al00aa

Allocates and initializes internal arrays.

[called by: xspech.] [calls: ra00aa.]

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1.1 definition of internal variables

1.1.1 LGdof and NGdof : number of geometrical degrees-of-freedom;

1. LGdof ≡ the number of degrees-of-freedom in the geometry (i.e. Fourier harmonics) of each interface;

2. NGdof ≡ total number of degrees-of-freedom in geometry, i.e. of all interfaces;

1.1.2 iota and oita : rotational transform on interfaces;

1. The input variables iota and oita are the rotational transform on "inner-side" and on the "outer-side" of each interface;

2. These quantities are formally input

3. Note that if $q_l + \gamma q_r \neq 0$, then iota is given by

$$\iota \equiv \frac{p_l + \gamma p_r}{q_l + \gamma q_r}, \tag{1}$$

where $p_l \equiv$pl, $q_l \equiv$ql, etc.; and similarly for oita.

1.1.3 `dtflux(1:Mvol)` and `dpflux(1:Mvol)` : enclosed fluxes;

1. `dtflux` $\equiv \Delta\psi_{tor}/2\pi$ and `dpflux` $\equiv \Delta\psi_{pol}/2\pi$ in each volume.

2. (Note that the total toroidal flux enclosed by the plasma boundary is $\Phi_{edge} \equiv$ `phiedge`.)

3. $\psi_{tor} \equiv$ `tflux` and $\psi_{pol} \equiv$ `pflux` are immediately normalized (in global) according to $\psi_{tor,i} \rightarrow \psi_{tor,i}/\psi_0$ and $\psi_{pol,i} \rightarrow \psi_{pol,i}/\psi_0$, where $\psi_0 \equiv \psi_{tor,N}$ on input.

1.1.4 `sweight(1:Mvol)` : star-like angle constraint weight;

1. the "star-like" poloidal angle constraint weights (only required for toroidal geometry, i.e. `Igeometry=3`) are given by

$$\texttt{sweight}_v \equiv \texttt{upsilon} \times \psi_v^w, \tag{2}$$

where $\psi_v \equiv$ `tflux(v)` is the normalized toroidal flux enclosed by the v-th interface, and $w \equiv$ `wpoloidal`.

1.1.5 `TT(0:Mrad,0:1,0:1)` : Chebyshev polynomials at inner/outer interface;

1. `TT(0:Lrad,0:1,0:1)` gives the Chebyshev polynomials, and their first derivative, evaluated at $s = -1$ and $s = +1$.

2. Precisely, `TT(l,i,d)` $\equiv T_l^{(d)}(s_i)$ for $s_0 = -1$ and $s_1 = +1$.

3. Note that $T_l^{(0)}(s) = s^l$ and $T_l^{(1)}(s) = s^{l+1} l^2$ for $s = \pm 1$.

4. Note that

$$T_l(-1) = \begin{cases} +1, & \text{if } l \text{ is even,} \\ -1, & \text{if } l \text{ is odd;} \end{cases} \qquad T_l(+1) = \begin{cases} +1, & \text{if } l \text{ is even,} \\ +1, & \text{if } l \text{ is odd;} \end{cases} \tag{3}$$

$$T_l'(-1) = \begin{cases} -l^2, & \text{if } l \text{ is even,} \\ +l^2, & \text{if } l \text{ is odd;} \end{cases} \qquad T_l'(+1) = \begin{cases} +l^2, & \text{if } l \text{ is even,} \\ +l^2, & \text{if } l \text{ is odd.} \end{cases} \tag{4}$$

5. `TT(0:Mrad,0:1,0:1)` is used in routines that explicity require interface information, such as

   (a) the interface force-balance routine, bb00aa;

   (b) the virtual casing routine, vc00aa;

   (c) computing the rotational-transform on the interfaces, tr00ab;

   (d) computing the covariant components of the interface magnetic field, sc00aa;

   (e) enforcing the constraints on the Beltrami fields, ma02ag; and

   (f) computing the enclosed currents of the vacuum field, ig00aa.

1.1.6 `ImagneticOK(1:Mvol)` : Beltrami/vacuum error flag;

1. error flags that indicate if the magnetic field in each volume has been successfully constructed;

2. `ImagneticOK` is initialized to `.false.` in dforce before the Beltrami solver routines are called. If the construction of the Beltrami field is successful (in either ma02aa or mp00ac) then `ImagneticOK` is set to `.true.`.

1.1.7 `Lhessianallocated`

1. The internal logical variable, `Lhessianallocated`, indicates whether the "Hessian" matrix of second-partial derivatives (really, the first derivatives of the force-vector) has been allocated, or not!

