QC Reference Manual version 1.3

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Contents

1 Introduction

The quasicontinuum (QC) method is a multiscale method combining atomistic simulations with nonlinear continuum finite elements. Theoretical details about the method are given in a series of papers [1, 2, 3, 4, 5]. This manual describes the details of using the freely-available QC method code distributed on the QC website `www.qcmethod.com`. The code is written in Fortran 90 and is designed to be as portable as possible. It has been successfully tested with a variety of different Fortran compilers[1]. Porting to new compilers and architectures should be straightforward.

The current distribution version of the QC code has certain limitations:

- It is limited to two-dimensional boundary value problems that can be described with displacement fields of the form

  $$u_x(x, y), \quad u_y(x, y), \quad u_z(x, y).$$

  Despite the two-dimensional constraint, all atomistic calculations are performed in three dimensions. This corresponds to simulating a slab with periodic boundary conditions applied in the out-of-plane direction that has a thickness equal to the minimum crystallographic repeat distance in that direction. This can be used, for example, to correctly simulate a dislocation whose line is perpendicular to the simulation plane, but not one inclined to it.

- The code is limited to crystalline materials with a simple lattice structure, such as fcc and bcc metals. It is currently not possible to simulate complex crystal materials such as hcp metals or unit cells containing multiple species. (It is possible to simulate a system containing multiple simple crystals in separate grains.)

- The code is a static energy minimization code. It can be used to study equilibrium structures at zero temperature, but not dynamical processes or finite temperature

[1] See Section 1.2 of the *QC Tutorial Guide* for a list of supported compilers.

effects.

- The atomic interactions are limited to empirical potentials in which the energy of the total system can be decomposed as a sum over individual atom energies. The current implementation includes the embedded-atom method (EAM) potential [6]. It should be straightforward to implement other potential forms.

These issues do not constitute limitations to the QC methodology itself (see for example [7] for extension to three dimensions, [8, 9] for extension to complex crystals, [10] for extension to finite temperature, and [11] for incorporation of quantum mechanical calculations within QC). These developments are planned for future releases of the distribution code.

Performing a QC simulation requires the preparation of five user routines that are linked in with the QC code[2] and an input file containing a set of instructions to the QC program based on the simple command line interface originally provided with the program FEAP [12]. This manual provides the information necessary to complete these two tasks. Section 2 provides an overview of the QC program structure along with information on how to prepare the user routines. Sections 3 and 4 provide a listing of all the QC commands that can appear in the input file, with details of the command syntax, options and function. QC simulations are comprised of two stages, each with its own set of commands. Therefore, the listing is split into the `head` stage commands (Section 3) and the `macros` stage commands (Section 4). Within each stage, the commands are listed alphabetically.

For users that are unfamiliar with QC simulations, a good starting point is the *QC Tutorial Guide*, which traces through a simple example simulation. This reference manual is intended to provide complete detail of the user routines and input commands, but assumes that the user is already familiar with the QC approach.

[2]For many simulations only one of the five user routines is required and the rest can be left blank.

2 QC Code structure

The QC code consists of one main file `qcmain.f` and a large number of additional files beginning with the suffix `mod_` each containing one Fortran 90 module dedicated to a specific task or closely-related set of tasks. Each module contains routines and/or variables related to its task. The QC modules and the tasks they deal with are:

- `mod_adaption.f`: Automatic mesh refinement and coarsening.
- `mod_bandwidth.f`: Nodal renumbering to minimize the stiffness matrix bandwidth.
- `mod_boundary.f`: Model boundary and special-attribute zones. See a more detailed description in Section 2.3.
- `mod_check.f`: Numerical derivative checks for debugging purposes.
- `mod_cluster.f`: Building and manipulation of clusters of atoms.
- `mod_crystal.f`: Generation of crystal lattice structures.
- `mod_element.f`: Finite element routines.
- `mod_file.f`: File opening and handling routines.
- `mod_ghost.f`: Ghost force correction calculations.
- `mod_global.f`: Global variables and initialization. See a more detailed description in Section 2.1.
- `mod_grain.f`: Definition and calculations related to crystallographic grains. See a more detailed description in Section 2.4.
- `mod_head.f`: Processing of head stage commands.
- `mod_macros.f`: Processing of macro stage commands.
- `mod_material.f`: Definition of model materials.
- `mod_mesh.f`: Mesh generation (Delaunay triangulation). See a more detailed description in Section 2.5.
- `mod_nonstandard.f`: Non-standard Fortran routines.
- `mod_output.f`: QC output interface. See a more detailed description in Section 2.6.
- `mod_pload.f`: System time and load variables. See a more detailed description in Section 2.7.
- `mod_plotting.f`: Plot generation in Tecplot® format.
- `mod_poten_eam.f`: Atomic-interaction potential (embedded-atom method).
- `mod_qclib.f`: Library of miscellaneous routines. See a more detailed description in Section 2.8.

- `mod_repatom.f`: Definition and calculations related to representative atoms. See a more detailed description in Section 2.9.
- `mod_restart.f`: Simulation restart file manipulation.
- `mod_savemesh.f`: Auxiliary module to the adaption module used for storage of meshes and transferring of field data.
- `mod_solve.f`: : Conjugate gradient and Newton-Raphson solvers.
- `mod_stiff.f`: : Stiffness matrix storage and handling. See a more detailed description in Section 2.10.
- `mod_types.f`: : Fortran type declarations.

Unless the user is interested in modifying the QC code itself, it is not necessary to understand most of these routines to use the code. The important modules that a user must be familiar with are detailed below.

In addition to the modules that come with the code, the user must supply a file `user_APP.f` for every application (where `APP` is the application name) containing the following five routines:

- `user_mesh`: This routine produces the mesh. It is called by the command `mesh` and is discussed in Section 2.11.1 and in Section 3.7 of the *QC Tutorial Guide*.
- `user_bcon`: This routine applies application-specific boundary conditions. It is called by the command `bcon` and discussed in Section 2.11.2 and in Section 4.7 of the *QC Tutorial Guide*.
- `user_pdel`: This routine defines a scalar measure of the applied force for a given boundary condition. This is discussed in Section 2.11.3 and in Section 4.9 of the *QC Tutorial Guide*.
- `user_potential`: This routines computes the energy (and corresponding force and stiffness) associated with an external potential. These contributions are added to the total energy of the system and its derivatives. This is an alternative approach to applying boundary conditions. It is discussed in Section 2.11.4.

- `user_plot`: This routine gives the user the opportunity to create specialized plots for the defined application. This is discussed in Section 2.11.5.

Below we elaborate on the important variables and routines in modules that the user may need to use when constructing the user-specified routines. Following that details of the user routines themselves are given.

2.1 Module mod_global

`mod_global` provides access to globally-defined variables that do not neatly fit into other more specific modules. The most relevant of these for user routines are the following:

- `cmdunit` (Integer): File handle for the parsed command file. See Section 2.11.1.
- `dp` (Integer): Standard double precision kind value.[3]
- `hmin`, (Real, default=0.0): Minimum allowed element side size. Enforced by the adaption routine if different from zero.
- `iregion(1:numnp)` (Integer, default=1): The meshing region to which each node is assigned. See Section 2.11.1.
- `maxel` (Integer): Maximum number of elements in the mesh.
- `maxneq` (Integer): Maximum number of equations in the system, (`maxnp*ndf`).
- `maxnp` (Integer): Maximum number of nodes in the mesh.
- `ndf` (Integer, default=3): Number of degrees of freedom per node.

[3]This variable defines a standard double precision `kind` value to be used by QC. Instead of using the Fortran statement `double precision` to define real double precision variables, the statement `real(kind=dp)` is used. Double precision constants are written with `_dp` rather than the `d` exponent (e.g. `1.0_dp` instead of `1.d0`). Conversion of integers to double precision is done with `real(n,dp)` instead of `dble(n)`, where `n` is an integer. These changes have been introduced to make the QC code portable, since the Fortran standard does not contain a definition for the `double precision` statement. The current version of the code uses `dp=selected_real_kind(p=15,r=307)` for 15 digit precision and a decimal exponent range of 307. This is what corresponds to double precision on most platforms.

- `ndm` (Integer, default=2): Number of spatial dimensions.
- `nen` (Integer, default=3): Number of nodes per element.
- `nregion` (Integer, default=1): The number of unconnected separately meshed regions in the model. See Section 2.11.1.
- `numel` (Integer): Current number of elements in the mesh.
- `numnp` (Integer): Current number of nodes in the mesh.
- `nxdm` (Integer, default=3): Number of nodal coordinate dimensions.
- `neq` (Integer): Number of equations (`ndf*numnp`).
- `nq` (Integer, default=14): Dimension of element internal variable array, `q()`.
- `nstr` (Integer, default=6): Dimension of stress `str` and strain `eps` arrays.
- `SymmetricMesh` (Logical, default=.False.): Flag indicating whether the meshing routine `delaunay` should attempt to create a symmetric mesh. See Section 2.11.1.
- `SymmetryDof` (Integer): For a `SymmetricMesh` sets the symmetry plane (1: symmetric relative to $x =$ `SymmetryValue`, 2: symmetric relative to $y =$ `SymmetryValue`).
- `SymmetryValue` (Real): Symmetry value for a `SymmetricMesh`. See above.

For more detail on these and other variables, see the file `mod_global.f`.

2.2 QC Variables

In addition to variables stored in `mod_global`, QC passes many of its variables as subroutine arguments. A list of the most important ones is given below. The dimensions that appear in array variables are defined in Section 2.1.

- `b(ndf,numnp)`: (double precision) Nodal displacement array. `b(i,j)` stores the `i`th component of the displacement of the `j`th node. If desired, it can be initialized to some value during mesh generation. It is typically modified in the `user_bcon` routine as a means of applying an initial guess to the solution of the nonlinear problem at hand. See Section 4.2 for details. Note that `b` is initialized to zero at the start of the simulation.

- `db(ndf,numnp)`: (double precision) Nodal displacement increment. `db(i,j)` stores the most recent change in the `i`th component of the displacement of the `j`th node. This is typically the change due to an iterative step in the Newton-Raphson solver.

- `dr(ndf,numnp)`: (double precision) Out-of-balance force vector. `dr(i,j)` stores the `i`th component of the current out-of-balance force on the `j`th node. In equilibrium configurations this vector will be close to zero. The norm of this vector is often used as a convergence criterion during a Newton-Raphson solution phase. Note that `dr` is initialized to zero at the start of the simulation. See Section 2.11.4 for an example of how this variable is used.

- `eps(nstr,numel)`: (double precision) Elemental strain array. `eps(i,j)` stores the `i`th component of the Lagrangian finite strain in the `j`th element. Order of storage is E_{xx}, E_{yy}, E_{zz}, E_{xy}, E_{xz}, E_{yz}. `eps` is an output variable and will be computed from the current displacement values every time the energy or out-of-balance forces are computed.

- `f(ndf,numnp)`: (double precision) The boundary condition array. `f(i,j)` stores the `i`th component of a normalized force applied to node `j` (if `id(i,j)=0`) or of a normalized displacement (if `id(i,j)=1`) that is used to apply the boundary conditions. See Section 2.11.2 for a discussion on the application of boundary conditions in QC. For degrees of freedom that are unconstrained and have no applied force, the corresponding `f(i,j)` entry must be set to zero (which is the default value to which it is initialized).

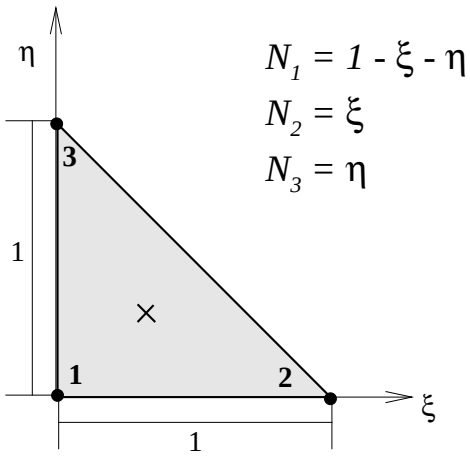


Figure 1: Parent element and shape functions used in the QC method.

- `id(ndf,numnp)`: (integer) The boundary constraint flag array `id(i,j)` stores a flag that identifies whether a node `j` is to have a fixed `i`th component of displacement (`id(i,j)=1`) or not (`id(i,j)=0`). This array is set by the user, either during the generation of the initial mesh in `user_mesh` (Section 2.11.1) or during application of boundary conditions in `user_bcon` (Section 2.11.2).[4]

- `itx(3,numel)`: (integer) The adjacency matrix. `itx(j,i)` stores the element number adjacent to the `j`th side of element `i`. The initial `itx` array is created during mesh generation in the `user_mesh` routine (Section 2.11.1).

