Verification of the Hessian calculation in SPEC

J. Loizu

(Dated: January 23, 2018)

This is a simple study aiming at verifying that the Hessian is calculated correctly in SPEC. To this aim, I consider 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 should be a scalar for which an analytical formula can be derived.

Model

Consider a slab, two-volume MRxMHD equilibrium. That implies a single ideal-inteface 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.
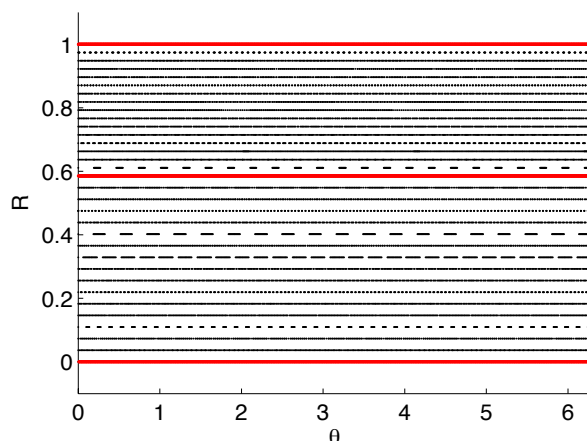

FIG. 1: Poincaré plot for the $N_{vol} = 2$ equilibrium. Red lines indicate lower and upper boundaries, and inner ideal interface.

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,

$$B_s = 0 \tag{1}$$

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

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

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,

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

which gives

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

Finally, the Hessian is thus given by:

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

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 equilibirium, $f = 0$, 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, 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 analyical solution with increasing L_{rad}. Figure 2 shows that this is the case for R_1, but for the hessian H the error saturates at about 10^{-8}. Perhaps this is because the hessian in the SPEC output is written in single-precision?

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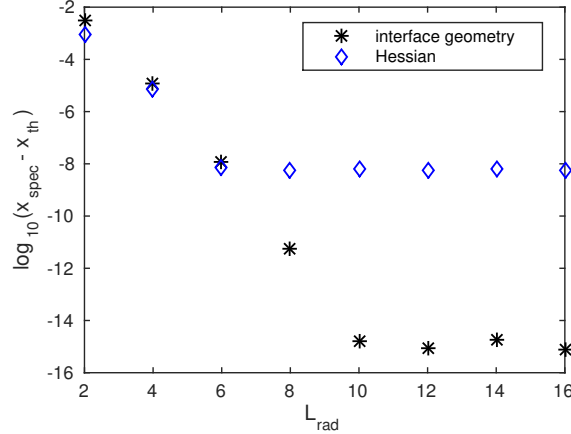
FIG. 2: Distance between SPEC and analytical theory for the $N_{vol} = 2$ equilibrium, as a function of the radial resolution.

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 $\{R_l \, , \; l = 1...N_{gdof}\}$, 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,

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

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

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

and therefore is expected to be symmetric, tridiagonal matrix.

SPEC calculation

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

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

$$(8)$$

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. While the order of magnitude and sign of the coefficients of H are in agreement, the Hessian in SPEC is *not symmetric* and *not tridiagonal*!
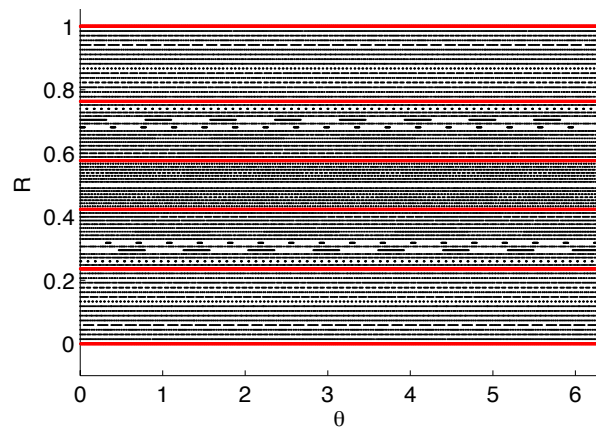
FIG. 3: Poincaré plot for the $N_{vol} = 5$ equilibrium. Red lines indicate lower and upper boundaries, and inner ideal interfaces.
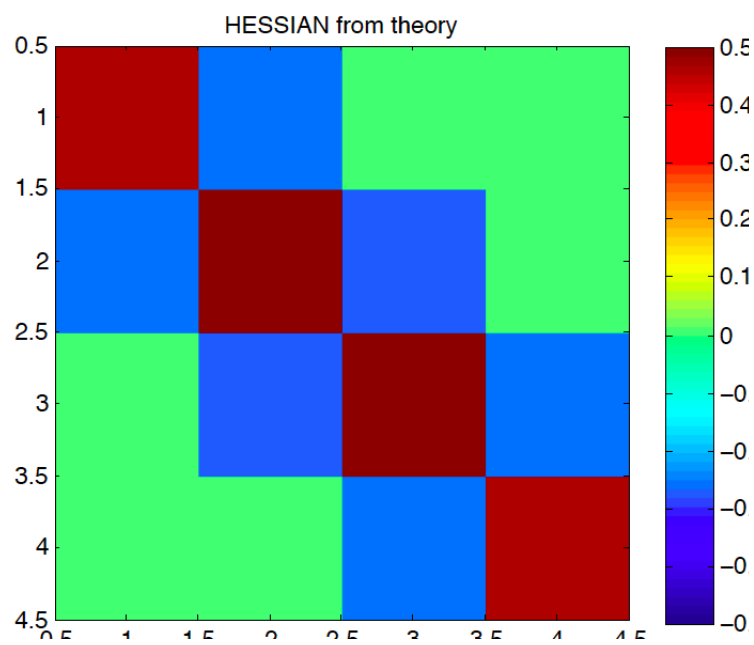

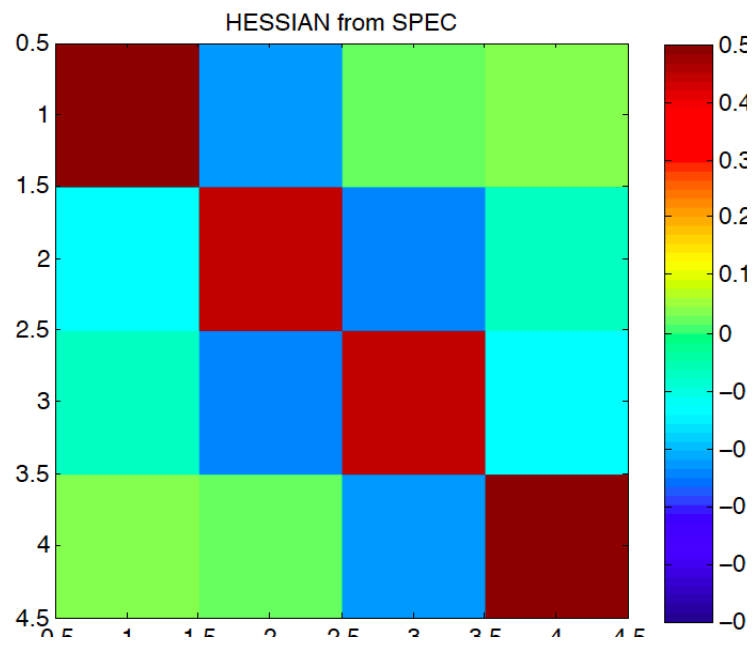FIG. 4: Coefficients of the 4x4 Hessian matrix from the theory.

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