0.1 stepped pressure equilibrium code : ma01ae

1. Constructs matrix that represents the Beltrami linear system.

0.1.1 gauge and boundary conditions

1. The helicity integral, $\int \mathbf{A}\cdot\mathbf{B}\,dv$, depends explicity on the vector potential. The gauge must be constrained and the boundary conditions enforced. First we consider an annular volume.

0.1.2 annular volume - gauge

1. The coordinates, (s,θ,ζ), are adapted to the interfaces, so that the interfaces coincide with coordinate surfaces $s = const.$ and θ,ζ are poloidal and toroidal angles.

2. In the l-th annulus, bounded by the $(l-1)$-th and l-th interfaces, a general covariant representation of the magnetic vector-potential is written

$$\bar{\mathbf{A}} = \bar{A}_s\nabla s + \bar{A}_\theta\nabla\theta + \bar{A}_\zeta\nabla\zeta. \tag{1}$$

To this add $\nabla g(s,\theta,\zeta)$, where g satisfies

$$\partial_s g(s,\theta,\zeta) = -\bar{A}_s(s,\theta,\zeta),\;\; \partial_\theta g(s_{l-1},\theta,\zeta) = -\bar{A}_\theta(s_{l-1},\theta,\zeta) + \psi_{t,l-1},\;\; \partial_\zeta g(s_{l-1},0,\zeta) = -\bar{A}_\zeta(s_{l-1},0,\zeta) + \psi_{p,l-1}, \tag{2}$$

for arbitrary constants $\psi_{t,l-1}$, $\psi_{p,l-1}$, which are the toroidal and poloidal-fluxes on the interior of surface $l-1$. Then $\mathbf{A} = \bar{\mathbf{A}} + \nabla g$ is given by $\mathbf{A} = A_\theta\nabla\theta + A_\zeta\nabla\zeta$ with

$$A_\theta(s_{l-1},\theta,\zeta) = \psi_{t,l-1},\;\; A_\zeta(s_{l-1},0,\zeta) = \psi_{p,l-1}. \tag{3}$$

This specifies the gauge.

3. The magnetic field is $\sqrt{g}\mathbf{B} = (\partial_\theta A_\zeta - \partial_\zeta A_\theta)\mathbf{e}_s - \partial_s A_\zeta\mathbf{e}_\theta + \partial_s A_\theta\mathbf{e}_\zeta$.

$$B^2 = B^sB^sg_{ss} + 2B^sB^\theta g_{s\theta} + 2B^sB^\zeta g_{s\zeta} + B^\theta B^\theta g_{\theta\theta} + 2B^\theta B^\zeta g_{\theta\zeta} + B^\zeta B^\zeta g_{\zeta\zeta} \tag{4}$$

$$\sqrt{g}\mathbf{A}\cdot\mathbf{B} = -A_\theta\partial_s A_\zeta + A_\zeta\partial_s A_\theta. \tag{5}$$

4. For stellarator symmetric equilibria, A_θ and A_ζ may be represented by cosine series

$$A_\theta(s,\theta,\zeta) = \sum_j A_{\theta,j}(s)\cos(m_j\theta - n_j\zeta),\;\; A_\zeta(s,\theta,\zeta) = \sum_j A_{\zeta,j}(s)\cos(m_j\theta - n_j\zeta), \tag{6}$$

where $A_{\theta,j}(s)$ and $A_{\zeta,j}(s)$ are represented using finite-elements, as described below.

5. Within each annulus, a regular, radial-sub-grid, $s_{l,i} \equiv$ `ss(l)%s(i)`, for $i = 0$, `Ni`, is established, see `al00aa`.

0.1.3 interface boundary condition

1. The condition that the field is tangential to the inner interface is

$$-m_jA_{\zeta,j}(s_{l-1}) - n_jA_{\theta,j}(s_{l-1}) = 0. \tag{7}$$

Combing the gauge constraints and the flux surface condition we have

$$A_{\theta,j}(s_{l-1}) = \begin{cases} \psi_{t,l-1} & , \;\; j = 1, \\ 0 & , \;\; j > 1, \end{cases} \tag{8}$$

$$A_{\zeta,j}(s_{l-1}) = \begin{cases} \psi_{p,l-1} & , \;\; j = 1, \\ 0 & , \;\; j > 1, \end{cases} \tag{9}$$

2. The condition that the field is tangential to the outer interface is similar to Eq.(7), but it cannot be simplified further and so at the outer interface we must constrain the vector potential to be of the form

$$A_\theta(s_l) = \partial_\theta f(\theta,\zeta)\,, \;\; A_\zeta(s_l) = \partial_\zeta f(\theta,\zeta), \tag{10}$$

for arbitrary f of the form

$$f = \psi_{t,l}\theta + \psi_{p,l}\zeta + \sum_j f_{l,j}\sin(m_j\theta - n_j\zeta) \tag{11}$$

and $\psi_{t,l} \equiv A_{\theta,1}(s_l)$ and $\psi_{p,l} \equiv A_{\zeta,1}(s_l)$. We have

$$A_{\theta,j}(s_l) = \begin{cases} \psi_{t,l} & , \quad j=1, \\ m_j f_{l,j} & , \quad j>1, \end{cases} \tag{12}$$

$$A_{\zeta,j}(s_l) = \begin{cases} \psi_{p,l} & , \quad j=1, \\ -n_j f_{l,j} & , \quad j>1, \end{cases} \tag{13}$$