- `ix(nen,numel)`: (integer) The connectivity array. `ix(j,i)` stores the global node number of the `j`th node defining element `i`. The initial `ix` array is generated by the `user_mesh` routine (Section 2.11.1).

- `jdiag(neq)`: (integer) Pointer into the stiffness matrix which is stored in a collapsed banded format. `jdiag` is used to efficiently store the sparse stiffness matrix.

[4]Note also that the mesh adaption routine will assign `id` values to new nodes as they are added to the mesh based on nearby existing nodes. Specifically, a node `j3` is added to the mesh by bisecting an edge between two existing nodes, `j1` and `j2`. The `i`th degree of freedom of the new node will be assigned `id(i,j3)=1` if (and only if) `id(j1,i)=1` and `id(j2,i)=1`.

- `shp(nshp,numel)`: (double precision) Shape functions. The QC method uses three-node linear elements, thus there is only one Gauss point at the centroid of each element. The isoparametric formulation is used, with the parent element, local node numbering and shape functions as shown in Fig. 1. More information on the finite element formulation can be found in, for example, [12]. For each element `i`, the following is stored in `shp`:
  - `shp(1,i)`: Derivative $\partial N_1/\partial x$.
  - `shp(2,i)`: Derivative $\partial N_1/\partial y$.
  - `shp(3,i)`: Value of N_1 at the Gauss point (`0.333_dp`).
  - `shp(4,i)`: Derivative $\partial N_2/\partial x$.
  - `shp(5,i)`: Derivative $\partial N_2/\partial y$.
  - `shp(6,i)`: Value of N_2 at the Gauss point (`0.333_dp`).
  - `shp(7,i)`: Derivative $\partial N_3/\partial x$.
  - `shp(8,i)`: Derivative $\partial N_3/\partial y$.
  - `shp(9,i)`: Value of N_3 at the Gauss point (`0.333_dp`).

  Here $N_i(x, y)$ is the shape function associated with node i.

- `str(nstr,numel)`: (double precision) Elemental stress array. `str(i,j)` stores the `i`th component of the Kirchhoff stress[5] in the `j`th element. Order of storage is τ_{xx}, τ_{yy}, τ_{zz}, τ_{xy}, τ_{xz}, τ_{yz}. `str` is an output variable and will be updated each time the energy or out-of-balance forces are computed for a given set of nodal displacements. The elemental stresses are only computed in elements which touch local nodes.

- `q(nq,numel)`: (double precision) Elemental internal variable array. `q` stores several elemental quantities. For element `iel`:

[5]Note that the Kirchhoff stress $\boldsymbol{\tau}$ is related to the Cauchy stress (or true stress) $\boldsymbol{\sigma}$ that is more commonly used through the relation $\boldsymbol{\tau} = J\boldsymbol{\sigma}$, where J is the determinant of the deformation gradient $\boldsymbol{F}$, which is stored in the internal variable array `q`.

  - `q(1,iel)`: Strain energy density.
  - `q(2:10,iel)`: Deformation gradient components in Fortran column order (F_{11}, F_{21}, F_{31}, F_{12}, F_{22}, F_{32}, F_{13}, F_{23}, F_{33}).
  - `q(11:13,iel)`: Eigenvalues of the right Cauchy-Green deformation tensor, $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$.
  - `q(14,iel)`: Grain number containing the centroid of the element.

- `x(nxdm,numnp)`: (double precision) The reference coordinate array. `x(1..nxdm,i)` stores the reference coordinates of the `i`th repatom (node). Note that even though the fields in the current QC implementation are limited to two dimensions, the `x` array has three components (`nxdm=3`) in order to store the correct atomic crystal structure. The initial `x` array is generated by the `user_mesh` routine (Section 2.11.1).

- `xsj(numel)`: (double precision) Elemental areas. `xsj(i)` stores the area (in the undeformed configuration) of element `i`.

2.3 Module mod_boundary

Module `mod_boundary` contains information and routines related to the boundaries of the QC model. Particularly relevant for the user are the variables `ncb`, `nce`, `NCEMAX` and `elist()` used to define outer and inner boundaries of the model that must be respected by the mesh generation routine. The variable `active()` is used to define boundary segments that trigger nonlocality. These variables are described in detail in Section 2.11.1.

2.4 Module mod_grain

Module `mod_grain` contains data and routines related to the definition and processing of the crystallographic grains making up the system. The data in this module is not directly accessible to the user (to prevent inadvertent errors being introduced). However, a series of routines have been defined to allow a user to query the values of variables stored there.

Some of these variables can be very useful for generating the initial arrangement of nodes in `user_mesh`. This is discussed further in Section 2.11.1. See also Section 3.5 of the *QC Tutorial Guide* where the grain definition and associated variables are defined. The data query routines in `mod_grain` are:

- `NumGrains`: number of grains
- `GetGrainCellSize`: repeating cell dimensions for a given grain
- `GetGrainNumCell`: number of atoms in the repeating cell for a given grain
- `GetGrainCellAtom`: coordinates of a given atom in the repeating cell for a given grain
- `GetGrainBvec`: Bravais vector matrix for a given grain
- `GetGrainBinv`: inverse Bravais vector matrix for a given grain
- `GetGrainRefStiff`: reference stiffness matrix for a given grain
- `GetGrainRefatom`: reference atom for a given grain
- `GetGrainSpecies`: atomic species for a given grain
- `GetGrainNumVrts`: number of vertices for polygon of a given grain
- `GetGrainVertex` : given vertex of the polygon of a given grain
- `GetGrainXlatvect`: crystallographic axes for a given grain

Another useful routine in `mod_grain` is `NearestBSite` that returns the nearest Bravais site to a given point. This routine is used to ensure the requirement normally imposed in QC that nodes must occupy lattice sites in the reference configuration. The use of this routine and its calling format are discussed in Section 2.11.1.

2.5 Module mod_mesh

Module `mod_mesh` contains routines related to the generation of two-dimensional triangular meshes. This module is built around `contri`, a constrained Delaunay triangulation program developed by Sloan [13, 14]. Two routines in `mod_mesh` are accessed by users:

- `delaunay`: the main triangulation routine that calls `contri`. This routine is discussed in Section 2.11.1.
- `PerturbMesh`: a routine for slightly perturbing (or unperturbing) the nodes in a mesh prior to (or after) triangulation to obtain uniform or symmetric meshes. This is discussed in Section 2.11.1.

2.6 Module mod_output

Module `mod_output` provides a standardized interface for generating output in QC. Rather than printing directly to the output stream, a set of routines and associated variables are provided that allow the user to generate output in the user routines consistent with the QC format. This includes an indentation hierarchy that positions the output in way that makes reading output files much easier. The output interface has three main components for generating (1) standard output, (2) error messages, and (3) log file entries.

1. To generate standard output, the desired output is stored in the `character(len=160)` variable `string` and then a `call output` statement is issued. For example,

   ```
   string = 'Message from the user!'
   call output
   ```

   will print the text "Message from the user!" in the appropriate place in the QC output file. Variable data can be printed in the following manner:

   ```
   write(string,'(a,i5)')'**numnp = ',numnp
   call output
   ```

The `write` statement places the formatted output in `string`, which is then sent to the output file by `call output`.

2. To generate an error message, the `nerror` lines of the message are stored in the `character(len=160)` array `error(nerrmax)`. Note that `nerror` must be less than the maximum allowed value `nerrmax` (currently set to 25). The output is generated by issuing a `call erroroutput` statement. Typically this statement is followed by a `stop` statement to terminate program execution. For example,

```
 if (kount > maxnp) then
    nerror = 2
    error(1) =
&      'Number of nodes exceeds maxnp in subroutine user_mesh'
    write(error(2),'(a,i5)')'**maxnp = ',maxnp
    call erroroutput
    stop
 endif
```

This code segment from a `user_mesh` routine checks whether the number of nodes generated by the meshing routine (given by `kount`) exceeds the maximum allowed value of `maxnp`. If it does, an appropriate error message is issued and execution terminates. The `call erroroutput` statement will send the error message to the output file and will also generate a log entry in the log file. As for standard output, variable data can be stored in `error()` lines using `write` statements.

3. The log file `qc.log` is used to output large amounts of data that would clutter up the standard output file. To generate a log file entry, the desired output is stored in the `character(len=160)` variable `string` and then a `call logoutput` statement is issued. For example,

```
 ! Check for repeating nodes
 do i = 1, numnp
    do j = i+1, numnp
       if ( abs(x(1,i)-x(1,j)) < tol .and.
&           abs(x(2,i)-x(2,j)) < tol ) then
          nerror = 2
          write(error(1),'(a,i5,a,i5)')'Node',j,' coincides with',i
```

```
            error(2) =
     &           'Node list sent to log file (subroutine user_mesh)'
            call erroroutput
            ! list nodes to log file
            string = 'Node List:'; call logoutput
            string = ' node        x             y     '
            call logoutput
            do k=1,numnp
               write(string,'(i5,2x,f12.5,2x,f12.5)')k,x(1:2,k)
               call logoutput
            enddo
            stop
          endif
        enddo
      enddo
```

This code segment checks for coincident nodes (two nodes located at the same position) in the `user_mesh` routine for `Friction_example`[6]. If a coincident node is found, an error message is issued and the complete list of nodes is sent to the log file to facilitate debugging. A typical output to the log file is given below:

```
--Log Entry    2      2007-05-12 13:50
QC simulation terminated due to error.
*** ERROR: Node  364 coincides with  363
           Node list sent to log file (subroutine user_mesh)
Node List:
 node        x             y
    1    -499.73534    -498.98750
    2    -400.04389    -498.98750
    3    -300.35244    -498.98750
    4    -200.66099    -498.98750
    .         .             .
    .         .             .
    .         .             .
```

Note that the error message is also sent to the log file as explained above. The error statement created a new `Log Entry` indicated by a number and time stamp. The output generated by `logoutput` simply follows this. In some cases it may be necessary to generate log file output without a preceding error message. In this case a `call logentry` statement must be issued before the first `logoutput` to create a new log entry to separate the generated output from earlier entries in the log file.

[6]See *QC Tutorial Guide* for more information.

2.7 Module mod_pload

Module `mod_pload` provides access to variables and routines related to the proportional loading table and time[7] management. The data in this module is not directly accessible to the user (to prevent inadvertent errors being introduced). However, a series of routines have been defined to allow a user to query the values of variables stored there. Some of these variables can be necessary to the user when applying boundary conditions. See Section 2.11.2 for a discussion of how boundary conditions are applied in QC. The data query routines in `mod_pload` are:

- `GetLoadTime`: current loading time (`time`)
- `GetLoadTimeStep`: current loading timestep (`dt`)
- `GetLoadPropFact`: current loading proportional factor (`prop`)
- `GetLoadOldPropFact`: previous loading proportional factor (`propol`)
- `TimeStepMax`: compute the maximum possible time step that after the application of boundary conditions will just result in a node being pushed onto the opposite element side, i.e. that will cause element warping.
- `PropToTime`: given a current time and a desired property value, returns the required future time.

See module `mod_pload` for details on the calling format for these routines. Some examples of their use are given below in Section 2.11.2.

2.8 Module mod_qclib

Module `mod_qclib` is a library of general-purpose routines used by other modules in QC. There are a variety of vector and matrix manipulation routines, geometric routines, character

[7]This version of QC is a static zero temperature implementation. "time" refers to an arbitrary load step counter and not an actual measure of time.

string manipulation routines, and miscellaneous routines (such as a pseudo random number generator). Details of these routines are given in `mod_qclib` and will not be reproduced here, except for three routines that are particularly important for the user programs. The first two are routines used to parse input lines from the input file:

- `next`: integer function to find the next delimiter (comma or space) in a string.
- `freein`: subroutine to parse free-form input lines.

These two commands work in tandem to extract variables from the comma delimited variables on QC input lines. Examples of how these routines are used are given in Sections 2.11.1 and 2.11.2.

