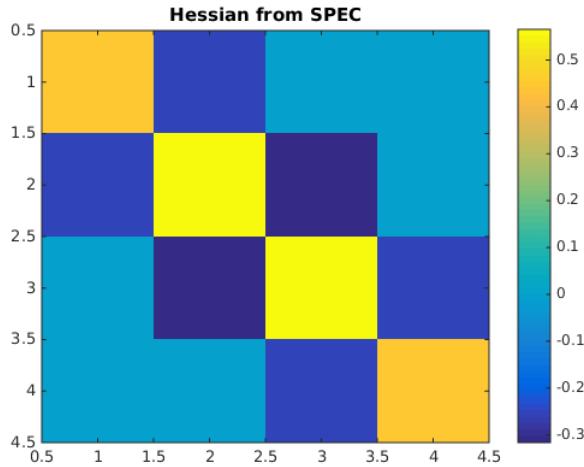


FIG. 5: Coefficients of the 4x4 Hessian matrix from SPEC.

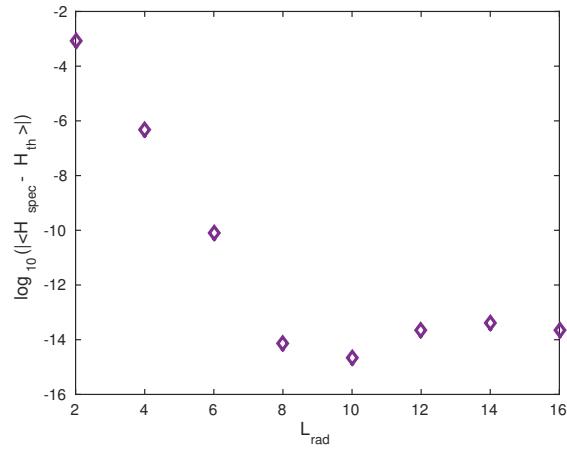


FIG. 6: Average distance in the Hessian coefficients between SPEC and the analytical prediction for the $N_{\text{vol}} = 5$ equilibrium, as a function of the radial resolution.

the Hessian around the unperturbed equilibrium, which is

$$H_{ij} = \frac{\partial f_i}{\partial R_j} \quad (10)$$

where $f_k = f_{l_k, m_k}$ and $R_k = R_{l_k, m_k}$, with $k = 1 \dots N_{\text{dof}}$ and $l_k = [1 + (k-1)/\mathcal{N}]$ and $m_k = k - 1 - (l_k - 1)\mathcal{N}$.

From [Loizu et al, Physics of Plasmas 22, 022501, 2015], we have that

$$f_{l,0} = \frac{1}{32\pi^2} \left(\frac{\mu_{l+1}^2}{\sin^2(\bar{\mu}_{l+1})} (\Psi_{t,l+1}^2 + \Psi_{p,l+1}^2) - \frac{\mu_l^2}{\sin^2(\bar{\mu}_l)} (\Psi_{t,l}^2 + \Psi_{p,l}^2) \right), \quad (11)$$

where $\bar{\mu}_l = \mu_l(R_{l,0} - R_{l-1,0})/2$, and

$$f_{l,1} = (\mathcal{C}_{l+1}^- - \mathcal{C}_l^+)R_{l,1} - \mathcal{D}_{l+1}R_{l+1,1} - \mathcal{D}_lR_{l-1,1} \quad (12)$$

where

$$\mathcal{C}_l^\pm = \frac{\mu_l^2}{32\pi^2} [\pm\sigma_l(\Psi_t \pm \Psi_p \cot(\bar{\mu}_l))^2 (\tan(\bar{\sigma}_l) - \cot(\bar{\sigma}_l)) + 2\mu_l(\pm(\Psi_t^2 - \Psi_p^2) \cot(\bar{\mu}_l) + \Psi_t\Psi_p(\cot^2(\bar{\mu}_l) - 1))] \quad (13)$$

$$\mathcal{D}_l = \frac{\mu_l^2}{32\pi^2} \sigma_l [(\Psi_p^2 \cot^2(\bar{\mu}_l) - \Psi_t^2)(\tan(\bar{\sigma}_l) + \cot(\bar{\sigma}_l))] \quad (14)$$

for $\mu_l \geq 1$, and

$$\mathcal{C}_l^\pm = \frac{\mu_l^2}{32\pi^2} [\mp 2\sigma_l(\Psi_t \pm \Psi_p \cot(\bar{\mu}_l))^2 \coth(2\bar{\sigma}_l) + 2\mu_l(\pm(\Psi_t^2 - \Psi_p^2) \cot(\bar{\mu}_l) + \Psi_t \Psi_p (\cot^2(\bar{\mu}_l) - 1))] \quad (15)$$

$$\mathcal{D}_l = \frac{\mu_l^2}{32\pi^2} \frac{2\sigma_l}{\sinh(2\bar{\sigma}_l)} [\Psi_p^2 \cot^2(\bar{\mu}_l) - \Psi_t^2] \quad (16)$$

for $\mu_l \leq 1$. Here $\sigma_l = \sqrt{|\mu_l^2 - 1|}$ and $\bar{\sigma}_l = \sigma_l \Delta_l / 2$.

