

jk03aa

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](#), [packed](#) and [global:wrtend](#).]

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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 it's 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 .	