1.1.8 `ki(1:mn,0:1)` : Fourier identification;

1. Consider the 'abbreviated' representation for a double Fourier series,

$$\sum_i f_i \cos(m_i\theta - n_i\zeta) \equiv \sum_{n=0}^{N_0} f_{0,n} \cos(-n\zeta) + \sum_{m=1}^{M_0} \sum_{n=-N_0}^{N_0} f_{m,n} \cos(m\theta - n\zeta), \tag{5}$$

and the same representation but with enhanced resolution,

$$\sum_k \bar{f}_k \cos(\bar{m}_k\theta - \bar{n}_k\zeta) \equiv \sum_{n=0}^{N_1} f_{0,n} \cos(-n\zeta) + \sum_{m=1}^{M_1} \sum_{n=-N_1}^{N_1} f_{m,n} \cos(m\theta - n\zeta), \tag{6}$$

with $M_1 \geq M_0$ and $N_1 \geq N_0$;
then $k_i \equiv$ `ki(i,0)` is defined such that $\bar{m}_{k_i} = m_i$ and $\bar{n}_{k_i} = n_i$.

1.1.9 `kija(1:mn,1:mn,0:1)`, `kijs(1:mn,1:mn,0:1)` : Fourier identification;

1. Consider the following quantities, which are computed in ma00aa, where $\bar{g}^{\mu\nu} = \sum_k \bar{g}_k^{\mu\nu} \cos\alpha_k$ for $\alpha_k \equiv m_k\theta - n_k\zeta$,

$$\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \cos\alpha_i \;\; \cos\alpha_j \;\; = \;\; \frac{1}{2}\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(+\cos\alpha_{k_{ij+}} + \cos\alpha_{k_{ij-}}), \tag{7}$$

$$\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \cos\alpha_i \;\; \sin\alpha_j \;\; = \;\; \frac{1}{2}\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(+\sin\alpha_{k_{ij+}} - \sin\alpha_{k_{ij-}}), \tag{8}$$

$$\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \sin\alpha_i \;\; \cos\alpha_j \;\; = \;\; \frac{1}{2}\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(+\sin\alpha_{k_{ij+}} + \sin\alpha_{k_{ij-}}), \tag{9}$$

$$\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu} \sin\alpha_i \;\; \sin\alpha_j \;\; = \;\; \frac{1}{2}\oint\oint d\theta d\zeta \;\; \bar{g}^{\mu\nu}(-\cos\alpha_{k_{ij+}} + \cos\alpha_{k_{ij-}}), \tag{10}$$

   where $(m_{k_{ij+}}, n_{k_{ij+}}) = (m_i + m_j, n_i + n_j)$ and $(m_{k_{ij-}}, n_{k_{ij-}}) = (m_i - m_j, n_i - n_j)$;
   then `kija(i,j,0)`$\equiv k_{ij+}$ and `kijs(i,j,0)`$\equiv k_{ij-}$.

2. Note that Eqn.(6) does not include $m < 0$; so, if $m_i - m_j < 0$ then k_{ij-} is re-defined such that $(m_{k_{ij-}}, n_{k_{ij-}}) = (m_j - m_i, n_j - n_i)$; and similarly for the case $m = 0$ and $n < 0$. Also, take care that the sign of the sine harmonics in the above expressions will change for these cases.

1.1.10 `djkp`

1.1.11 `iotakki`

1.1.12 `cheby(0:Lrad,0:2)` : Chebyshev polynomial workspace;

1. `cheby(0:Lrad,0:2)` is global workspace for computing the Chebyshev polynomials, and their derivatives, using the recurrence relations $T_0(s) = 1$, $T_1(s) = s$ and $T_l(s) = 2\,s\,T_{l-1}(s) - T_{l-2}(s)$.

2. These are computed as required, i.e. for arbitrary s, in bfield, jo00aa and ma00aa.

3. (Note that the quantities required for ma00aa are for fixed s, and so these quantities should be precomputed.)

1.1.13 `Iquad`, `gaussianweight`, `gaussianabscissae` : Gaussian quadrature;

1. The volume integrals are computed using a "Fourier" integration over the angles and by Gaussian quadrature over the radial, i.e. $\displaystyle\int f(s)ds = \sum_k \omega_k f(s_k)$.

