newton

Employs Newton method to find $\mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{x} \equiv \{\text{geometry}\}$ and $\mathbf{F}$ is defined in dforce.

[called by: xspech.] [calls: dforce, packxi and global:wrtend.]

contents

1.0.1 iterative, reverse communication loop

1. The iterative, Newton search to find $\mathbf{x} \equiv \{\text{geometry}\} \equiv \{R_{i,l}, Z_{i,l}\}$ such that $\mathbf{F}(\mathbf{x}) = 0$, where $\mathbf{F}$ and its derivatives, $\nabla_{\mathbf{x}}\mathbf{F}$, are calculated by dforce, is provided by either

   i. NAG: C05NDF if `Lfindzero=1`, which only uses function values; or

   ii. NAG: C05PDF if `Lfindzero=2`, which uses user-provided derivatives.

2. The iterative search will terminate when the solution is within `c05xtol` of the true solution (see NAG documentation).

3. The input variable `c05factor` is provided to determine the initial step bound (see NAG documentation).

1.0.2 logic, writing/reading from file

1. Before proceeding with iterative search, dforce is called to determine the magnitude of the initial force imbalance, and if this is less than `forcetol` then the iterative search will not be performed.

2. As the iterations proceed, global:wrtend will be called to save itermediate information (also see xspech).

3. If the derivative matrix, $\nabla_{\mathbf{x}}\mathbf{F}$, is required, i.e. if `Lfindzero=2`, and if `LreadGF=.true.` then the derivative matrix will initially be read from `.ext.sp.DF`, if it exists, or from `.sp.DF`.

4. As the iterations proceed, the derivative matrix will be written to `.ext.sp.DF`.