0.1.4 finite element radial basis functions

1. Within each annulus a regular, radial-sub-grid, s_i, is established.
2. In the region $s \in [s_{i-1}, s_i]$, the vector potential is $\mathbf{A} = A_\theta \nabla\theta + A_\zeta \nabla\zeta$ where

$$A_\theta(s,\theta,\zeta) = \sum_{j,l,p} A_{\theta,j,i-1+l,p}\;\varphi_{l,p}(s)\;\cos(m_j\theta - n_j\zeta), \tag{14}$$

$$A_\zeta(s,\theta,\zeta) = \sum_{j,l,p} A_{\zeta,j,i-1+l,p}\;\varphi_{l,p}(s)\;\cos(m_j\theta - n_j\zeta), \tag{15}$$

where j labels the Fourier harmonic, and $l = 0,1$ and p identify the radial basis functions, $\varphi_{l,p}(s)$.

3. Near the coordinate singularity (described in more detail below) this representation needs to be modified.

0.1.5 metric information

1. The geometric information required in the following is

$$\bar{g}_{ss} \equiv g_{ss}/\sqrt{g} = \sum_i \bar{g}_{ss,i}(s)\cos(m_i\theta - n_i\zeta), \tag{16}$$

$$\bar{g}_{s\theta} \equiv g_{s\theta}/\sqrt{g} = \sum_i \bar{g}_{s\theta,i}(s)\sin(m_i\theta - n_i\zeta), \tag{17}$$

$$\bar{g}_{s\zeta} \equiv g_{s\zeta}/\sqrt{g} = \sum_i \bar{g}_{s\zeta,i}(s)\sin(m_i\theta - n_i\zeta), \tag{18}$$

$$\bar{g}_{\theta\theta} \equiv g_{\theta\theta}/\sqrt{g} = \sum_i \bar{g}_{\theta\theta,i}(s)\cos(m_i\theta - n_i\zeta), \tag{19}$$

$$\bar{g}_{\theta\zeta} \equiv g_{\theta\zeta}/\sqrt{g} = \sum_i \bar{g}_{\theta\zeta,i}(s)\cos(m_i\theta - n_i\zeta), \tag{20}$$

$$\bar{g}_{\zeta\zeta} \equiv g_{\zeta\zeta}/\sqrt{g} = \sum_i \bar{g}_{\zeta\zeta,i}(s)\cos(m_i\theta - n_i\zeta). \tag{21}$$

2. For any function $f(s,\theta,\zeta)$, in particular the metrics, we write

$$\begin{aligned}
\langle s_j\,|f|\,s_k\rangle &= \oint\!\!\oint d\theta d\zeta \;\; \sin(m_j\theta - n_j\zeta)\, f(s,\theta,\zeta)\, \sin(m_k\theta - n_k\zeta) \\
\langle s_j\,|f|\,c_k\rangle &= \oint\!\!\oint d\theta d\zeta \;\; \sin(m_j\theta - n_j\zeta)\, f(s,\theta,\zeta)\, \cos(m_k\theta - n_k\zeta) \\
\langle c_j\,|f|\,c_k\rangle &= \oint\!\!\oint d\theta d\zeta \;\; \cos(m_j\theta - n_j\zeta)\, f(s,\theta,\zeta)\, \cos(m_k\theta - n_k\zeta)
\end{aligned}$$

0.1.6 volume integral

1. Consider the integral $P = \sum_{i=1}^{N_i} P_i$, where

$$
\begin{aligned}
P_i \quad = \quad & \\
& + \frac{1}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\theta A_\zeta \quad \partial_\theta A_\zeta \quad \bar{g}_{ss} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\theta A_\zeta \quad \partial_\zeta A_\theta \quad \bar{g}_{ss} \\
& + \frac{1}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\zeta A_\theta \quad \partial_\zeta A_\theta \quad \bar{g}_{ss} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\theta A_\zeta \quad \partial_s A_\zeta \quad \bar{g}_{s\theta} \\
& + \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\zeta A_\theta \quad \partial_s A_\zeta \quad \bar{g}_{s\theta} \\
& + \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\theta A_\zeta \quad \partial_s A_\theta \quad \bar{g}_{s\zeta} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\zeta A_\theta \quad \partial_s A_\theta \quad \bar{g}_{s\zeta} \\
& + \frac{1}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\zeta \quad \partial_s A_\zeta \quad \bar{g}_{\theta\theta} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\zeta \quad \partial_s A_\theta \quad \bar{g}_{\theta\zeta} \\
& + \frac{1}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\theta \quad \partial_s A_\theta \quad \bar{g}_{\zeta\zeta} \\
& + \frac{\mu}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad A_\theta \quad \partial_s A_\zeta \\
& - \frac{\mu}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad A_\zeta \quad \partial_s A_\theta \quad .
\end{aligned}
\tag{22}
$$