The third useful routine in `mod_qclib` is `qsortr`. This routine sorts the first column of a `list` containing two columns and `n` rows according to a key variable `xkey`. The sorting direction is determined by the variable `sign` (= 1.0 for ascending sort, = −1.0 for descending sort). For an ascending sort, upon return from `qsortr` all elements satisfy: `xkey(list(1,i))` ≤ `xkey(list(1,i+1))`. The calling format is:

```
call qsortr(n,list,xkey,sign,listdim,keydim)
```

Here `listdim` is the allocated dimension of `list` (`n` ≤ `listdim`) and `keydim` is the allocated dimension of `xkey` (`keydim` ≥ max{`list(1,1:n)`}). This routine is used in `user_mesh` to sort the nodes defining outer and inner boundaries (i.e holes) in the model in counter-clockwise and clockwise directions, respectively. See Section 2.11.1 for more information on this.

2.9 Module mod_repatom

Module `mod_repatom` is one of the main modules in the QC code dealing with many aspects of the definition and processing of representative atoms. Users should not need to directly access variables in this module. The exception is the logical array `protected()` that allows a user to mark certain representative atoms as permanent, i.e. ones that cannot be deleted

by the adaption routine during its coarsening phase. For example, to protect node `i` from deletion set

```
protected(i) = .true.
```

in `user_mesh`. Normally the reason for doing this is to maintain a "skeleton" of the model even if the coarsening algorithm determines that most nodes are not necessary. It is also possible to set `protected` from the input file. This is discussed in Section 4.15.

2.10 Module mod_stiff

Module `mod_stiff` is used to store the tangential stiffness matrix `tang`. To minimize storage requirements the symmetric banded nature of the stiffness matrix is exploited. Only the main diagonal of the stiffness matrix and columns of numbers above the diagonal that terminate in a non-zero element are stored. This list of numbers is stored in concatenated form in `tang` with the associated vector `jdiag(i)` pointing to the position of the `(i,i)`-th element of the stiffness matrix. A function `istiff` that is also located in `mod_stiff` returns the index into `tang` for a specific element. See Section 2.11.4 for an example how these variables are used.

2.11 User-Specified Routines

As noted above the user must supply QC with a `user_APP.f` containing five routines. At the top of this file is a module `mod_uservars` that can be used by the user to pass variables between the different user routines. For reasons of downward compatibility the module always contains the following two arrays:[8]

- `user_iparam(10)` (Integer): Array of integers available for storage of user-specific parameters to pass information between the user routines. See Section 2.11.1.
- `user_rparam(10)` (Real): Same as above for real (double precision) variables.

[8] In earlier versions of QC these variables were stored in module `mod_global`.

See Section 2.11.4 for an example how module `uservars` is used. The required user routines are described in the following sections.

Note: In order to facilitate the porting of `user_mesh`, `user_bcon` and `user_pdel` routines from earlier versions of QC (where they were stored in separate files), a `user_template.f` file is supplied with the distribution code in the `QC` directory. This file is complete except for blank places left for these routines along with helpful instructions on the changes that must be introduced to port over old files.

2.11.1 user_mesh

Other than the mesh generators provided with specific examples in the QC package, there are no mesh-generating capabilities in QC. Instead, the user is required to write a mesh generating routine `user_mesh` and compile and link it with the main QC routines. QC does include a number of tools, most notably a constrained Delaunay triangulation routine [13], that facilitate mesh generation. These tools are described below.

The `user_mesh` routine is initiated by a `mesh` statement in the head stage of the input file (see Section 3.7). The calling format for this macro is

```
mesh[,key][,data]
```

where `key` and `data` are problem-specific data that are passed to `user_mesh` as explained below. In addition, the lines immediately following the `mesh` command in the input file can be read by this routine to provide additional input to the mesh generator. See below under the heading "Direct input to the `user_mesh` routine" for more information on this.

The header of a typical `user_mesh` subroutine is as follows:

```
 subroutine user_mesh(id,x,ix,f,b,itx,key,input)
 use mod_uservars
 use mod_global,   only : dp,maxel,maxnp,ndf,ndm,nen,numel,numnp,
&                         nxdm
 use mod_output,   only : erroroutput,nerror,output,string,error
 use mod_boundary, only : ncb,nce,NCEMAX,elist
 use mod_repatom,  only : protected
 use mod_qclib,    only : next,freein,qsortr
```

```
      use mod_mesh,     only : delaunay,PerturbMesh
      use mod_grain,    only : NumGrains,GetGrainNumVrts,GetGrainVertex,
     &                         NearestBSite
      implicit none

!-- Transferred variables
      integer,           intent(inout)  :: id(ndf,maxnp),
     &                                     ix(nen,maxel),
     &                                     itx(3,maxel)
      real(kind=dp),     intent(inout)  :: x(nxdm,maxnp),
     &                                     f(ndf,maxnp),
     &                                     b(ndf,maxnp)
      character(len=4),  intent(in)     :: key
      character(len=80), intent(in)     :: input
```

The header begins with a list of modules used by `user_mesh`. Note the use of the `only` clause for all modules indicating the specific variables and routines accessed from the module. This is good programming practice, both from a readability standpoint and as an aid to the compiler to detect errors. The important variables and routines in these module are described in Section 2.1, and Sections 2.3 to 2.9. More details are also available in the comments at the top of the module files.

Variables passed to `user_mesh`. The variables passed to `user_mesh` (except for `key` and `input` are described in Section 2.2. Here a brief definition is given with additional comments specific to the `user_mesh` routine.

- `id(ndf,numnp)`: (integer) The boundary constraint flag array. This array can be initialized either here in `user_mesh` or in `user_bcon`.
- `x(nxdm,numnp)`: (double precision) The reference coordinate array. The initial `x` array must be generated here by the `user_mesh` routine. Details and useful tools are discussed below.
- `ix(nen,numel)`: (integer) The connectivity array. The initial `ix` array must be generated here by the `user_mesh` routine. Details and useful tools are discussed below.
- `f(ndf,numnp)`: (double precision) The boundary condition array. This array can be initialized either here in `user_mesh` or in `user_bcon`.

- `b(ndf,numnp)`: (double precision) Nodal Displacement Array. This array can be initialized here in `user_mesh` or in `user_bcon` if desired. (By default it is initialized to zero at the start of the simulation.)

- `itx(3,numel)`: (integer) The adjacency matrix. The initial `itx` array must be generated here by the `user_mesh` routine. Details and useful tools are discussed below.

- `key`: (character(len=4)) Key passed from the input file command line. Can be used to implement various options in the mesh generator. By convention, `key='dire'` indicates that additional input to `user_mesh` follows the `mesh` command line. See below under the heading "Direct input to the `user_mesh` routine". **Note that this variable should not be modified by the `user_mesh` routine.**

- `input`: (character(len=80)) Input data passed from the input file command line. `input` can be used to pass character, double precision, integer or logical data directly from the command line to the `user_mesh` routine. It is left to the user to parse this data. Routines in `mod_qclib` (see Section 2.8) facilitate this as shown below. **Note that this variable should not be modified by the `user_mesh` routine.**

As an example of how the `input` variable can be parsed, consider the `user_mesh` routine for `GB_example`[9]. This routine defines the following calling format for the input file:

```
mesh,,nx,ny
```

where `nx` and `ny` are the number of divisions along the x and y axes. Everything beyond the second comma will be passed to the `user_mesh` subroutine in the variable `input`. For example, if the input file contains

```
mesh,,8,8
```

the variable `input` passed to `user_mesh` contains `'8,8'`. The following code segment in `user_mesh` parses this input into the variables `nx` and `ny`:

[9]See *QC Tutorial Guide* for more information.

```
integer lower,upper,nx,ny
real(kind=dp) dum
.
.
.
! Parse input
lower = 0
upper = next(lower,input)
call freein(input,lower,upper,nx,dum,1)
lower = upper
upper = next(lower,input)
call freein(input,lower,upper,ny,dum,1)
```

The function `next` simply starts from the integer position `lower` in the string `input`, and returns the position of the next `','` or end-of-line character in the string. The routine `freein` parses a string between positions `lower+1` and `upper-1` as either an integer if the last variable in the list is `'1'` or a double precision real is the last variable in the list is `'2'`. If the return value is to be an integer, it is returned in the fourth variable on the list (`'nx'` or `'ny'` in this case), while a double precision return value is returned in the fifth variable. Another example of a code segment parsing input that also reads in double precision variables is given in Section 2.11.2.

Note that the text-parser routine `freein` expects the characters between each pair of commas (*i.e.* from `lower+1` to `upper-1`) to be consistent with `integer` or `double precision` formatting. For example, no letters (a-z) should appear in an `integer` field.

Expected output from the `user_mesh` routine. The user-routine for mesh generation must define the following variables:

- `numnp`: (integer). The number of repatoms in the mesh. This is a global variable in `mod_global`.
- `numel`: (integer). The number of elements in the mesh. This is a global variable in `mod_global`.
- `ix`: (integer). The connectivity matrix, as described above. Note that the constrained Delaunay triangulator that is provided with QC is a great help in generating this

matrix. How to use this triangulator is described under the heading "Constrained Delaunay triangulation" below.

- `itx`: (integer). The adjacency matrix, as described above. Note that the constrained Delaunay triangulator that is provided with QC is a great help in generating this matrix. How to use this triangulator is described under the heading "Constrained Delaunay triangulation" below.

- `nregion`: (integer). It is possible to define a model with several separately meshed regions. For example, in a nano-indentation simulation, one may wish to mesh the indenter separately from the indented substrate. The global variable `nregion` is found in the `mod_global` module, and must be defined to be the number of regions. The default value is set to `nregion=1`, so for a simple mesh with one region, nothing needs to be done in the `user_mesh routine`.

  Note that modeling contact problems between two regions requires some care. QC will only reliably detect contact between two nonlocal regions, so the surfaces expected to come into contact must be made nonlocal.

- `iregion(numnp)`: (integer). Related to the `nregion` variable described above, this array assigns each repatom in the problem to one of the regions to be meshed. Thus `iregion(i)` is the region to which repatom `i` belongs. The default value is set to `iregion(i)=1` for all `i`, so for a simple mesh with one region, nothing needs to be done in the `user_mesh` routine. Once `nregion` and `iregion` is set in `user_mesh`, it will be kept up to date by the code automatically during subsequent mesh adaption.

- `x`: (double precision). The reference coordinates of all repatoms, as discussed in the list of input variables above. Note that the QC normally requires repatoms to lie on Bravais lattice sites. The requirement is only relaxed for a fully *local* QC simulation, in which case the user can set choose to set `NodesOnBSites=.false.` (see the `flag` command). Two items available to the `user_mesh` routine simplify the generation of

conforming points. First, there is a subroutine `NearestBsite` which, given a point in the simulation plane, returns the nearest Bravais site. (See Section 2.4). Its header is as follows:

```
subroutine NearestBSite(u,CheckModel,xa,igrain,iel,x,b,ix,itx)
use mod_global, only : dp,maxel,maxnp,ndf,ndm,nen,nxdm,NodesOnBsites
implicit none

!-- Transferred variables
real(kind=dp) u(ndm), xa(3),x(nxdm,maxnp),b(ndf,maxnp)
integer   igrain,iel,ix(nen,maxel),itx(3,maxel)
Logical CheckModel
```

The variables `x, b, ix, itx` are as previously defined and are not modified by the routine. The others are:

- `u(ndm)`: (double precision, in). Coordinates of the point. In the 2D QC implementation, `ndm=2`.
- `CheckModel`: (logical, in). If `CheckModel=.true.`, the routine will return the closest point that is *inside* the current model boundaries, otherwise it will not check whether the new point lies in the model. In the `user_mesh` routine, the model is in the process of being defined and therefore this flag is typically `.false.`. Note that if `CheckModel=.false.` then the variables `iel,x,b,ix,itx` are not used by the `NearestBSite` routine. Thus, dummy arguments can be passed to the subroutine in this case, which is important when `NearestBSite` is being used during initial mesh generation.
- `xa(nxdm)`: (double precision, out), Returned coordinates of the Bravais site.
- `igrain`: (integer, out), Returned grain number in which the site resides.
- `iel`: (integer, in/out) : If `checkmodel` is `.true.`, `iel` returns the element in which the returned point sits. Also, `iel` is used as the element from which to start searching (breadth-first search) to determine if the point is in the model. It can be initialized to `0` if an intelligent guess for a starting element is not known.

