The SPD correction factor for the Newton solver

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In Newton iterations, the top-left block of the system Jacobian is given by

$$J_{IJ}^{uu} := \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{\varphi}_I^{\boldsymbol{u}}) : [2\eta\boldsymbol{\varepsilon}(\boldsymbol{\varphi}_J^{\boldsymbol{u}}) + 2\mathbb{E} : \boldsymbol{\varepsilon}(\boldsymbol{\varphi}_J^{\boldsymbol{u}})] \, \mathrm{d}\Omega, \tag{1}$$

where $\boldsymbol{\varepsilon}(\cdot)$ is the symmetric gradient operator, $\boldsymbol{\varphi}_I^{\boldsymbol{u}}$ is the shape function of velocity, and the fourth-order tensor $\mathbb{E}$ is defined as

$$\mathbb{E} := \boldsymbol{\varepsilon} \otimes \frac{\partial \eta}{\partial \boldsymbol{\varepsilon}}. \tag{2}$$

To inverse the top-left block with the CG solver, we must guarantee the symmetry and positive definiteness of (1). As suggested by Fraters et al. [2019], we can modify the top-left block by

$$\widetilde{J}_{IJ}^{uu} := \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{\varphi}_I^{\boldsymbol{u}}) : [2\eta\boldsymbol{\varepsilon}(\boldsymbol{\varphi}_J^{\boldsymbol{u}}) + 2\alpha\mathbb{E}^{\mathrm{sym}} : \boldsymbol{\varepsilon}(\boldsymbol{\varphi}_J^{\boldsymbol{u}})] \, \mathrm{d}\Omega, \tag{3}$$

where

$$\mathbb{E}^{\mathrm{sym}} := \frac{1}{2}\left(\boldsymbol{\varepsilon} \otimes \frac{\partial \eta}{\partial \boldsymbol{\varepsilon}} + \frac{\partial \eta}{\partial \boldsymbol{\varepsilon}} \otimes \boldsymbol{\varepsilon}\right), \tag{4}$$

and $\alpha \in (0, 1]$ is a scaling factor which ensures that the eigenvalues of $\eta\boldsymbol{\varepsilon}(\boldsymbol{\varphi}^{\boldsymbol{u}}) + \mathbb{E} : \boldsymbol{\varepsilon}(\boldsymbol{\varphi}^{\boldsymbol{u}})$ are positive.

To determine the value of α, we first define $\boldsymbol{n}$ and $\hat{\boldsymbol{n}}$ as unit tensors "parallel" to $\boldsymbol{\varepsilon}$ and $\partial\eta/\partial\boldsymbol{\varepsilon}$, respectively, i.e.

$$\boldsymbol{n} := \frac{\boldsymbol{\varepsilon}}{\|\boldsymbol{\varepsilon}\|}, \qquad \hat{\boldsymbol{n}} := \frac{\partial \eta}{\partial \boldsymbol{\varepsilon}} \bigg/ \left\|\frac{\partial \eta}{\partial \boldsymbol{\varepsilon}}\right\|. \tag{5}$$

In general cases, $\boldsymbol{n}$ and $\hat{\boldsymbol{n}}$ are not identical. Thus, we can decompose $\hat{\boldsymbol{n}}$ into two vectors $\boldsymbol{n}^{//}$ and $\boldsymbol{n}^{\perp}$, the former parallel with $\boldsymbol{n}$ and the latter perpendicular to $\boldsymbol{n}$. Assume that $\boldsymbol{n} : \hat{\boldsymbol{n}} = \cos\psi$ ($\psi \in [0, \pi]$), then we have

$$\boldsymbol{n}^{\perp} = \hat{\boldsymbol{n}} - (\hat{\boldsymbol{n}} : \boldsymbol{n})\boldsymbol{n} = \hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi. \tag{6}$$

The norm of $\boldsymbol{n}^{\perp}$ can be calculated by

$$\|\boldsymbol{n}^{\perp}\| = \sqrt{\boldsymbol{n}^{\perp} : \boldsymbol{n}^{\perp}} = \sqrt{1 - \cos^2\psi} = \sin\psi. \tag{7}$$

Thus, we obtain a unit tensor $(\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi)/\sin\psi$ which is perpendicular to $\boldsymbol{n}$, and any unit symmetric tensor can be expressed as

$$\boldsymbol{n}\cos\theta + \frac{\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi}{\sin\psi}\sin\theta, \tag{8}$$

where θ is an arbitrary angle.