0.1.7 derivatives of volume integral – annular regions

1. The first derivatives are as follows:

$$
\begin{aligned}
\frac{\partial}{\partial A_{\theta,j,i-1+l,p}} P_i \quad = \quad & \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\theta A_\zeta \quad n_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{ss} \\
& + \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\zeta A_\theta \quad n_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{ss} \\
& + \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\zeta \quad n_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{s\theta} \\
& + \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\theta A_\zeta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{s\zeta} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\theta \quad n_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{s\zeta} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_\zeta A_\theta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{s\zeta} \\
& - \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\zeta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{\theta\zeta} \\
& + \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\theta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{\zeta\zeta} \\
& + \frac{\mu}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad \partial_s A_\zeta \quad \varphi_{l,p} \quad c_j \\
& - \frac{\mu}{2} \int_{s_{i-1}}^{s_i} ds \oint\!\!\oint d\theta d\zeta \quad A_\zeta \quad \varphi'_{l,p} \quad c_j
\end{aligned}
\tag{23}
$$

$$
\begin{aligned}
\frac{\partial}{\partial A_{\zeta,j,i-1+l,p}} P_i \quad = \quad & \\
- \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_\theta A_\zeta \quad m_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{ss} \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_\zeta A_\theta \quad m_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{ss} \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_s A_\zeta \quad m_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{s\theta} \\
- \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_\theta A_\zeta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{s\theta} \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_\zeta A_\theta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{s\theta} \\
- \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_s A_\theta \quad m_j \quad \varphi_{l,p} \quad s_j \quad \bar{g}_{s\zeta} \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_s A_\zeta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{\theta\theta} \\
- \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_s A_\theta \quad \varphi'_{l,p} \quad c_j \quad \bar{g}_{\theta\zeta} \\
+ \quad \tfrac{\mu}{2} \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad A_\theta \quad \varphi'_{l,p} \quad c_j \\
- \quad \tfrac{\mu}{2} \quad & \int_{s_{i-1}}^{s_i} ds \oiint d\theta d\zeta \quad \partial_s A_\theta \quad \varphi_{l,p} \quad c_j
\end{aligned}
\tag{24}
$$

2. The second derivatives are required for construction of the Beltrami matrix, which are given

$$
\begin{aligned}
\frac{\partial}{\partial A_{\theta,k,i-1+r,q}} \frac{\partial}{\partial A_{\theta,j,i-1+l,p}} P_i \quad = \quad & \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad n_k \quad n_j \quad \varphi_{r,q} \quad \varphi_{l,p} \quad \langle s_j | \bar{g}_{ss} | s_k \rangle \\
- \quad & \int_{s_{i-1}}^{s_i} ds \quad n_j \quad \varphi'_{r,q} \quad \varphi_{l,p} \quad \langle s_j | \bar{g}_{s\zeta} | c_k \rangle \\
- \quad & \int_{s_{i-1}}^{s_i} ds \quad n_k \quad \varphi_{r,q} \quad \varphi'_{l,p} \quad \langle c_j | \bar{g}_{s\zeta} | s_k \rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad \varphi'_{r,q} \quad \varphi'_{l,p} \quad \langle c_j | \bar{g}_{\zeta\zeta} | c_k \rangle
\end{aligned}
\tag{25}
$$

$$
\begin{aligned}
\frac{\partial}{\partial A_{\zeta,k,i-1+r,q}} \frac{\partial}{\partial A_{\theta,j,i-1+l,p}} P_i \quad = \quad & \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad m_k \quad n_j \quad \varphi_{r,q} \quad \varphi_{l,p} \quad \langle s_j | \bar{g}_{ss} | s_k \rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad n_j \quad \varphi'_{r,q} \quad \varphi_{l,p} \quad \langle s_j | \bar{g}_{s\theta} | c_k \rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad m_k \quad \varphi_{r,q} \quad \varphi'_{l,p} \quad \langle c_j | \bar{g}_{s\zeta} | s_k \rangle \\
- \quad & \int_{s_{i-1}}^{s_i} ds \quad \varphi'_{r,q} \quad \varphi'_{l,p} \quad \langle c_j | \bar{g}_{\theta\zeta} | c_k \rangle \\
+ \quad \tfrac{\mu}{2} \quad & \int_{s_{i-1}}^{s_i} ds \quad \varphi'_{r,q} \quad \varphi_{l,p} \quad \langle c_j | 1 | c_k \rangle \\
- \quad \tfrac{\mu}{2} \quad & \int_{s_{i-1}}^{s_i} ds \quad \varphi_{r,q} \quad \varphi'_{l,p} \quad \langle c_j | 1 | c_k \rangle
\end{aligned}
\tag{26}
$$