The second item that is useful for generating a set of nodes `x` that are on lattice sites is the `periodic cell` for each grain, as discussed in Section 3.5 of the *QC Tutorial Guide*. This cell is useful because it can be used to "tile" the model with all the possible lattice sites in space for the given orientation of the grains. This tiling can serve as a template for choosing a sensible location for each repatom in the mesh. The following code segments use the routines described in Section 2.4 to extract the cell variables for grain `igrain`:

- The number of atom sites in the cell `ncell`:

```
integer ncell
call GetGrainNumCell(igrain,ncell)
```

- The coordinates of the atoms in the cell. `cellatom(1:3)` contains the coordinates of the `j`th atom (`j` $\leq$ `ncell`):

```
real(kind=dp) cellatom(3)
call GetGrainCellAtom(igrain,j,cellatom)
```

- The periodic lengths of the cell `dcell(3)` in the three coordinate directions:

```
real(kind=dp) dcell(3)
call GetGrainCellSize(igrain,dcell)
```

Constrained Delaunay triangulation. Relatively speaking, the selection of a set of repatoms is a simple task while correctly generating a mesh of these points (i.e. generating connectivity and adjacency matrices) can be difficult. Therefore, QC includes a constrained Delaunay triangulator called `contri` [13, 14]. To use `contri`, the user needs only to define the coordinates of all the repatoms in the problem. If the mesh is relatively simple (specifically if it is a simply-connected convex hull) no more information is needed. For multiply-connected regions (i.e. with holes) or non-convex outer boundaries, the user must also generate a set of *constrained edges and boundaries* for the mesh.

A boundary is made up of a series of edges, each of which is defined by the repatoms at the start and end of the edge. The edges that define the boundaries may be listed in any

order, but the repatoms defining external boundary edges must be listed counter-clockwise around the boundary, while edges for internal boundaries (holes) must be listed clockwise. In addition to boundaries, internal edges can also be specified to insure that these edges appear in the final mesh. For example, it may be desirable that the path of a grain boundary is closely followed by the edges of the elements in a bi-crystal simulation.

Constrained boundary and edge information is stored in `mod_boundary`. (See Section 2.3.) The information that the user must generate before calling the triangulator is as follows:[10]

- `nce`: (integer). The number of constrained edges. For convex hull triangulation, `nce=0`
- `ncb`: (integer). The number of constrained boundary edges. For convex hull triangulation, `ncb=0`. Note that `nce` must be greater than or equal to `ncb`.
- `elist(2,nce)`: (integer). The repatom numbers defining each edge. Constrained boundary edges must appear in the list before any internal constrained edges. Each edge `i` goes from repatom `elist(1,i)` to `elist(2,i)`. As mentioned earlier, boundary edges can appear in any order but must be listed in their counter-clockwise sense if they are external boundaries and in their clockwise sense if they are internal boundaries (holes). There are different ways for ensuring this. One approach that uses the routine `qsortr` described in Section 2.8 is to identify all of the nodes on a boundary, sort them in counter-clockwise fashion (for an outer boundary) and then defined the edges by connecting the nodes in series. A code segment that does this, taken from the `GB_example`[11], is given below:

```
real(kind=dp), allocatable :: vtmp(:)
real(kind=dp) xmin,xmax,ymin,ymax,xx,yy,xc,yc
integer i
.
.
.
! Identify nodes lying on the boundaries and sort
! in counterclockwise fashion for constrained Delaunay algorithm
```

[10] See also the discussion under the heading "The model boundary" below.
[11] See *QC Tutorial Guide* for more information.

```
 1    xmax=xmax-0.2_dp*dx
 2    xmin=xmin+0.2_dp*dx
 3    ymax=ymax-0.2_dp*dy
 4    ymin=ymin+0.2_dp*dy
 5    nce = 0
 6    allocate(vtmp(numnp))
 7    do i=1,numnp
 8       xx=x(1,i)
 9       yy=x(2,i)
10       if (xx.lt.xmin .or. xx.gt.xmax .or.
     &       yy.lt.ymin .or. yy.gt.ymax) then
11          nce=nce+1
12          if (nce.gt.NCEMAX) then
13             nerror = 1
14             error(1) = 'nce exceeds NCEMAX in subroutine user_mesh'
15             call erroroutput
16             stop
17          endif
18          elist(1,nce)=i
19          vtmp(i)=datan2(yy-yc,xx-xc)
20       endif
21    enddo
22    call qsortr(nce,elist,vtmp,1.0_dp,NCEMAX,numnp)
23    deallocate(vtmp)

      ! Finish defining boundary
24    elist(2,nce)=elist(1,1)
25    ncb = nce
26    do i=1,nce-1
27       elist(2,i)=elist(1,i+1)
28    enddo
```

The domain to be meshed in this case is a simple rectangle with minimum and maximum dimensions in the x and y directions, `xmin`, `xmax`, `ymin`, and `ymax`. The spacing between nodes is `dx` and `dy`, so lines 1–4 ensure that the test in line 10 is true for any nodes lying on the outer boundary (the perimeter of the rectangle). The nodes on the boundary are added to `elist` in line 18. For each node `i` on the boundary, `vtmp(i)` computed in line 19, contains the angle to this point from the center of the rectangle `(xc,yc)`. The boundary nodes are sorted in counter-clockwise order in line 22 using the routine `qsortr`. The boundary list is completed in lines 24–27. Note that since a rectangle is a convex region, the entire procedure of identifying the nodes on the boundary and sorting them is unnecessary. The default behavior of `contri` with no boundary defined would have given the same result. This is only done in this routine

as an example.

Once these data are generated (normally within the `user_mesh`) routine, the triangulator is executed. In QC, this is done by calling the subroutine `delaunay` with the following header:

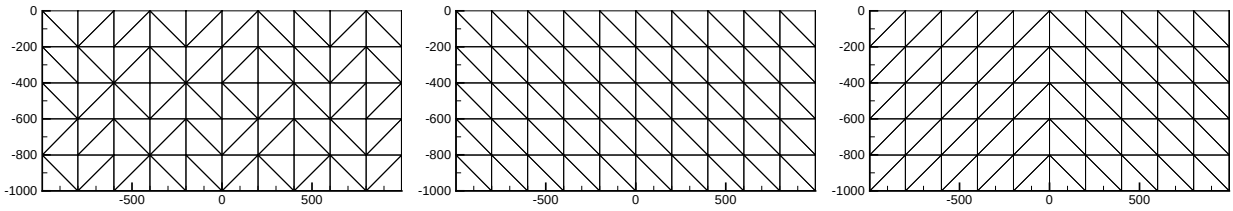
```
      subroutine delaunay(x,ix,b,f,id,itx)
      use mod_global,   only : dp,iregion,maxel,maxnp,ndf,nen,neq,
     &                         nregion,numel,numelast,numnp,nxdm,NeedItx
      use mod_output,   only : erroroutput,nerror,output,string,error
      use mod_boundary, only : IncreaseElist,nce,ncb,elist,active,NCEMAX
      implicit none

!-- Transferred variables
      integer,       intent(inout) :: ix(nen,maxel)
      integer,       intent(inout) :: id(ndf,maxnp)
      real(kind=dp), intent(inout) :: x(nxdm,maxnp),b(ndf,maxnp),
     &                                f(ndf,maxnp)
      integer,       intent(out)   :: itx(3,maxel)
```

where `x, ix, b` and `itx` are as previously defined. If the global logical variable `DefMesh` is `.false.` (the default), the mesh is generated using the reference configuration of points (`x`), otherwise the deformed configuration is used (`x+b`). Upon successful completion of this routine, the matrices `ix` and `itx` will be defined.

Symmetric and regular mesh generation. It is often desirable that the orientation of the triangular elements in a finite element mesh be as regular[12] or symmetric as possible. The QC program includes a utility routine that can be used by the `user_mesh` routine to generate regular or symmetric meshes.

The Delaunay triangulation algorithm can be coaxed into producing a regular or symmetric mesh by introducing a bias in the nodal locations prior to calling the meshing routine. For example, a regular square array of nodal points will be meshed with randomly oriented triangles depending on the numerical precision to which the nodal coordinates are specified (see Fig. 2(a)). On the other hand, if the square array is slightly sheared so that the squares become parallelograms, the mesh will become perfectly regular (see Fig. 2(b)). If

[12]Here *regular* means that all elements are oriented in the same direction.



(a) (b) (c)

Figure 2: Three uniform meshes obtained from `delaunay` depending on whether `PerturbMesh` was called and the setting of `SymmetricMesh`. (a) Random mesh (`PerturbMesh` not called, `SymmetricMesh=.false.`), (b) Regular mesh (`PerturbMesh` called, `SymmetricMesh=.false.`), (c) Symmetric mesh (`PerturbMesh` called, `SymmetricMesh=.true.` with `SymmetryDof` = 1 and `SymmetryValue` = 0.0_dp).

the perturbation is selected in a symmetric manner, a symmetric mesh can be obtained (see Fig. 2(c)).

The QC program provides a utility routine `PerturbMesh` and several global variables (`SymmetricMesh`, `SymmetryDof`, `SymmetryValue`) that control the mesh morphology. The `Perturbmesh` subroutine header is as follows:

```
      subroutine PerturbMesh(x,perturb)
      use mod_global, only : dp,nxdm,maxnp,numnp,
     &                       SymmetricMesh,SymmetryDof,SymmetryValue
      implicit none

!--Transferred variables
      logical,       intent(in)    :: perturb
      real(kind=dp), intent(inout) :: x(nxdm,maxnp)
```

where `x` is as previously defined and `perturb` is a logical flag. When `perturb=.true.`, the nodal coordinates are modified to produce a bias for the Delaunay algorithm. When `perturb=.false.`, the opposite bias is applied, canceling the effect of the previous perturbation.

Code segments that produce random, regular and symmetric meshes are shown below. A random mesh (Fig. 2(a)) is the default behavior obtained from simply calling `delaunay`:

```
      call delaunay(x,ix,b,f,id,itx)
```

A regular mesh (Fig. 2(b)) is obtained by applying `PerturbMesh` with symmetry off:

```
SymmetricMesh=.false.
call PerturbMesh(x,.true.)
call delaunay(x,ix,b,f,id,itx)
call PerturbMesh(x,.false.)
```

A symmetric mesh (Fig. 2(c)) is obtained by applying `PerturbMesh` with symmetry on:

```
SymmetricMesh=.true.
SymmetryDof=1
SymmetryValue=0.0_dp
call PerturbMesh(x,.true.)
call delaunay(x,ix,b,f,id,itx)
call PerturbMesh(x,.false.)
```

Here, the first three lines are global variables (found in the module `mod_global`) provided to the `PerturbMesh` routine. `SymmetricMesh` is a logical flag set to true if the symmetric mesh option is desired. `SymmetryDof` is an integer that defines the coordinate (`1=x` or `2=y`) used to define the plane of symmetry and `SymmetryValue` is a double-precision value defining the coordinate of the plane of symmetry. The call to `PerturbMesh` modifies the `x` values prior to the call to `delaunay`, which produces the mesh. Finally, the second call to `PerturbMesh` restores the correct values in `x`. In this example, the nodal points are temporarily sheared in such a way as to make the elements appear symmetrical about the plane `x=0.0_dp`.

It is important to note that regular (or symmetric) meshes can only be obtained if the nodes themselves are regular (or symmetric). Due to the constraint that nodes must lie on lattice sites, sometimes even arrangements of nodes that appear regular (or symmetric) are not exactly so as a result of small adjustments to the positions of nodes. To prevent this problem, nodes for regular (or symmetric) meshes, should be generated to be consistent with the underlying lattice structure from the start by using the grain repeating cell information as explained above.

The model boundary. The definition of the mesh, and more specifically the assignment of the variables `ncb`, `nce`, and `elist` described above also defines the spatial extent of the model. Prior to the assignment of these variables by the `user_mesh` routine, there is only the definition of the regions containing each grain as defined by the `grain` command. The QC

program does not require that the grain shapes match the mesh shape, but every element must lie inside one or more grains. Thus, it is often convenient to define grains that are much larger than the intended region to be modeled, allowing the `user_mesh` routine to effectively "cut out" a region of this space to define the actual model.

Once the mesh is defined, the list of boundary edges contained in `elist` defines the true boundary of the model. This has ramifications for mesh adaption, as any repatoms added during adaption will lie inside this model boundary.

The model boundary is also used by the QC to determine the location of free surfaces. Specifically, each boundary segment `j` stored in the array `elist` is also associated with a logical variable `active(j)` found in the module `mod_boundary`. It is left to the user, during the execution of the `user_mesh` routine, to define the `active` variable for each boundary segment. If a segment of the boundary is "active" (*i.e.* `active(j)=.true.`), this free surface will trigger a region of nonlocality within a distance `PROXFACT*rcut`. Thus, the model will automatically refine the mesh in this region down to the atomic scale and make every repatom in the region nonlocal. Also see Sections 3.3 and 3.4 for discussions of the model parameters `PROXFACT` and `SurfOn`.