Following the idea of Fraters et al. [2019], we calculate the Rayleigh quotient of $\mathbb{E}^{\mathrm{sym}}$:

$$
\begin{aligned}
R(\theta) =& \left(\boldsymbol{n}\cos\theta + \frac{\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi}{\sin\psi}\sin\theta\right) : \frac{1}{2}\left(\boldsymbol{\varepsilon}\otimes\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}} + \frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\otimes\boldsymbol{\varepsilon}\right) : \left(\boldsymbol{n}\cos\theta + \frac{\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi}{\sin\psi}\sin\theta\right) \\
=& \frac{1}{2}\|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|\left(\boldsymbol{n}\cos\theta + \frac{\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi}{\sin\psi}\sin\theta\right) : (\boldsymbol{n}\otimes\hat{\boldsymbol{n}} + \hat{\boldsymbol{n}}\otimes\boldsymbol{n}) : \left(\boldsymbol{n}\cos\theta + \frac{\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi}{\sin\psi}\sin\theta\right) \\
=& \frac{1}{2}\|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|\left[(\hat{\boldsymbol{n}} + \boldsymbol{n}\cos\psi)\cos\theta + \boldsymbol{n}\sin\psi\sin\theta\right] : \left(\boldsymbol{n}\cos\theta + \frac{\hat{\boldsymbol{n}} - \boldsymbol{n}\cos\psi}{\sin\psi}\sin\theta\right) \\
=& \|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|\left(\cos\psi\cos^2\theta + \sin\psi\cos\theta\sin\theta\right) \\
=& \|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|\cos\theta\cos(\theta-\psi) \\
=& \frac{1}{2}\|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|\left[\cos(2\theta-\psi) + \cos\psi\right].
\end{aligned}
\tag{9}
$$

Since θ is arbitrary, the minimum value of (9) is

$$
R_{\min} = \frac{1}{2}\|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|(-1+\cos\psi), \tag{10}
$$

which is the lower bound of the eigenvalues of $\mathbb{E}^{\mathrm{sym}}$. Therefore, the scaling factor can be defined as

$$
\alpha = \begin{cases} 1 & \text{if } \|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|(-1+\boldsymbol{n}:\hat{\boldsymbol{n}}) \geq -2c_{\mathrm{safety}}\eta, \\ c_{\mathrm{safety}}\dfrac{2\eta}{\|\boldsymbol{\varepsilon}\|\left\|\frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}\right\|(1-\boldsymbol{n}:\hat{\boldsymbol{n}})} & \text{otherwise}, \end{cases} \tag{11}
$$

where c_{safety} is a safety factor determined by the user.

It is worth noting that the expression of α is very similar to that in Fraters et al. [2019] (Eq. [18]). If we define

$$
\boldsymbol{a} := \boldsymbol{\varepsilon}, \qquad \boldsymbol{b} = \frac{\partial\eta}{\partial\boldsymbol{\varepsilon}}, \tag{12}
$$

then (11) can be rewritten as

$$
\alpha = \begin{cases} 1 & \text{if } \left(1 - \dfrac{\boldsymbol{a}:\boldsymbol{b}}{\|\boldsymbol{a}\|\|\boldsymbol{b}\|}\right)\|\boldsymbol{a}\|\|\boldsymbol{b}\| < 2c_{\mathrm{safety}}\eta, \\ c_{\mathrm{safety}}\dfrac{2\eta}{\left(1 - \dfrac{\boldsymbol{a}:\boldsymbol{b}}{\|\boldsymbol{a}\|\|\boldsymbol{b}\|}\right)\|\boldsymbol{a}\|\|\boldsymbol{b}\|} & \text{otherwise}. \end{cases} \tag{13}
$$

It can be found that the only difference between Eq. (13) and Eq. [18] in Fraters et al. [2019] is the power of $\left(1 - \frac{\boldsymbol{a}:\boldsymbol{b}}{\|\boldsymbol{a}\|\|\boldsymbol{b}\|}\right)$.

References

M R T Fraters, W Bangerth, C Thieulot, A C Glerum, and W Spakman. Efficient and practical Newton solvers for non-linear Stokes systems in geodynamic problems. *Geophysical Journal International*, 218(2): 873–894, August 2019. ISSN 0956-540X. doi: 10.1093/gji/ggz183.