$$
\begin{aligned}
\frac{\partial}{\partial A_{\theta,k,i-1+r,q}}\frac{\partial}{\partial A_{\zeta,j,i-1+l,p}}P_i \quad = \quad & \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad n_k \quad m_j \quad \varphi_{r,q} \quad \varphi_{l,p} \quad \langle s_j \,|\bar{g}_{ss}|\, s_k\rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad n_k \quad \quad \varphi_{r,q} \quad \varphi'_{l,p} \quad \langle c_j \,|\bar{g}_{s\theta}|\, s_k\rangle \\
- \quad & \int_{s_{i-1}}^{s_i} ds \quad \quad m_j \quad \varphi'_{r,q} \quad \varphi_{l,p} \quad \langle s_j \,|\bar{g}_{s\zeta}|\, c_k\rangle \\
- \quad & \int_{s_{i-1}}^{s_i} ds \quad \quad \quad \varphi'_{r,q} \quad \varphi'_{l,p} \quad \langle c_j \,|\bar{g}_{\theta\zeta}|\, c_k\rangle \\
+ \quad \tfrac{\mu}{2} & \int_{s_{i-1}}^{s_i} ds \quad \quad \quad \varphi_{r,q} \quad \varphi'_{l,p} \quad \langle c_j \,|1|\, c_k\rangle \\
- \quad \tfrac{\mu}{2} & \int_{s_{i-1}}^{s_i} ds \quad \quad \quad \varphi'_{r,q} \quad \varphi_{l,p} \quad \langle c_j \,|1|\, c_k\rangle
\end{aligned}
\tag{27}
$$

$$
\begin{aligned}
\frac{\partial}{\partial A_{\zeta,k,i-1+r,q}}\frac{\partial}{\partial A_{\zeta,j,i-1+l,p}}P_i \quad = \quad & \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad m_k \quad m_j \quad \varphi_{r,q} \quad \varphi_{l,p} \quad \langle s_j \,|\bar{g}_{ss}|\, s_k\rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad \quad m_j \quad \varphi'_{r,q} \quad \varphi_{l,p} \quad \langle s_j \,|\bar{g}_{s\theta}|\, c_k\rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad m_k \quad \quad \varphi_{r,q} \quad \varphi'_{l,p} \quad \langle c_j \,|\bar{g}_{s\theta}|\, s_k\rangle \\
+ \quad & \int_{s_{i-1}}^{s_i} ds \quad \quad \quad \varphi'_{r,q} \quad \varphi'_{l,p} \quad \langle c_j \,|\bar{g}_{\theta\theta}|\, c_k\rangle
\end{aligned}
\tag{28}
$$

0.1.8 matrix elements – annular regions

1. The required matrix elements take the form, where $\alpha = \theta, \zeta$ and $\beta = \theta, \zeta$,

$$
\begin{aligned}
\frac{\partial}{\partial A_{\beta,k,i-1,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P &= \frac{\partial}{\partial A_{\beta,k,i-1,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P_i \\
\frac{\partial}{\partial A_{\beta,k,i,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P &= \frac{\partial}{\partial A_{\beta,k,i,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P_i + \frac{\partial}{\partial A_{\beta,k,i,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P_{i+1} \\
\frac{\partial}{\partial A_{\beta,k,i+1,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P &= \frac{\partial}{\partial A_{\beta,k,i+1,q}}\frac{\partial}{\partial A_{\alpha,j,i,p}}P_{i+1}
\end{aligned}
\tag{29}
$$

0.1.9 gauge and regularity conditions near coordinate origin

1. Near the polar coordinate origin, which is *not* required to coincide with the magnetic axis (the location of which is as yet not known apriori), we may exploit the regularity constraints and gauge freedom [1] to write $\mathbf{A} = A_\theta \nabla\theta + A_\zeta \nabla\zeta$ where

$$
A_\theta(s,\theta,\zeta) = \sum_{j=1}\sum_{p=0} A_{\theta,j,0,p} s^{m_j+2+2p}\cos(m_j\theta - n_j\zeta), \tag{30}
$$

$$
A_\zeta(s,\theta,\zeta) = \sum_{j=1}\sum_{p=0} A_{\zeta,j,0,p} s^{m_j \quad +2p}\cos(m_j\theta - n_j\zeta), \tag{31}
$$

where the $A_{\theta,j,0,p}$ and $A_{\zeta,j,0,p}$ are degrees of freedom, except $A_{\zeta,j,0,0} = 0$ if $m_j = 0$.

2. Note that the location of the coordinate axis is determined by `ex00aa`.

3. The factor s^{m_j} can become very small and cause finite-precision errors unless it is treated carefully. Introducing the scaled independent variables

$$
a_{j,p} \equiv A_{\theta,j,0,p}\,\rho^{m_j}, \quad b_{j,p} \equiv A_{\zeta,j,0,p}\,\rho^{m_j}, \tag{32}
$$

[1] This was done using Mathematica, and further details will be provided on demand.

where $\rho \equiv s_{1,1}$, and for $s \in [0, \rho]$ we have

$$A_\theta(s,\theta,\zeta) = \sum_{j=1}\sum_{p=0} a_{j,p} s^{m_j+2+2p}/\rho^{m_j} \cos(m_j\theta - n_j\zeta), \tag{33}$$

$$A_\zeta(s,\theta,\zeta) = \sum_{j=1}\sum_{p=0} b_{j,p} s^{m_j \quad +2p}/\rho^{m_j} \cos(m_j\theta - n_j\zeta), \tag{34}$$