Regions of the model where boundaries are set to be inactive (`active(j)=.false.`) will not correctly include surface energetics, but can significantly reduce the computational effort where these energetics are not expected to have an important effect on the phenomena of interest. For example, in studying crack tip phenomena, it is sensible to include the surface effects only for a short distance along the crack faces near the tip, turning the surfaces off for the majority of the traction free crack faces.

If the user's mesh is a simply-connected convex region, the constrained Delaunay routine does not need any defined boundaries to produce the correct mesh of the points. In this case, the variables `nce`, `ncb` and `elist` are assigned automatically by the program during the Delaunay triangulation so that the correct model boundary is stored. In this case, all model boundaries are set to be inactive (`active(j)=.false.`) unless the user specifies

otherwise following the call to the Delaunay triangulator.

Optional output from the `user_mesh` routine. The user may choose to define the variables `f` and `id` either during mesh generation, or during the application of the boundary conditions in the `user_bcon` routine. See Section 2.11.2 for an explanation how boundary conditions are applied in QC.

It is sometimes convenient to pass mesh-specific information to the boundary condition routine (`user_bcon`, see Section 2.11.2) that can only be determined at the time of mesh generation. To facilitate this passage of information, module `uservars` is included in the `user_APP.f` file. As noted earlier, to be compatible with earlier versions of QC it contains by default the following two variables:[13]

- `user_iparam(10)`: (integer). Storage for up to 10 integer parameters.
- `user_rparam(10)`: (double precision). Storage for up to 10 double precision parameters.

Since both the `user_mesh` and `user_bcon` routines use the `mod_uservars` module, parameters stored in these variables during the execution of `user_mesh` will be accessible to the `user_bcon` routine later in the simulation.

Direct input to the `user_mesh` routine. Additional input for the meshing routine can be listed in the lines immediately following the `mesh` command in the input file. By convention, if this is the case, no input should be given on the command line itself and `key` should be set to `'dire'`. The additional input is read in from the input stream in the `user_mesh` routine using Fortran `read` statements:

`read(cmdunit,`*format-spec*`)` *list*

where `cmdunit` is the file handle for the input stream (a global QC variable defined in `mod_global`), *format-spec* is the format specifier (use `*` for unformatted input), and *list* is the

[13] Of course the user may opt to add on any additional variables.

list of data variables to be read in. For example to read in two integers `nx` and `ny`, indicating perhaps the number of divisions along the x and y directions, the following statement could be used:

```
read(cmdunit,*) nx,ny
```

Each read statement corresponds to one line following the `mesh` command and as many read statements as wanted can be used.

2.11.2 user_bcon

The `user_bcon` routine is called by macro `bcon` (see Section 4.2) to apply special boundary conditions to the simulation. Before this routine can be discussed it is necessary to explain how boundary conditions are applied in QC. Two variables in QC are related to the application of boundary conditions:

- `time`: (double precision) A scalar measure of the load step. Despite its name, this is a dimensionless variable that merely serves as a load step counter. It is increment by macro `time` that is discussed in Section 4.24.

- `prop`: (double precision) The value corresponding to `time` in the proportional load table (see Section 4.14). This table is a graph relating `time` to a physical property `prop` that is used to defined the boundary conditions. For example, `prop` could be the vertical displacement of an indenter in a nanoindentation simulation, the stress intensity factor in a fracture simulation, the shear strain in a shearing test, etc.

QC automatically uses `prop` to apply boundary conditions at each load step. Just prior to invoking the solver, the QC program executes two code segments to assign displacements to constrained degrees of freedom and external forces to free degrees of freedom:

```
! Set displacements of constrained nodes
do i=1,numnp
   do j=1,ndf
      if (id(j,i)==1) b(j,i) = prop*f(j,i)
   enddo
```

```
enddo
.
.
.
! Set external forces applied to free nodes
do i=1,numnp
   do j=1,ndf
      if (id(j,i)==0) then
         dr(j,i) = prop*f(j,i)
      else
         dr(j,i) = 0.0_dp
      endif
   enddo
enddo
```

The variable `id(j,i)` indicates whether the `j`-th degree of freedom of node `i` is constrained or free and `f(j,i)` is the corresponding normalized displacement of force. See Section 2.2 for a discussion of the variables appearing above.

For simulations where all force and displacement boundary conditions are proportional the single variable `prop`, no further boundary conditions need to be specified. In this case `bcon` need not appear in the input file and `user_bcon` can be left as an empty routine (although it must be present in the `user_APP.f` file). In other cases, however, more elaborate boundary conditions need to be applied, and `f(j,i)` needs to be correctly modified at every load step so that the above code segment leads to the desired boundary loads and displacements. The `user_bcon` routine provides the user with means for applying completely general and arbitrarily complex boundary condition in these cases.

Another case where `user_bcon` is necessary is when constructing an initial guess for a new load step based on the converged solution of the previous load step. Note however that changing `b(j,i)` for a boundary node (one for which `id(j,i)=1`) inside `user_bcon` will have no effect: it is overwritten by the above code segment when the solver is invoked. As such, `f(j,i)` must also be correctly set to impose the boundary displacements consistent with the initial guess to the solution.

The `user_bcon` routine is initiated by a `bcon` statement in the macros stage of the input file (see Section 4.2). The calling format for this macro is

```
bcon[,key][,data]
```

where `key` and `data` are problem-specific parameters that are passed to `user_bcon` as explained below.

The header of a typical `user_bcon` subroutine is as follows:

```
      subroutine user_bcon(id,x,ix,f,jdiag,str,eps,q,b,dr,db,shp,
     &   xsj,key,input,flag)
      use mod_uservars
      use mod_global, only : dp,maxel,maxneq,maxnp,ndf,ndm,nen,nq,nstr,
     &                       numnp,nxdm
      use mod_output, only : output,string
      use mod_pload,  only : GetLoadPropFact,GetLoadOldPropFact,
     &                       GetLoadTime,GetLoadTimeStep
      implicit  none

!-- Transferred variables
      real(kind=dp),     intent(inout) :: b(ndf,maxnp),str(nstr,maxel),
     &                                    eps(nstr,maxel),q(nq,maxel),
     &                                    x(nxdm,maxnp),f(ndf,maxnp),
     &                                    dr(ndf,maxnp),db(maxneq),
     &                                    shp(3,nen,maxel),xsj(maxel)
      integer,           intent(inout) :: jdiag(maxneq),ix(nen,maxel),
     &                                    id(ndf,maxnp)
      character(len=80), intent(in)    :: input
      character(len=4),  intent(in)    :: key
      logical,           intent(inout) :: flag
```

The header begins with a list of modules used by `user_bcon`. The use of the `only` clause is encouraged as a good programming practice (see Section 2.11.1 for more on this). The important variables and routines in these module are described in Section 2.1, 2.6 and 2.7. More details are also available in the comments at the top of the module files.

The variables passed to `user_bcon` (except for `key`, `input` and `flag`) are described in Section 2.2. Here a brief definition is given with additional comments specific to the `user_bcon` routine including details on how `user_bcon` normally operates on these variables.

- `id(ndf,numnp)`: (integer) The boundary constraint flag array. This array is set by the user, either during the generation of the initial mesh in `user_mesh` (Section 2.11.1) or here in the `user_bcon` routine.

- `x(nxdm,numnp)`: (double precision) The reference coordinate array. **Note that the `x` array should not be modified by the `user_bcon` routine.**

- `ix(nen,numel)`: (integer) The connectivity array. **Note that the `ix` array should not be modified by the `user_bcon` routine.**

- `f(ndf,numnp)`: (double precision) The boundary condition array. This array is set by the user, either during the generation of the initial mesh in `user_mesh` (Section 2.11.1) or here in the `user_bcon` routine.

- `jdiag(neq)`: (integer) Pointer into the stiffness matrix which is stored in a collapsed banded format. **Note that this variable should not be modified by the `user_bcon` routine.**

- `str(nstr,numel)`: (double precision) Elemental Stress array. This variable may be useful for an application where the applied boundary conditions vary in response to the stress in the material. **Note that this variable should not be modified by the `user_bcon` routine.**

- `eps(nstr,numel)`: (double precision) Elemental strain array. This variable may be useful for an application where the applied boundary conditions vary in response to the strain in the material. **Note that this variable should not be modified by the `user_bcon` routine.**

- `q(nq,numel)`: (double precision) Elemental internal variable array. **Note that this variable should not be modified by the `user_bcon` routine.**

- `b(ndf,numnp)`: (double precision) Nodal Displacement Array. This variable is typically modified in the `user_bcon` routine as a means of applying an initial guess to the solution of the nonlinear problem at hand. Judicious initial guesses to the equilibrium solution can significantly enhance convergence rates and prevent nonphysical energy minima from being reached by the nonlinear solver.

  Depending on the problem, the initial guess may simply be the solution field from the previous load step, or that same previous solution incremented in some sensible way.

For example, consider a fracture analysis in which each load step i is characterized by an applied far-field stress σ^i. In solving for the displacement field u^{i+1} due to stress σ^{i+1}, it may be sensible to start from an initial guess of the displacement field solution u^i due to σ^i plus a linear elastic displacement field associated with the change in the applied stress, Δu due to $\Delta\sigma = \sigma^{i+1} - \sigma^i$. The natural place to make this modification to the displacement field before starting the solution algorithm is in the routine `user_bcon`.

Generally, the displacement array can be modified in either a *total* or *incremental* manner depending on the simulation details. Total re-assignment of the `b` array is typically done by making use of the current proportional load `prop`, whereas incremental modifications start from the current displacements stored in `b` (which, for example, may be the equilibrium solution from the previous load step) and then add a displacement increment based on the difference between the current and previous proportional loads, `prop-propol`. For example, here is a code segment from `user_bcon` routine of the the `GB_example` given in the *QC Tutorial Guide* that applies an incremental shear strain to the system:

```
1     integer i,j
2     real(kind=dp) propfact,propolfact

3     propfact = GetLoadPropFact()
4     propolfact = GetLoadOldPropFact()
5     do i=1,numnp
6        b(1,i)=b(1,i)+(propfact-propolfact)*x(2,i)
7        if (id(1,i)==1) f(1,i)=x(2,i)
8     enddo
```

The query routines `GetLoadPropFact` and `GetLoadOldPropFact` in lines 3–4 (discussed in Section 2.7) are used to obtained current values of `prop` and `propol` that are stored in the local variables `propfact` and `propolfact`. The loop in lines 5–8 increments the x displacement u_x of every node by a shear strain increment proportional to the y-coordinate of the node,

$$u_x^i = u_x^{i-1} + (\gamma^i - \gamma^{i-1})y.$$

Here the superscript i is a load step counter. In this case `prop` is interpreted as the shear parameter γ imposed on the system. Note the substitution in line 7 of the y coordinate into the boundary condition array `f()` for degrees of freedom with fixed displacement boundary conditions. This is necessary since any modification to displacement degrees of freedom for which `id(i,j)=1` will be overwritten by the next call to compute the total energy or solve the system (see the discussion of the application of boundary conditions above).

- `dr(ndf,numnp)`: (double precision) Out-of-balance force vector. **Note that this variable should not be modified by the `user_bcon` routine.**
- `db(ndf,numnp)`: (double precision) Nodal displacement increment. **Note that this variable should not be modified by the `user_bcon` routine.**
- `shp(nshp,numel)`: (double precision) Shape functions. **Note that this variable should not be modified by the `user_bcon` routine.**
- `xsj(numel)`: (double precision) Element areas. **Note that this variable should not be modified by the `user_bcon` routine.**
- `key`: (character(len=4)) Key passed from the input file command line. Can be used to implement various options in `user_bcon`. **Note that this variable should not be modified by the `user_bcon` routine.**
- `input`: (character(len=80)) Input data passed from the input file command line. `input` can be used to pass character, double precision, integer or logical data directly from the command line to the `user_bcon` routine. It is left to the user to parse this data, however the following is a useful example of how this can be efficiently achieved.

  Suppose that the user has written a `bcon` routine that, in addition to the `key` option, requires 3 data entries: a character `filename`, an integer `index` and a double precision `scale`. The `bcon` command appears in the input file as:

```
bcon,key,filename,0,1.0
```

Everything beyond the second comma will be passed to the `user_bcon` subroutine as the `input` variable. Thus, in this example,

```
input='filename,0,1.0'
```

The following code segment will effectively parse this input string:

```
integer lower,upper,next,index,idum
real(kind=dp) scale,dum
character(len=80) input,filename
.
.
.
lower = 0
upper = next(lower,input)
filename = input(lower+1:upper-1)
lower = upper
upper = next(lower,input)
call freein(input,lower,upper,index,dum,1)
lower = upper
upper = next(lower,input)
call freein(input,lower,upper,idum,scale,2)
```

See Section 2.11.1 for an explanation of the integer function `next` and subroutine `freein` used here.