2. The quadrature resolution in each volume is give by `Iquad(1:Mvol)` which is determined as follows:

   - if `Nquad.gt.0`, then `Iquad(vvol) = Nquad`;
   - if `Nquad.le.0 and .not.Lcoordinatesingularity`, then `Iquad(vvol) = 2*Lrad(vvol)-Nquad`;
   - if `Nquad.le.0 and Lcoordinatesingularity`, then `Iquad(vvol) = 2*Lrad(vvol)-Nquad+Mpol`;

3. The Gaussian weights and abscissae are given by `gaussianweight(1:maxIquad,1:Mvol)` and `gaussianabscissae(1:maxIquad,1:Mv` which are computed using NAG: D01BCF.

4. `Iquad`$_v$ is passed through to ma00aa to compute the volume integrals of the metric elements; also see jo00aa, where `Iquad`$_v$ is used to compute the volume integrals of $||\nabla \times \mathbf{B} - \mu\mathbf{B}||$;

1.1.14 `LBsequad`, `LBnewton` and `LBlinear`

1. `LBsequad`, `LBnewton` and `LBlinear` depend simply on `LBeltrami`, which is described in global.

1.1.15 `BBweight(1:mn)` : weighting of force-imbalance harmonics

1. weight on force-imbalance harmonics;

$$\texttt{BBweight}_i \equiv \texttt{opsilon} \times \exp\left[-\texttt{escale} \times (m_i^2 + n_i^2)\right] \tag{11}$$

2. this is only used in dforce in constructing the force-imbalance vector;

1.1.16 `mmpp(1:mn)` : spectral condensation weight factors

1. spectral condensation weight factors;

$$\texttt{mmpp(i)} \equiv m_i^p, \tag{12}$$

   where $p \equiv$ `pcondense`.

1.1.17 `NAdof`, `Ate`, `Aze`, `Ato` and `Azo` : degrees-of-freedom in magnetic vector potential

1. `NAdof(1:Mvol)` $\equiv$ total number of degrees-of-freedom in magnetic vector potential, including Lagrange multipliers, in each volume. This can de deduced from ma02ag.

2. The components of the vector potential, $\mathbf{A} = A_\theta \nabla + A_\zeta \nabla\zeta$, are

$$A_\theta(s,\theta,\zeta) = \sum_{i,l} A_{\theta,e,i,l}\, \overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\theta,o,i,l}\, \overline{T}_{l,i}(s)\sin\alpha_i, \tag{13}$$

$$A_\zeta(s,\theta,\zeta) = \sum_{i,l} A_{\zeta,e,i,l}\, \overline{T}_{l,i}(s)\cos\alpha_i + \sum_{i,l} A_{\zeta,o,i,l}\, \overline{T}_{l,i}(s)\sin\alpha_i, \tag{14}$$

   where $\overline{T}_{l,i}(s) \equiv \bar{s}^{m_i/2} T_l(s)$, $T_l(s)$ is the Chebyshev polynomial, and $\alpha_j \equiv m_j\theta - n_j\zeta$. The regularity factor, $\bar{s}^{m_i/2}$, where $\bar{s} \equiv (1+s)/2$, is only included if there is a coordinate singularity in the domain (i.e. only in the innermost volume, and only in cylindrical and toroidal geometry.)

3. The Chebyshev-Fourier harmonics of the covariant components of the magnetic vector potential are kept in
   $A_{\theta,e,v,j,l} \equiv$ `Ate(v,0,j)%s(l)`,
   $A_{\zeta,e,v,j,l} \equiv$ `Aze(v,0,j)%s(l)`,
   $A_{\theta,o,v,j,l} \equiv$ `Ato(v,0,j)%s(l)`, and
   $A_{\zeta,o,v,j,l} \equiv$ `Azo(v,0,j)%s(l)`;
   where $v = 1,$`Mvol` labels volume, $j = 1,$`mn` labels Fourier harmonic, and $l = 0,$ `Lrad`(v) labels Chebyshev polynomial. (These arrays also contains derivative information.)

4. If `Linitguess=1`, a guess for the initial state for the Beltrami fields is constructed. An initial state is required for iterative solvers of the Beltrami fields, see `LBeltrami`.

5. If `Linitguess=2`, the initial state for the Beltrami fields is read from file (see ra00aa). An initial state is required for iterative solvers of the Beltrami fields, see `LBeltrami`.