0.1.10 matching regularity/gauge at first grid

1. By matching at the first grid point, $\rho \equiv s_{1,1}$, we see that the $A_{\theta,j,1,p}$ depend on the $a_{j,p}$ and the $A_{\zeta,j,1,p}$ depend on the $b_{j,p}$.
2. For example, consider the quintic case, where `Nofe` $= 2$. For the $A_{\theta,j}$, matching at $s = \rho$ gives

$$\begin{pmatrix} A_{\theta,j,1,0} \\ A_{\theta,j,1,1} \\ A_{\theta,j,1,2} \end{pmatrix} = \begin{pmatrix} \rho^2 & , & \rho^4 & , & \rho^6 \\ (m+2)\rho^1 & , & (m+4)\rho^3 & , & (m+6)\rho^5 \\ (m+1)(m+2)\rho^0 & , & (m+3)(m+4)\rho^2 & , & (m+5)(m+6)\rho^4 \end{pmatrix} \begin{pmatrix} a_{j,0} \\ a_{j,1} \\ a_{j,2} \end{pmatrix} \tag{35}$$

and for the $A_{\zeta,j}$ we have

$$\begin{pmatrix} A_{\zeta,j,1,0} \\ A_{\zeta,j,1,1} \\ A_{\zeta,j,1,2} \end{pmatrix} = \begin{pmatrix} \rho^{+0} & , & \rho^2 & , & \rho^4 \\ (m+0)\rho^{-1} & , & (m+2)\rho^1 & , & (m+4)\rho^3 \\ (m-1)(m+0)\rho^{-2} & , & (m+1)(m+2)\rho^0 & , & (m+3)(m+4)\rho^2 \end{pmatrix} \begin{pmatrix} b_{j,0} \\ b_{j,1} \\ b_{j,2} \end{pmatrix} \tag{36}$$

3. Whether linear, cubic, quintic or septemtic polynomials are used, we may write

$$A_{\theta,j,1,p} = \sum_{q=0}^{N} \mathcal{A}^j_{p,q}\, a_{j,q} \quad , \quad A_{\zeta,j,1,p} = \sum_{q=0}^{N} \mathcal{B}^j_{p,q}\, b_{j,q}, \tag{37}$$

where $\mathcal{A}^j_{p,q} \equiv$ `Ajpq(j,p,q)` and $\mathcal{B}^j_{p,q} \equiv$ `Bjpq(j,p,q)`, which are assigned in `al00aa`.

4. The $A_{\theta,j,0,0}$ and $A_{\zeta,j,0,0}$ are not degrees of freedom. These terms, which are related to the toroidal and poloidal fluxes, contribute to the 'right-hand-side'. Also, the $A_{\theta,j,N_i,0}$ and $A_{\zeta,j,N_i,0}$ are not independent.

0.1.11 derivatives near coordinate singularity

1. The innermost volume, $l = 1$, contains the coordinate singularity, so for $l = 1$ and $i = 1$ the following expressions must be used.
2. The first derivative with respect to $a \equiv a_{j,p}$ is, where $\bar{s} \equiv s/\rho$,

$$\begin{aligned}
\frac{\partial P_1}{\partial a} = & \\
& - \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \; n_j \; \sin\alpha_j \qquad\qquad \bar{s}^{m_j} s^{2+2p+0} \; \partial_\theta A_\zeta \; \bar{g}_{ss} \\
& - \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \; n_j \; \sin\alpha_j \qquad\qquad \bar{s}^{m_j} s^{2+2p+0} \; \partial_\zeta A_\theta \; \bar{g}_{ss} \\
& - \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \; n_j \; \sin\alpha_j \qquad\qquad \bar{s}^{m_j} s^{2+2p+0} \; \partial_s A_\zeta \; \bar{g}_{s\theta} \\
& + \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \; (m_j+2+2p) \; \bar{s}^{m_j} s^{2+2p-1} \; \partial_\theta A_\zeta \; \bar{g}_{s\zeta} \\
& + \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \; n_j \; \sin\alpha_j \qquad\qquad \bar{s}^{m_j} s^{2+2p+0} \; \partial_s A_\theta \; \bar{g}_{s\zeta} \\
& - \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \; (m_j+2+2p) \; \bar{s}^{m_j} s^{2+2p-1} \; \partial_\zeta A_\theta \; \bar{g}_{s\zeta} \\
& - \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \; (m_j+2+2p) \; \bar{s}^{m_j} s^{2+2p-1} \; \partial_s A_\zeta \; \bar{g}_{\theta\zeta} \\
& + \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \; (m_j+2+2p) \; \bar{s}^{m_j} s^{2+2p-1} \; \partial_s A_\theta \; \bar{g}_{\zeta\zeta} \\
& + \tfrac{\mu}{2} \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \qquad\qquad \bar{s}^{m_j} s^{2+2p+0} \; \partial_s A_\zeta \\
& - \tfrac{\mu}{2} \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \; (m_j+2+2p) \; \bar{s}^{m_j} s^{2+2p-1} \; A_\zeta
\end{aligned} \tag{38}$$