- `flag`: (logical) `user_bcon` flag. `flag` is a global (static) logical variable reserved for the `user_bcon` subroutine. It can be set as the user likes, for example as an indication of whether the `bcon` routine is being called for the first time. It is initialized to `.false.` once at the start of the simulation.

2.11.3 user_pdel

The routine `user_pdel` is associated with macro `pdel` (see Section 4.12) that outputs the current value of `prop` (see Section 2.7) and a scalar, user-defined, `force` measure of the current applied loading. The calling format for `pdel` is:

```
pdel,[key],fileprefix[,data]
```

Macro `pdel` calls `user_pdel` to computes `force`. `user_pdel` has the following header:

```
      subroutine user_pdel(id,x,ix,f,jdiag,str,eps,q,b,dr,db,shp,
     &   xsj,key,input,force)
      use mod_uservars
      use mod_global, only : dp,maxel,maxneq,maxnp,ndf,ndm,nen,nq,nstr,
     &                       numnp,nxdm
      implicit  none

!-- Transferred Variables
      real(kind=dp),     intent(inout) :: b(ndf,maxnp),str(nstr,maxel),
     &                                    eps(nstr,maxel),q(nq,maxel),
     &                                    x(nxdm,maxnp),f(ndf,maxnp),
     &                                    dr(ndf,maxnp),db(maxneq),
     &                                    shp(3,nen,maxel),xsj(maxel)
      integer,           intent(inout) :: jdiag(maxneq),ix(nen,maxel),
     &                                    id(ndf,maxnp)
      character(len=80), intent(in)    :: input
      character(len=4),  intent(in)    :: key
      real(kind=dp),     intent(out)   :: force
```

The routine uses `mod_global`, which contains dimensioning variables for the transferred arguments, and `dp`, the double precision kind variables. These variables are described in Section 2.1. Note the use of the `only` clause in the `use` statement. This is encouraged as a good programming practice (see Section 2.11.1 for more on this). The variables passed to `user_pdel` as arguments are defined in Section 2.2, except for the last three that are:

- `key`: (character(len=4)) The `key` from the `pdel` command line.
- `input`: (character(len=80)) The input string from the `pdel` command line, including the `fileprefix` and `[data]` exactly as it appears.
- `force`: (double precision) The scalar measure of the applied force. This is the only expected output from the routine and is the only external variable that should be modified by `user_pdel`.

Typically, the force measure can be extracted directly from the values of `prop*f(j,i)` for the degrees of freedom to which forces are applied externally, or from `dr(j,i)` for degrees of freedom that are constrained to fixed displacements. The units of force in QC are derived

from the energy and length units of the underlying atomistic potentials, typically they are eV/Å.

As an example, here is a code segment from the `user_pdel` routine of the the `GB_example` given in the *QC Tutorial Guide*:

```
integer i

force = 0.0_dp
do i = 1,numnp
   if (id(1,i)==1 .and. x(2,i)>0.0_dp) force=force-dr(1,i)
enddo
```

This routine computes the total force in the x direction for nodes with fixed displacements that have $y > 0$. In this problem the model is a rectangular region with the bottom at $y = 0$ held fixed at zero displacement and the top at $y = h$ pulled to the right and held fixed. (See Section 4.2 and Section 4.2 of the *QC Tutorial Guide*.) The only nodes with `id(1,i)==1` and $y > 0$ are then the nodes at the top of the model. Therefore the `force` computed is the total force that must be applied to the top of the model to hold it at the current shear strain defined by `prop`.[14] One thing to note is that `force` is computed as the negative of `dr()`. This is due to the sign convention adopted for `dr`.

Note that even though the QC code is a 2D implementation (see Section 1 for more details), it has a finite thickness in the out-of-plane direction (this thickness can be found from the variable `dcell(3)` discussed in Section 3.5 of the *QC Tutorial Guide*). However forces in QC are *not* forces per unit depth as is commonly the case in 2D finite element codes. In QC they are nodal forces with units of energy per length.

2.11.4 user_potential

The routine `user_potential` allows the user to define an additional external potential energy, called `user_energy` that is added to the total energy of the system. This can be used to include additional boundary conditions that cannot be included using `user_bcon`.

[14] Without the condition `x(2,i)>0.0_dp` the force computed would be zero, since the load applied to the top of the model is balanced by the reaction forces at the support.

WARNING: If a `user_energy` is defined in `user_potential`, the user must also add the gradient of this energy to the out-of-balance force vector `dr` and the second gradient to the stiffness matrix `tang`. Otherwise gradient-based solvers (such as conjugate gradients) or second-gradient based solvers (such as Newton-Raphson) will fail. It is recommended to perform a numerical derivative checks using the `chec` macro (see Section 4.3) to verify that the forces (`chec,forc`) and stiffness matrix (`chec,stif`) are computed correctly when `user_potential` is used.

As an example, consider the repulsive force-field approach used to model cylindrical and spherical indenters proposed by [15]. The idea is to add to the total energy a potential of the form,

$$P = \sum_{\substack{i=1 \\ r^i<R}}^{N} \frac{1}{2} K (R - r^i)^2,$$

where N is the number of nodes in the mesh, R is the radius of the indenter, K is a stiffness associated with the repulsive field, and r^i is the distance between the current position of node i ($\boldsymbol{x}^i$) and the current position of the center of the indenter ($\boldsymbol{c}$),

$$r^i = |\boldsymbol{x}^i - \boldsymbol{c}|.$$

The first and second gradients of P follow as

$$\frac{\partial P}{\partial x^i_m} = K(\frac{R}{r^i} - 1)(c_m - x^i_m) \tag{1}$$

$$\frac{\partial^2 P}{\partial x^i_m \partial x^j_n} = \delta_{ij} K \left[\frac{R}{(r^i)^3} (c_m - x^i_m)(c_n - x^i_n) - \delta_{mn} \left(\frac{R}{r^i} - 1 \right) \right] \tag{2}$$

In the QC implementation, the variables defining the indenter are stored in module `uservars` (see Section 2.11):

```
module mod_uservars
use mod_global, only : dp

save
public

integer user_iparam(10)
real(kind=dp) user_rparam(10)
```

```
      real(kind=dp) indent_radius,indent_radius2,indent_stiffness,
     &   indent_orig(2),indent_force(2)=0.0_dp

      end module mod_uservars
```

Here `indent_radius`=R, `indent_stiffness`=K, and `indent_orig(2)`=$\boldsymbol{c}_0$, where $\boldsymbol{c}_0$ is the original position of the indenter center at the start of the loading. The other variables are `indent_radius2`=R^2 (stored for computational efficiency) and `indent_force(2)`, which is the force the indenter is applying to the surface (this is returned by `user_pdel`). The `user_potential` code implementing the repulsive potential is given below:

```
 1    subroutine user_potential(id,x,ix,f,jdiag,str,eps,q,b,dr,shp,xsj,
 2   &                          fls,flt,flw)
 3    use mod_uservars
 4    use mod_global, only : dp,maxneq,maxnp,maxel,ndf,nen,nq,nstr,
 5   &                       numnp,nxdm,user_energy
 6    use mod_pload,  only : GetLoadPropFact,GetLoadOldPropFact,
 7   &                       GetLoadTime,GetLoadTimeStep
 8    use mod_stiff,  only : tang,istiff
 9    implicit  none

!-- Transferred Variables
10    real(kind=dp), intent(inout) :: b(ndf,maxnp),str(nstr,maxel),
11   &                                eps(nstr,maxel),q(nq,maxel),
12   &                                x(nxdm,maxnp),f(ndf,maxnp),
13   &                                dr(ndf,maxnp),shp(3,nen,maxel),
14   &                                xsj(maxel)
15    integer,       intent(inout) :: jdiag(maxneq),ix(nen,maxel),
16   &                                id(ndf,maxnp)
17    logical,       intent(in)    :: fls,flt,flw

!-- Local Variables
18    integer i,idf,m,n,is
19    real(kind=dp) r,r2,del(2),grad_node(2),indent_loc(2),R_over_r,
20   &              stif_node

21    ! update indenter position
22    indent_loc(1) = indent_orig(1)
23    indent_loc(2) = indent_orig(2) - GetLoadPropFact()

24    ! compute external potential and forces
25    if (flw) user_energy = 0.0_dp
26    indent_force = 0.0_dp
27    do i=1,numnp
28       del(1:2) = x(1:2,i) + b(1:2,i) - indent_loc(1:2)
29       r2 = del(1)*del(1) + del(2)*del(2)
30       if (r2<=indent_radius2) then
31          r = sqrt(r2)
```

```
32          R_over_r = indent_radius/r
33          if (flw) user_energy = user_energy +
34   &                0.5_dp*indent_stiffness*(indent_radius-r)**2
35          grad_node(1:2)= -indent_stiffness*(R_over_r - 1.0_dp)*del(1:2)
36          indent_force = indent_force + grad_node
37          if (fls) dr(1:2,i) = dr(1:2,i) - grad_node(1:2)
38          if (flt) then
39             idf = (i-1)*ndf
40             do m=1,2
41             do n=m,2
42                stif_node = R_over_r/r2*del(m)*del(n)
43                if (m == n) stif_node = stif_node - (R_over_r - 1.0_dp)
44                is=istiff(idf+m,idf+n,jdiag)
45                tang(is) = tang(is) + indent_stiffness*stif_node
46             enddo
47             enddo
58          endif
49       endif
50    enddo

51    return
52    end
```

The variables `id` to `xsj` passed to `user_potential` contain information on the model (nodal positions, boundary conditions, mesh connectivity, etc.) and the current state of the simulation (displacements, stress, strain, etc.). They are described in Section 2.2. Additional variables passed to `user_potential` are:

- `fls`: (logical) Force calculation flag. (True means calculate force.)
- `flt`: (logical) Tangential stiffness calculation flag. (True means calculate stiffness.)
- `flw`: (logical) Energy calculation flag. (True means calculate energy.)

It is important that `user_potential` respect these flags and not modify variables unless asked to. The rest of the QC code depends on this convention. The current position of the indenter is computed in lines 22–23. Note that `prop` is interpreted as the the vertical displacement of the indenter downwards. The calculation of the potential energy and its derivatives is done in the loop over the nodes in lines 27–50. This is largely self-explanatory, however, two subtleties are worth pointing out:

- Notice that the gradient `grad_node(1:2)` ($\partial P/\partial \boldsymbol{x}^i$) is *subtracted* from `dr(1:2,i)` instead of being added. This is due to the sign convention of `dr`, which is defined as the negative of the gradient of the potential energy.

- From Eqn. (2) it is clear that P only contributes to the four terms ($m = 1, 2$, $n = 1, 2$) associated with each of the diagonal terms of stiffness matrix (i.e. terms for which $i = j$). However, note that in `user_potential` the symmetry of the stiffness matrix is exploited and only three terms are looped over due to the bounds of `n` in line 41. This is important because `tang` also exploits symmetry and stores only the upper half and diagonal of the stiffness matrix. In fact, if `m>n`, the function `istiff` returns zero indicating that no such term is stored in `tang`. For more details on `tang` and `istiff` see Section 2.10.

2.11.5 user_plot

The routine `user_plot` provides the user with the opportunity to generate an application-specific plot. `user_plot` is called whenever a `plot,user` statement appears in the input file. The calling format for this statement is

```
plot,key,filepref,[index],[umag],[scale],[append][,data]
```

where `key=user` in this case. The variables `filepref` and `append` have their usual meanings for a `plot` statement (see Section 4.13 for more information). The file `filepref_Uxxx.plt` is opened and the file handle pointing to it is passed to `user_plot`. The variables `index`, `scale` and `append` are also passed to `user_plot` (see below). In addition, variables specific to `user_plot` may follow the `append` variable at the end of the input list as indicated by `[,data]` above.