Since $f_{l,0} = f_{l,0}(R_{l,0}, R_{l-1,0}, R_{l+1,0})$ and $f_{l,1} = f_{l,1}(R_{l,m}, R_{l-1,m}, R_{l+1,m}; m = 0, 1)$, there are many terms in the Hessian that are automatically zero. Since Eq. (11) is also Eq. (7), the derivatives of $f_{l,0}$ have already been calculated. The derivatives of $f_{l,1}$ are simply

$$\frac{\partial f_{l,1}}{\partial R_{l,1}} = \mathcal{C}_{l+1}^- - \mathcal{C}_l^+ \quad (17)$$

$$\frac{\partial f_{l,1}}{\partial R_{l-1,1}} = -\mathcal{D}_l \quad (18)$$

$$\frac{\partial f_{l,1}}{\partial R_{l+1,1}} = -\mathcal{D}_{l+1} \quad (19)$$

and

$$\frac{\partial f_{l,1}}{\partial R_{l,0}} = 0 \quad (20)$$

$$\frac{\partial f_{l,1}}{\partial R_{l-1,0}} = 0 \quad (21)$$

$$\frac{\partial f_{l,1}}{\partial R_{l+1,0}} = 0 \quad (22)$$

since we are assuming that our equilibrium has $R_{l,1} = 0$ for all l .

Figure 7 shows the coefficients of the Hessian matrix as calculated analytically for the input parameters (μ_l , $\Psi_{t,l}$, etc.) for the $N_{vol} = 5$ case considered previously. Figure 8 shows the coefficients of the Hessian matrix as calculated by SPEC for the corresponding system. The agreement is excellent and the distance between the two matrices converges to machine precision as L_{rad} is increased (Figure 9).

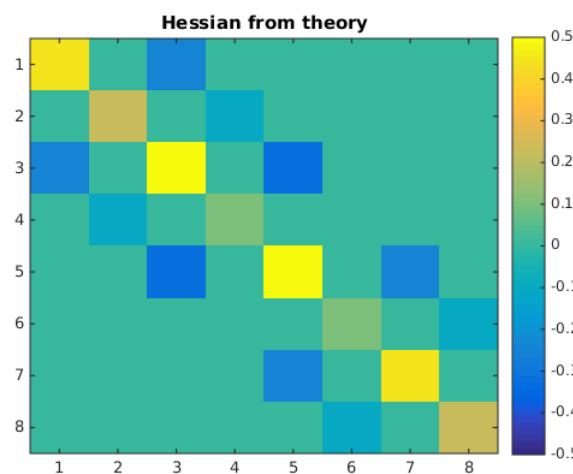


FIG. 7: Coefficients of the 8x8 Hessian matrix from the theory ($N_{vol} = 5, m = 1$).

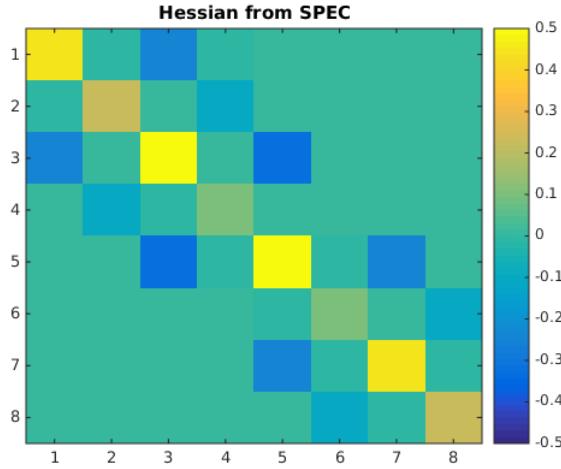


FIG. 8: Coefficients of the 8x8 Hessian matrix from SPEC ($N_{vol} = 5, m = 1$).

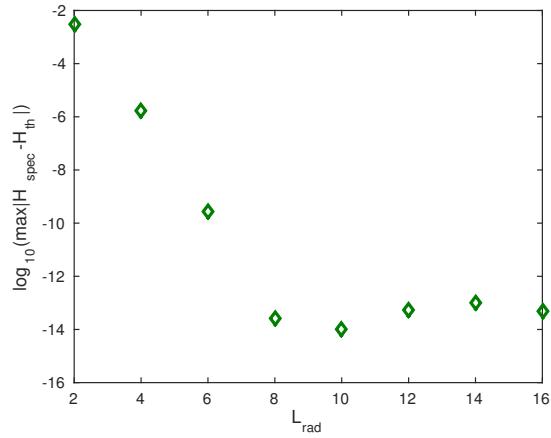


FIG. 9: Maximum distance in the Hessian coefficients between SPEC and the analytical prediction for the $N_{vol} = 5, m = 1$ equilibrium, as a function of the radial resolution.