1.1.18 `workspace`

1.1.19 `goomne`, `goomno` : metric information

1.1.20 `gssmne`, `gssmno` : metric information

1.1.21 `gstmne`, `gstmno` : metric information

1.1.22 `gszmne`, `gszmno` : metric information

1.1.23 `gttmne`, `gttmno` : metric information

1.1.24 `gtzmne`, `gtzmno` : metric information

1.1.25 `gzzmne`, `gzzmno` : metric information

1. The metric information are:

   `goomne(0:mne)`, `goomno(0:mne)`

   `gssmne(0:mne)`, `gssmno(0:mne)`

   `gstmne(0:mne)`, `gstmno(0:mne)`

   `gszmne(0:mne)`, `gszmno(0:mne)`

   `gttmne(0:mne)`, `gttmno(0:mne)`

   `gtzmne(0:mne)`, `gtzmno(0:mne)`

   `gzzmne(0:mne)`, `gzzmno(0:mne)`

2. These are defined in metrix, and used in ma00aa.

1.1.26 `cosi(1:Ntz,1:mn)` and `sini(1:Ntz,1:mn)`

1. Trigonometric factors used in various Fast Fourier transforms, where

$$\texttt{cosi}_{j,i} = \cos(m_i\theta_j - n_i\zeta_j), \tag{15}$$

$$\texttt{sini}_{j,i} = \sin(m_i\theta_j - n_i\zeta_j). \tag{16}$$

1.1.27 `psifactor(1:mn,1:Mvol)` : coordinate "pre-conditioning" factor

1. In toroidal geometry, the coordinate "pre-conditioning" factor is

$$f_{j,v} \equiv \begin{cases} \psi_{t,v}^{0} & , \quad \text{for } m_j = 0, \\ \psi_{t,v}^{m_j/2} & , \quad \text{otherwise.} \end{cases} \tag{17}$$

   where $\psi_{t,v} \equiv$ `tflux` is the (normalized?) toroidal flux enclosed by the v-th interface.

2. `psifactor` is used in packed, dforce and hesian.

1.1.28 `Bsupumn` and `Bsupvmn`

1.1.29 `diotadxup` and `glambda` : transformation to straight fieldline angle

1. Given the Beltrami fields in any volume, the rotational-transform on the adjacent interfaces may be determined (in tr00ab) by constructing the straight fieldline angle on the interfaces.

2. The rotational transform on the inner or outer interface of a given volume depends on the magnetic field in that volume, i.e. $\iota_\pm = \iota(\mathbf{B}_\pm)$, so that

$$\delta\,\iota_\pm = \frac{\partial\,\iota_\pm}{\partial \mathbf{B}_\pm} \cdot \delta \mathbf{B}_\pm. \tag{18}$$

3. The magnetic field depends on the Fourier harmonics of both the inner and outer interface geometry (represented here as x_j), the helicity multiplier, and the enclosed poloidal flux, i.e. $\mathbf{B}_\pm = \mathbf{B}_\pm(x_j, \mu, \Delta\psi_p)$, so that

$$\delta \mathbf{B}_\pm = \frac{\partial \mathbf{B}_\pm}{\partial x_j}\delta x_j + \frac{\partial \mathbf{B}_\pm}{\partial \mu}\delta\mu + \frac{\partial \mathbf{B}_\pm}{\partial \Delta\psi_p}\delta\Delta\psi_p. \tag{19}$$

4. The rotational-transforms, thus, can be considered to be functions of the geometry, the helicity-multiplier and the enclosed poloidal flux, $\iota_\pm = \iota_\pm(x_j, \mu, \Delta\psi_p)$.

5. The rotational-transform, and its derivatives, on the inner and outer interfaces of each volume is stored in `diotadxup(0:1,-1:2,1:Mvol)`. The arguments label:

   i. the first argument labels the inner or outer interface,

   ii. the the second labels derivative, with

   -1 : indicating the derivative with respect to the interface geometry, i.e. $\dfrac{\partial\,\iota_\pm}{\partial x_j}$,

   0 : the rotational-transform itself,

   1,2 : the derivatives with respec to μ and $\Delta\psi_p$, i.e. $\dfrac{\partial\,\iota_\pm}{\partial \mu}$ and $\dfrac{\partial\,\iota_\pm}{\partial \Delta\psi_p}$;

   iii. the third argument labels volume.

6. The values of `diotadxup` are assigned in mp00aa after calling tr00ab.

1.1.30 `vvolume`, `lBBintegral` and `lABintegral`

1. volume integrals

$$\texttt{vvolume(i)} = \int_{\mathcal{V}_i} dv \tag{20}$$

$$\texttt{lBBintegral(i)} = \int_{\mathcal{V}_i} \mathbf{B}\cdot\mathbf{B}\, dv \tag{21}$$

$$\texttt{lABintegral(i)} = \int_{\mathcal{V}_i} \mathbf{A}\cdot\mathbf{B}\, dv \tag{22}$$