3. The second derivative with respect to $a \equiv a_{j,p}$ and $b \equiv a_{k,q}$ is

$$
\begin{aligned}
\frac{\partial^2 P_1}{\partial a \partial b} = & \\
+ \quad & \rho^{1+2+2p+0+2+2q+0} \int_0^1 d\bar{s}\; n_j \qquad\qquad \bar{s}^{m_j}\,\bar{s}^{2+2p+0} \quad n_k \qquad\qquad \bar{s}^{m_k}\,\bar{s}^{2+2q+0} \quad \langle s_j\,|\bar{g}_{ss}|\,s_k\rangle \\
- \quad & \rho^{1+2+2p+0+2+2q-1} \int_0^1 d\bar{s}\; n_j \qquad\qquad \bar{s}^{m_j}\,\bar{s}^{2+2p+0} \qquad (m_k+2+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2+2q-1} \quad \langle s_j\,|\bar{g}_{s\zeta}|\,c_k\rangle \\
- \quad & \rho^{1+2+2p-1+2+2q+0} \int_0^1 d\bar{s} \qquad (m_j+2+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2+2p-1} \quad n_k \qquad\qquad \bar{s}^{m_k}\,\bar{s}^{2+2q+0} \quad \langle c_j\,|\bar{g}_{s\zeta}|\,s_k\rangle \\
+ \quad & \rho^{1+2+2p-1+2+2q-1} \int_0^1 d\bar{s} \qquad (m_j+2+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2+2p-1} \qquad (m_k+2+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2+2q-1} \quad \langle c_j\,|\bar{g}_{\zeta\zeta}|\,c_k\rangle
\end{aligned}
\tag{39}
$$

4. The second derivative with respect to $a \equiv a_{j,p}$ and $b \equiv b_{k,q}$ is

$$
\begin{aligned}
\frac{\partial^2 P_1}{\partial a \partial b} = & \\
+ \quad & \rho^{1+2+2p+0+0+2q+0} \int_0^1 d\bar{s}\; n_j \qquad\qquad \bar{s}^{m_j}\,\bar{s}^{2+2p+0} \quad m_k \qquad\qquad \bar{s}^{m_k}\,\bar{s}^{2q+0} \quad \langle s_j\,|\bar{g}_{ss}|\,s_k\rangle \\
+ \quad & \rho^{1+2+2p+0+0+2q-1} \int_0^1 d\bar{s}\; n_j \qquad\qquad \bar{s}^{m_j}\,\bar{s}^{2+2p+0} \qquad (m_k+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2q-1} \quad \langle s_j\,|\bar{g}_{s\theta}|\,c_k\rangle \\
- \quad & \rho^{1+2+2p-1+0+2q+0} \int_0^1 d\bar{s} \qquad (m_j+2+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2+2p-1} \quad m_k \qquad\qquad \bar{s}^{m_k}\,\bar{s}^{2q+0} \quad \langle c_j\,|\bar{g}_{s\zeta}|\,s_k\rangle \\
- \quad & \rho^{1+2+2p-1+0+2q-1} \int_0^1 d\bar{s} \qquad (m_j+2+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2+2p-1} \qquad (m_k+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2q-1} \quad \langle c_j\,|\bar{g}_{\zeta\zeta}|\,c_k\rangle \\
+\tfrac{\mu}{2} \quad & \rho^{1+2+2p+0+0+2q-1} \int_0^1 d\bar{s} \qquad\qquad \bar{s}^{m_j}\,\bar{s}^{2+2p+0} \qquad (m_k+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2q-1} \quad \langle c_j\,|1|\,c_k\rangle \\
-\tfrac{\mu}{2} \quad & \rho^{1+2+2p-1+0+2q+0} \int_0^1 d\bar{s} \qquad (m_j+2+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2+2p-1} \qquad\qquad \bar{s}^{m_k}\,\bar{s}^{2q+0} \quad \langle c_j\,|1|\,c_k\rangle
\end{aligned}
\tag{40}
$$

5. The first derivative with respect to $a \equiv b_{j,p}$ is

$$
\begin{aligned}
\frac{\partial P_1}{\partial a} = & \\
- \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \;\; m_j \quad \sin\alpha_j \qquad\qquad \bar{s}^{m_j}\,s^{0+2p+0} \quad \partial_\theta A_\zeta \quad \bar{g}_{ss} \\
+ \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \;\; m_j \quad \sin\alpha_j \qquad\qquad \bar{s}^{m_j}\,s^{0+2p+0} \quad \partial_\zeta A_\theta \quad \bar{g}_{ss} \\
+ \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \;\; m_j \quad \sin\alpha_j \qquad\qquad \bar{s}^{m_j}\,s^{0+2p+0} \quad \partial_s A_\zeta \quad \bar{g}_{s\theta} \\
- \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \quad (m_j+2p) \quad \bar{s}^{m_j}\,s^{0+2p-1} \quad \partial_\theta A_\zeta \quad \bar{g}_{s\theta} \\
+ \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \quad (m_j+2p) \quad \bar{s}^{m_j}\,s^{0+2p-1} \quad \partial_\zeta A_\theta \quad \bar{g}_{s\theta} \\
- \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \;\; m_j \quad \sin\alpha_j \qquad\qquad \bar{s}^{m_j}\,s^{0+2p+0} \quad \partial_s A_\theta \quad \bar{g}_{s\zeta} \\
+ \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \quad (m_j+2p) \quad \bar{s}^{m_j}\,s^{0+2p-1} \quad \partial_s A_\zeta \quad \bar{g}_{\theta\theta} \\
- \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \quad (m_j+2p) \quad \bar{s}^{m_j}\,s^{0+2p-1} \quad \partial_s A_\theta \quad \bar{g}_{\theta\zeta} \\
+\tfrac{\mu}{2} \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \quad (m_j+2p) \quad \bar{s}^{m_j}\,s^{0+2p-1} \quad A_\theta \\
-\tfrac{\mu}{2} \quad & \int_0^\rho ds \oint\!\!\oint d\theta d\zeta \qquad \cos\alpha_j \qquad\qquad \bar{s}^{m_j}\,s^{0+2p+0} \quad \partial_s A_\theta
\end{aligned}
\tag{41}
$$