The header of the `user_plot` routine is

```
 subroutine user_plot(id,x,ix,itx,f,jdiag,str,eps,q,b,dr,db,shp,
&                     xsj,index,umag,scale,logic,input,upper)
 use mod_uservars
 use mod_global, only : dp,maxnp,maxel,maxneq,ndf,nen,nq,nstr,nxdm
```

```
      implicit  none

!-- Transferred Variables
      real(kind=dp),     intent(in)    :: b(ndf,maxnp),str(nstr,maxel),
     &                                     eps(nstr,maxel),q(nq,maxel),
     &                                     x(nxdm,maxnp),f(ndf,maxnp),
     &                                     dr(ndf,maxnp),db(maxneq),
     &                                     shp(3,nen,maxel),xsj(maxel),
     &                                     umag,scale
      integer,           intent(in)    :: jdiag(maxneq),ix(nen,maxel),
     &                                     id(ndf,maxnp),itx(3,maxel),
     &                                     index,logic
      integer,           intent(inout) :: upper
      character(len=80), intent(in)    :: input
```

The variables `id` to `xsj` contain information on the model (nodal positions, boundary conditions, mesh connectivity, etc.) and the current state of the simulation (displacements, stress, strain, etc.). They are described in Section 2.2. These variables are passed to `user_plot` in case they are needed for the calculations performed there. **They should not be modified.** The variables `index`, `umag` and `scale` are defined in Section 4.13. Note that it is up to the user to use these variables in `user_plot` in a manner consistent with their definition. (See `subroutine dumpit` in module `mod_plotting` for an example how these variables are used.) Additional plot-specific variables passed to `user_plot` are:

- `logic`: (integer) File handle to an open plot file. Data is sent to this file using standard Fortran output statements:

  `write(logic,`*format-spec*`)` *list*

  where *format-spec* is the format specifier (use `*` for unformatted output), and *list* is the list of data variables to be written.

- `input`: (character(len=80)) The input line containing all of the variables and delimiters after the `key` parameter (i.e. `input = 'filepref,index,umag,scale,append,data'`). The user may parse this string to obtain additional variables in `data` specific to `user_plot`. See the discussion for the `upper` variable appearing next.

- `upper`: (integer) A pointer to the last comma or end-of-line symbol that was processed in the input line. (This is the comma between `append` and `data`.) The user may continue parsing the string from this point as shown in Sections 2.11.1 and 2.11.2.

3 `Head` Stage Commands

The following is an alphabetical listing of the commands that are available during the `head` stage of the QC simulation. For additional detail, please see the *QC Tutorial Guide*.

3.1 Macro `'cons'` : read in potential specific constitutive input

The default module for the `cons` routine is a module that reads a general EAM [6] potential from a file in either `setfl` or `funcfl` format. These formats are standard with the MD code DYNAMO [16]. Potentials from other sources can be converted to the `setfl` format using the utility program `dynpots.f` provided with the QC code. The `dynpots.f` file can be found in the QC subdirectory `Potentials/FortranSource`. The QC method expects all interatomic potential files to have the `.fcn` extension.

`Funcfl` files contain only the potential information for a single atom type, while all pair-potential interactions between dissimilar nuclei are modeled as the geometric mean of the homonuclear pair interactions. `Setfl` files contain all the potential information for a complete alloy set, including the pair-potential interactions between the dissimilar nuclei. They can also be used for potentials defining a single atomic species.

calling format: `cons,key,nfiles,fprefix_1,...,fprefix_nfiles`

- `key`:
  - `'setf'` : File containing constitutive information is in `setfl` format.
  - `'func'` : Files containing constitutive information are in `funcfl` format.
- `nfiles` : (integer) The number of files required to read all the necessary constitutive information. Note that if the `key` is `'setf'`, this value must be `1`.

- fprefix_i : (character(len=80)) The file prefix for the name of a file, fprefix_i.fcn, containing the constitutive information. The number of file prefixes must equal nfiles.

After all the constitutive information has been read in, the cons command computes several values for each of the previously defined grains in the model. Specifically, it computes the cohesive energy per unit volume, the initial stresses and the initial elastic moduli for the infinite, undistorted lattice. The stresses and moduli are given in relation to the global x-y-z coordinate system, and the moduli are presented in the compact Voigt notation using a 6×6 matrix. These values are often known from atomistic simulations of the same material and serve as a useful check that the grains and constitutive information have been read in correctly. The user can access the elastic constants (perhaps in order to apply boundary conditions in user_bcon) using the routine GetGrainRefStiff in mod_grain (see Section 2.4). The initial stresses in the perfect lattice should be zero. Often, very small differences between the lattice constant used to define the grains and the optimal lattice constant can lead to nonzero residual stresses in the lattice.

3.2 Macro 'end ' : terminate head stage

calling format: end

This command is required to signal the end of the head stage.

3.3 Macro 'fact' : sets global run factors

There are a number of factors that need to be set by the user at the start of a QC simulation. This is achieved using the fact command. In a typical input file, a list of these commands will appear near the start of the file. Factors can be set in any order. Even if the default value is to be used, it is often useful (for clarity) to include these commands in the simulation.

calling format: fact,key,value

- key :

  - `'prox'` : Proximal nonlocality factor (`PROXFACT`). See Section 4.20 for more details.
  - `'adap'` : Adaption nonlocal padding factor (`ADAPFACT`). See Section 4.1 for more details.
  - `'cutf'` : Effective cutoff factor (`CUTFACT`). See Section 4.20 for more details
  - `'epsc'` : Nonlocality criterion strain tolerance (`epscr`). See Section 4.20 and Section 3.2 of the *QC Tutorial Guide* for more details.

- `value` : (double precision) The factor will be set to this value.

Note: For more information on the run factors, see the file `mod_global.f`.

3.4 Macro `'flag'` : sets global run flags

The `flag` command is exactly like the `fact` command, except that it is reserved for simulation parameters that are of logical type. These are typically switches that determine whether or not a particular feature of the QC will be activated for the current simulation.

In a typical input file, a list of `flag` commands will appear near the start of the file. Flags can be set in any order. Even if the default value is to be used, it is often useful for clarity to include these commands in the simulation.

calling format: `flag,key,value`

- `key` :
  - `'nloc'` : Nonlocal effects flag. (Default, `NlocOn=T`)
  - `'surf'` : Surface effects flag. See Section 2.11.1 for more details. (Default, `SurfOn=T`)
  - `'grai'` : Grain boundary effects flag. See Section 3.5 for more details. (Default, `GrainOn=T`)
  - `'ghos'` : Ghost force correction flag. (Default, `GhostOn=T`)

- `'node'` : Nodes on Bravais sites flag. Note that this flag must be set to `T` if nonlocal effects on being included in the simulation. (Default, `NodesOnBsites=T`)
- `'prev'` : Element warping prevention flag. (Default, `PreventWarping=F`) Element warping occurs when the deformation is so severe that the volume of an element becomes zero or negative (the element is turned "inside-out"). This is not permitted in continuum finite elements and in QC elements touching local repatoms. However, elements between nonlocal repatoms contain no atoms and can warp without any non-physical consequences. Typically then, `PreventWarping` is set to `false`. In a fully local simulation, setting this flag to `true` can be a useful check for errors in the model.
- `'defm'` : Perform mesh adaptions in the deformed configuration. (Default, `DefMesh=F`)
- `'dumm'` : Flag indicating that "dummy atoms" are permitted. Dummy atoms are atoms stored inside local elements near that local/nonlocal interface. They are required to ensure the nonlocal repatoms see all their neighbors unless the local elements are fully refined in this region. Usually, allowing dummy atoms permits more rapid coarsening of the local elements but they will lead to larger ghost forces at the interface. If this flag is set to false, it forces the adaption routine to fully refine the local region immediately surrounding any nonlocal region, out to one cutoff radius of the potentials.

  NOTE: If this flag is set to false it may result in premature termination of conjugate gradient minimization. The reason for this is that during conjugate gradient minimization dummy atoms may move into the cutoff radius of nonlocal atoms. This is detected by periodic neighbor list updates that are carried out. If this occurs the conjugate gradient routine will exit with a warning. To ensure that minimization is completed with the DummysAllowed flag set to false, the conjugate gradient solver call needs to be placed inside a loop:

```
loop,,5
   solve,cg,1.0,10000,1
   status,update
   convergence,force
next
```

No change is required for Newton-Raphson minimizations.
(Default, DummysAllowed=T).

- value : logical, true sets the flag to true, turning on the effect it controls. False turns the effect off.

Note: For more information on the run flags, see the file mod_global.f.

3.5 Macro 'grai' : read in grain structure information, initialize grains

calling format: grai,key[,fileprefix]

- key:
  - 'file' : Read the grain structure data from a file called fileprefix.geo.
  - 'dire' : Read the grain structure data from the input stream in the lines following the grai command.
- fileprefix: (character(len=80)) Name of the file to be read if key='file'. Note that the program appends the extension .geo to form the filename.

Note: For information on grain structure data format, see Section 3.5 of the *QC Tutorial Guide* and subroutine ReadGrainData in the file QC/Code/mod_grain.f.

3.6 Macro 'mate' : material data input

calling format: mate,key[,nfiles,fprefix1,fprefix2,...]

- key :
  - 'file' : Read the material data from a files whose names appear in the command line, (fprefix1,fprefix2,...).

  - 'dire' : Read the material data from the input stream in the lines following the mate command.

- nfiles : (integer) The number of files to be read to obtain all the material definitions if key='file'.

- fprefix : (character(len=80)) The prefix of the name of the file to be read if key='file'. There must be nfiles names in the list. Note that the program automatically appends the extension .mat to create the filename.

Note: For more detail, see the discussion of this command in Section 3.3 of the *QC Tutorial Guide*.

3.7 Macro 'mesh' : generate mesh (user_mesh routine)

calling format: mesh[,key][,data]

This routine calls a user-supplied routine user_mesh to generate the initial mesh. See Section 2.11.1 for a detailed description of this routine. The optional parameters key and data are passed to user_mesh. By convention key='dire' implies that any data to user_mesh is given in the lines following the mesh statement, otherwise the data is expected to be in the remainder of the statement that is stored in data. It is up to the user to insure that user_mesh conforms to these conventions. Upon return from this routine an initial mesh will have been defined including the coordinates of all nodes and the mesh connectivity.

WARNING: QC only performs limited validation checks on the results of the user_mesh routine. If this routine is faulty it could results in erratic behavior of the code.

3.8 Macro 'zone' : define special-attribute zones

calling format: zone,key,[fprefix][,index]

Special-attribute zones are regions in the model where a user can introduce special constraints on the nodes. Currently, two possibilities exist. *No-adaption zones* are regions where no

adaption is allowed and all nodes are required to be local. These zones are typically placed to cap nonlocal regions that would otherwise continue to extend throughout the model further than desirable. An example of this is shown in Section 3.4 of the *QC Tutorial Guide* for a grain boundary. *Nonlocal zones* are regions where all atoms must be nonlocal. This is a convenient way for introducing a nonlocal region where it otherwise would not be triggered.

- `key` :
  - `'file'` : Read special-attribute zone data from a file named `fprefix.zon`.
  - `'dire'` : Read special-attribute zone data from the input stream in the lines following the `zone` command.
- `fprefix` : (character(len=80)) Prefix of the file to be read if `key='file'`. Note that the program automatically appends the extension `.zon` to create the filename.
- `index`:
  - `0,1` : No-adaption zone. All nodes in this region must be local. No adaption is allowed in this region.
  - `2` : Nonlocal zone. All nodes in this region must be nonlocal. If there is at least one node in the zone, it will result in the entire region being refined down to the atomic scale and made nonlocal.

Note: For information on the special-attribute zone data format, see Section 3.4 of the *QC Tutorial Guide* and subroutine `ReadZone` in file `Code/mod_boundary.f`.

4 `Macros` Stage Commands

The following is an alphabetical listing of the commands that are available during the `macros` stage of the QC simulation. For additional detail, please see the *QC Tutorial Guide*.

4.1 Macro 'adap' : Automatically adapt the mesh, through mesh refining and coarsening

The adap command is the starting point for all mesh adaption, including both mesh refinement and mesh coarsening. Related commands include prot and the mesh command in the head stage of the simulation. The adaption uses an estimator for the error in the deformation gradients, based on the error estimator of Zienkiewicz and Zhu [17] and described in more detail in [3].

Note that the last action of the adap command is a forced call to the status command to re-compute the repatom statuses. If necessary, this will trigger iterative adaption to make sure all nonlocal repatoms represent only themselves. See Section 4.20 for more details.

calling format: adap,,vartol,icoarse

- vartol : (double precision, default=0.075) Adaption criterion trigger value. Any element with a refinement criterion value greater than vartol will be refined. If coarsening is active, then any element that can be removed without creating new elements which would satisfy the refinement criterion is removed.

- icoarse : (integer, default=0) Specifies whether mesh coarsening is active.