6. The second derivative with respect to $a \equiv b_{j,p}$ and $b \equiv a_{k,q}$ is

$$
\begin{aligned}
\frac{\partial^2 P_1}{\partial a \partial b} &= \\
&+ \rho^{1+0+2p+0+2+2q+0} \int_0^1 d\bar{s}\; m_j \quad \bar{s}^{m_j}\,\bar{s}^{2p+0} \quad n_k \quad \bar{s}^{m_k}\,\bar{s}^{2+2q+0} \quad \langle s_j\,|\bar{g}_{ss}|\,s_k\rangle \\
&+ \rho^{1+0+2p-1+2+2q+0} \int_0^1 d\bar{s} \quad (m_j+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2p-1} \quad n_k \quad \bar{s}^{m_k}\,\bar{s}^{2+2q+0} \quad \langle c_j\,|\bar{g}_{s\theta}|\,s_k\rangle \\
&- \rho^{1+0+2p+0+2+2q-1} \int_0^1 d\bar{s}\; m_j \quad \bar{s}^{m_j}\,\bar{s}^{2p+0} \quad (m_k+2+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2+2q-1} \quad \langle s_j\,|\bar{g}_{s\zeta}|\,c_k\rangle \\
&- \rho^{1+0+2p-1+2+2q-1} \int_0^1 d\bar{s} \quad (m_j+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2p-1} \quad (m_k+2+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2+2q-1} \quad \langle c_j\,|\bar{g}_{\theta\zeta}|\,c_k\rangle \\
&+\tfrac{\mu}{2}\; \rho^{1+0+2p-1+2+2q+0} \int_0^1 d\bar{s} \quad (m_j+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2p-1} \quad \bar{s}^{m_k}\,\bar{s}^{2+2q+0} \quad \langle c_j\,|1|\,c_k\rangle \\
&-\tfrac{\mu}{2}\; \rho^{1+0+2p+0+2+2q-1} \int_0^1 d\bar{s} \quad \bar{s}^{m_j}\,\bar{s}^{2p+0} \quad (m_k+2+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2+2q-1} \quad \langle c_j\,|1|\,c_k\rangle
\end{aligned}
\tag{42}
$$

7. The second derivative with respect to $a \equiv b_{j,p}$ and $b \equiv b_{k,q}$ is

$$
\begin{aligned}
\frac{\partial^2 P_1}{\partial a \partial b} &= \\
&+ \rho^{1+0+2p+0+0+2q+0} \int_0^1 d\bar{s}\; m_j \quad \bar{s}^{m_j}\,\bar{s}^{2p} \quad m_k \quad \bar{s}^{m_k}\,\bar{s}^{2q} \quad \langle s_j\,|\bar{g}_{ss}|\,s_k\rangle \\
&+ \rho^{1+0+2p+0+0+2q-1} \int_0^1 d\bar{s}\; m_j \quad \bar{s}^{m_j}\,\bar{s}^{2p} \quad (m_k+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2q-1} \quad \langle s_j\,|\bar{g}_{s\theta}|\,c_k\rangle \\
&+ \rho^{1+0+2p-1+0+2q+0} \int_0^1 d\bar{s} \quad (m_j+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2p-1} \quad m_k \quad \bar{s}^{m_k}\,\bar{s}^{2q} \quad \langle c_j\,|\bar{g}_{s\theta}|\,s_k\rangle \\
&+ \rho^{1+0+2p-1+0+2q-1} \int_0^1 d\bar{s} \quad (m_j+2p) \quad \bar{s}^{m_j}\,\bar{s}^{2p-1} \quad (m_k+2q) \quad \bar{s}^{m_k}\,\bar{s}^{2q-1} \quad \langle c_j\,|\bar{g}_{\theta\theta}|\,c_k\rangle
\end{aligned}
\tag{43}
$$

0.1.12 matrix elements near coordinate singularity

1. The first derivatives are

$$
\begin{aligned}
\frac{\partial}{\partial a_{j,p}} P &= \frac{\partial}{\partial a_{j,p}} P_1 + \sum_i \mathcal{A}^j_{i,p} \frac{\partial}{A_{\theta,j,1,i}} P_2 \\
\frac{\partial}{\partial b_{j,p}} P &= \frac{\partial}{\partial b_{j,p}} P_1 + \sum_i \mathcal{B}^j_{i,p} \frac{\partial}{A_{\zeta,j,1,i}} P_2 \\
\frac{\partial}{\partial A_{\theta,j,2,p}} P &= \frac{\partial}{A_{\theta,j,2,p}} P_2 + \frac{\partial}{A_{\theta,j,2,p}} P_3 \\
\frac{\partial}{\partial A_{\zeta,j,2,p}} P &= \frac{\partial}{A_{\zeta,j,2,p}} P_2 + \frac{\partial}{A_{\zeta,j,2,p}} P_3
\end{aligned}
\tag{44}
$$

2. The matrix elements required are the second derivatives, given as

$$
\begin{aligned}
\frac{\partial}{\partial a_{k,q}} \frac{\partial}{\partial a_{j,p}} P &= \frac{\partial}{\partial a_{k,q}} \frac{\partial}{\partial a_{j,p}} P_1 + \sum_{i,o} \mathcal{A}^k_{o,q} \mathcal{A}^j_{i,p} \frac{\partial}{\partial A_{\theta,k,1,o}} \frac{\partial}{\partial A_{\theta,j,1,i}} P_2 \\
\frac{\partial}{\partial b_{k,q}} \frac{\partial}{\partial a_{j,p}} P &= \frac{\partial}{\partial b_{k,q}} \frac{\partial}{\partial a_{j,p}} P_1 + \sum_{i,o} \mathcal{B}^k_{o,q} \mathcal{A}^j_{i,p} \frac{\partial}{\partial A_{\zeta,k,1,o}} \frac{\partial}{\partial A_{\theta,j,1,i}} P_2 \\
\frac{\partial}{\partial a_{k,q}} \frac{\partial}{\partial b_{j,p}} P &= \frac{\partial}{\partial a_{k,q}} \frac{\partial}{\partial b_{j,p}} P_1 + \sum_{i,o} \mathcal{A}^k_{o,q} \mathcal{B}^j_{i,p} \frac{\partial}{\partial A_{\theta,k,1,o}} \frac{\partial}{\partial A_{\zeta,j,1,i}} P_2 \\
\frac{\partial}{\partial b_{k,q}} \frac{\partial}{\partial b_{j,p}} P &= \frac{\partial}{\partial b_{k,q}} \frac{\partial}{\partial b_{j,p}} P_1 + \sum_{i,o} \mathcal{B}^k_{o,q} \mathcal{B}^j_{i,p} \frac{\partial}{\partial A_{\zeta,k,1,o}} \frac{\partial}{\partial A_{\zeta,j,1,i}} P_2 \\
\frac{\partial}{\partial A_{\theta,k,2,q}} \frac{\partial}{\partial a_{j,p}} P &= \sum_{i} \mathcal{A}^j_{i,p} \frac{\partial}{\partial A_{\theta,k,2,q}} \frac{\partial}{\partial A_{\theta,j,1,i}} P_2 \\
\frac{\partial}{\partial A_{\zeta,k,2,q}} \frac{\partial}{\partial a_{j,p}} P &= \sum_{i} \mathcal{A}^j_{i,p} \frac{\partial}{\partial A_{\zeta,k,2,q}} \frac{\partial}{\partial A_{\theta,j,1,i}} P_2 \\
\frac{\partial}{\partial A_{\theta,k,2,q}} \frac{\partial}{\partial b_{j,p}} P &= \sum_{i} \mathcal{B}^j_{i,p} \frac{\partial}{\partial A_{\theta,k,2,q}} \frac{\partial}{\partial A_{\zeta,j,1,i}} P_2 \\
\frac{\partial}{\partial A_{\zeta,k,2,q}} \frac{\partial}{\partial b_{j,p}} P &= \sum_{i} \mathcal{B}^j_{i,p} \frac{\partial}{\partial A_{\zeta,k,2,q}} \frac{\partial}{\partial A_{\zeta,j,1,i}} P_2 \\
\frac{\partial}{\partial a_{k,q}} \frac{\partial}{\partial A_{\theta,j,2,p}} P &= \sum_{o} \mathcal{A}^k_{o,q} \frac{\partial}{\partial A_{\theta,k,1,o}} \frac{\partial}{\partial A_{\theta,j,2,p}} P_2 \\
\frac{\partial}{\partial b_{k,q}} \frac{\partial}{\partial A_{\theta,j,2,p}} P &= \sum_{o} \mathcal{B}^k_{o,q} \frac{\partial}{\partial A_{\zeta,k,1,o}} \frac{\partial}{\partial A_{\theta,j,2,p}} P_2 \\
\frac{\partial}{\partial a_{k,q}} \frac{\partial}{\partial A_{\zeta,j,2,p}} P &= \sum_{o} \mathcal{A}^k_{o,q} \frac{\partial}{\partial A_{\theta,k,1,o}} \frac{\partial}{\partial A_{\zeta,j,2,p}} P_2 \\
\frac{\partial}{\partial b_{k,q}} \frac{\partial}{\partial A_{\zeta,j,2,p}} P &= \sum_{o} \mathcal{B}^k_{o,q} \frac{\partial}{\partial A_{\zeta,k,1,o}} \frac{\partial}{\partial A_{\zeta,j,2,p}} P_2
\end{aligned}
\tag{45}
$$

ma01ae.h last modified on 2011-08-31 ;