  - icoarse=0: indicates coarsening is off.

  - icoarse=1: indicates coarsening is on.

4.2 Macro 'bcon' : apply boundary conditions (user_bcon routine)

calling format: bcon[,key][,data]

The bcon command calls a user-supplied subroutine called user_bcon, and permits the user to define key options and input data as required. As a result, the input for the command will depend on the user routine. The details of the functions performed by the bcon routine are also largely dependent on the user's requirements. For a detailed description of this routine see Section 2.11.2.

4.3 Macro 'chec' : Numerical derivative check

chec computes the first and second derivatives of the total energy numerically and compares them to the analytically computed values. It is for debugging purposes only, and is helpful when implementing new potentials or other changes to the code.

Note that some small discrepancies in the stiffness elements will often occur with interatomic potentials in the tabulated form provided with the QC package. This is due to the interpolation of higher order derivatives of the tabulated potentials. These discrepancies have not been found to interfere substantially with solution convergence.

calling format: chec[,key][,code]

- key:
  - ' ' or 'forc' : Numerical derivative check of out-of-balance forces. Compares analytical derivative with numerical derivative. Results are sent to the log file and the Tecplot® file forcecheck.plt.

    Note: macro form must be called before this to set up the out-of-balance force vector.
  - 'stif' : Numerical derivative check of stiffness matrix. Results are sent to the log file. Any stiffness matrix components which fail the test are flagged with a <---*** marker. Parameter code sets the number of repatoms tested:
    - code=0 : Check is carried out for two arbitrary rep atoms, one local and one nonlocal, i.e. all stiffness matrix items associated with these atoms are tested. This option should be selected for large meshes where testing the entire stiffness matrix would be computationally prohibitive. This is the default.
    - code=1 : One local atom and all nonlocal atoms are tested. Use this for medium sized models.
    - code=2 : All atoms are tested. Use this for small models.

Note: macro `tang` must be called before this to set up the stiffness matrix.

– `'loca'` : Numerical derivative check of the stresses and moduli computed in the potential routine for the local limit. Parameter `code` sets the deformation gradient for which the test will be done:

  * `code = 0` : The check is done using a randomly selected deformation gradient hard-wired into the routine. This is the default.
  * `code = iel` : The check is done using the deformation gradient of element `iel`.

  Note: regardless of the deformation gradient selected by code the test will be carried out for all grains in model. This means that if code=iel is selected and there are more than one grains in the model, the deformation of element iel will also be used to test grains with which that element is not associated.

- `code`: (integer) See the `key`-dependent descriptions above.

4.4 Macro 'clea' : Re-initialize solution variables.

calling format: `clea`

`clea` sets the nodal displacement vector `b` and the last increment in the nodal displacements `db` to zero.

4.5 Macro 'conv' : Loop convergence test

The `conv` command is used within a `loop` ... `next` construct to test for convergence. If convergence has been achieved, the `loop` is terminated and the simulation proceeds from the first command following the `next` command of the terminated `loop`.

The `conv` command can also be used to force a load step to exit. At the start of each call to the `conv` routine, the program looks for a file `abort.dat` in the working directory of the simulation. If the first line of this file contains a single `T` (for `.true.`) a "converged" signal is returned from the `conv` command regardless of the current convergence measure.

In this way, the user can stop a simulation but still produce, for example, output of the last incomplete load step.

A related command is `tole`, which sets the value of `globaltol` used by the `conv` routine.

calling format: `conv,[key]`

- `key` :
  - `'  '` or `'forc'` : converge when out-of-balance force norm is reduced below `globaltol*rnmax` where `rnmax` is the largest force norm encountered in the current loop.
  - `'disp'` : converge when the norm of the last displacement increment taken in the solver is less than `globaltol`.
  - `'cdis'` : converge when the norm of the last displacement increment taken in the solver is less than a fraction (`globaltol`) of the maximum displacement increment norm encountered in the loop.
  - `'ener'` : converge when the change in energy in the last Newton-Raphson step is less than `globaltol`.
  - `'elem'` : converge when the current number of elements is the same as or less than the number of elements the mesh had the last time `conv` was called. Used as a check to see when mesh refinement is no longer occurring.
  - `'adel'` : same as `'elem'`, but current number of elements is compared to the number of elements that existed prior to the last mesh adaption.
  - `'pdel'` : converge when the difference between the current external load (computed by macro `'pdel'`) and the external load when `conv` was last called, is less than `globaltol`.

4.6 Macro 'dtim' : set time increment

calling format: `dtim,,dt`

Note that there is no `key` required for this command, and so the double-comma is required to denote an empty `key` field.

- `dt`: (double precision). Time increment to be used by the `time` command .

4.7 Macro 'form' : Form the out-of-balance force vector

calling format: `form`

The `form` command computes the out-of-balance forces and total energy for the current nodal displacements.

4.8 Macro 'ghos' : Compute ghost forces correction

calling format: `ghos`

The `ghos` command computes the ghost force corrections associated with the current mesh, repatoms statuses and displacements. In all subsequent computations of the out-of-balance forces, the ghost force corrections will be added as dead loads to minimize the spurious forces at interfaces between local and nonlocal regions. If the `status` or `adap` command is called after the `ghos` command, it will generally change the values of the ghost forces. For this reason, the execution of the `status` or `adapt` commands will automatically force a re-computation of the ghost force correction loads.

The ghost force correction is described in detail in [3]. Note that the magnitudes and directions of the spurious forces will change as the repatom displacements change, and thus the ghost forces should in principal be updated occasionally during the simulation. It is left to the user to determine when these ghost forces need to be updated.

Since the ghost force correction is an approximate fix, there is necessarily some level of error associated with a QC simulation, even with ghost forces corrected using this command. The main source of this error lies in the fact that the ghost force correction is only periodically updated (at all `status` calls and explicit calls to this `ghost` command) and added as dead loads. In fact, every change to the displacement fields during the solution algorithm will

change the ghost forces slightly, but the lack of a well-defined energy functional incorporating the ghost forces makes their complete elimination impractical.

In order for the `ghos` command to have an effect, the `GhostOn` flag must be set to `.true.` during the `head` stage of the simulation.

4.9 Macro 'loop' : set loop start indicators

The `loop` command indicates the start of a loop in the command structure, while the related command `next` (Section 4.10) indicates the end of the loop. The current QC implementation permits full loop nesting to any depth.

calling format: `loop,[label],nloop`

- `label` : (character) label name for the loop (only used as a guide to the eye - program does not verify `loop-next` labels match).
- `nloop`: (integer) number of times the loop is to be executed unless prematurely terminated due to a "converged" signal from the `conv` command.

4.10 Macro 'next' : loop terminator control

The `next` command indicates the end of a loop (started by a `loop` command) in the command structure.

calling format: `next[,label]`

Description of input variables:

- `label` : (character(len=4)) label name for the loop (only used as a guide to the eye - program does not verify that `loop-next` labels match).

4.11 Macro 'outp' : output nodal displacements to the log file

calling format: `outp`

The command `outp` writes the nodal displacements to the log file.

4.12 Macro 'pdel' : compute current external load and applied displacement

calling format: `pdel,[key],fileprefix[,data]`

The `pdel` command is used to produce output of a scalar measure of the applied force for a given configuration.[15] It opens a file `fileprefix.pde` at its first call and at this and subsequent calls writes a line of output to the file. The output line consists of two real numbers: the current value of `prop` (the proportional load level) and a user-defined measure of the applied force. The force is computed by the routine `user_pdel`, which must be supplied by the user and is documented in Section 2.11.3. More information on `prop` is given in Section 4.14. The arguments to the `pdel` command are:

- `key` : (character(len=4)) Optional parameter passed to the user routine `user_pdel`. This could be used, for example, to select a particular force when the routine has multiple options.
- `fileprefix` : (character(len=80), default = 'pdelta') Prefix of file to which the output should be written. The program will automatically append the extension `.pde` to create the filename `fileprefix.pde`.
- `data` : Optional data passed to the user routine `user_pdel`. This can include a list of variables separated by commas that will be parsed by `user_pdel`. See Section 2.11.3 for more information.

4.13 Macro 'plot' : generate plot files

calling format: `plot,key,filepref,[index],[umag | polyfile],[scale],[append]`

- `key` :
  - `'  '` or `'disp'` : Displacement field plot. The nodal x, y and z displacements are stored on a finite element mesh plot. For this `key`, `index` has no effect.

[15] The name "`pdel`" comes from the original use of this feature for plotting the load (P) versus depth (δ) in nanoindentation simulations.

– `'bcon'` : Boundary conditions plot. Finite element mesh plot with the following nodal values:

  * `index = 0,1` : applied loads.
  * `index = 2` : out-of-balance forces.
  * `index = 3` : boundary condition indicator (0 free, 1 constrained).

– `'stre'` : Kirchhoff stress field plot. Finite element mesh plot with the following nodal values:

  * `index = 0` : Von Mises effective stress.
  * `index = 1` : Kirchhoff stress components: σ_{xx}, σ_{yy}, σ_{zz}, σ_{xy}, σ_{xz}, σ_{yz}.

  Notes:

  1. Stresses are element quantities that are computed at the element integration points. The nodal values stored in the plot file are extrapolated and thus include an additional extrapolation error.
  2. Stresses are only computed in elements adjacent to local nodes. No stress information is available in nonlocal regions.
  3. The output stresses are components of the Kirchhoff stress tensor $\boldsymbol{\tau}$ *not* the more commonly used Cauchy stress tensor $\boldsymbol{\sigma}$. See variable `str` in Section 2.2 for the relation between these stress measures.

– `'stra'` : Lagrangian strain field plot. Finite element mesh plot with the following nodal values:

  * `index = 0` : Von Mises effective strain.
  * `index = 1` : Lagrangian Strain components: ϵ_{xx}, ϵ_{yy}, ϵ_{zz}, ϵ_{xy}, ϵ_{xz}, ϵ_{yz}.

  Notes 1 and 2 for `key='stre'` apply here as well.

– `'ener'`: Strain energy density field plot. Nodal values of the strain energy density are extrapolated from the element integration points. For this `key`, `index` has no

effect. Notes for `key='stre'` apply here as well. To plot the energies of individual nonlocal atoms, the `'repa'` key described below should be used.

– `'ghos'`: Ghost force correction plot. The nodal ghost force correction dead loads are plotted on a finite element mesh. `index` has no effect.

– `'patc'`: Patch plot of the internal element variables. This option allows the user to view the element variables without the extrapolation errors discussed in `key='stre'`. The generated mesh is patched with each element displaying a constant value. The displayed information is set by `index`:

  * `index = 0` : Mixed plot with generally useful values:
    · Strain energy density.
    · Eigenvalues of the right Cauchy-Green deformation tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$ (where $\boldsymbol{F}$ is the deformation gradient): λ_1 , λ_2, λ_3.
    · σ_{xy} (XY-component of the Kirchhoff stress tensor).
  * `index = 1` : Strain Energy Density plot.
  * `index = 2` : Eigenvalues of the deformation tensor $\boldsymbol{F}^T\boldsymbol{F}$, (where $\boldsymbol{F}$ is the deformation gradient). These values are used in the nonlocality criterion and indicate the degree of deformation in an element.
  * `index = 3` : Kirchhoff stress plot. Plotted values are: σ_{xx}, σ_{yy}, σ_{zz}, σ_{xy}, σ_{xz}, σ_{yz}.
  * `index = 4` : Lagrangian strain plot. Plotted values are: ϵ_{xx}, ϵ_{yy}, ϵ_{zz}, ϵ_{xy}, ϵ_{xz}, ϵ_{yz}.

– `'repa'`: Representative atom plot. Output the nonlocal representative atoms followed by the local representative atoms. For each atom its energy and the number of atoms it represents is included. Following the representative atom information, the tessellation for the current representation and the model boundaries are added. For this key, `index` has no effect.

  - 'atom': Atomic positions plot. Generates a plot of all atoms in a given polygon. The polygon vertex coordinates are read from file 'polyfile'. The positions of unrepresented atoms are obtained through finite element mesh interpolation. The type of plot generated is determined by index:
    * index = 1 : normal plot
    * index = 2 : "Vitek" plot - In addition to the atomic position, adds information on the relative slip between the atoms. This is inspired by Prof. V. Vitek's visualizations of screw dislocation cores (See, for example, [18]).
  - 'type': Atomic types plot. Plots the atomic number for each repatom, useful for models where there are more than one species of atom present. For this key, index has no effect.
  - 'user': User-specified output generated by the routine user_plot. The parameters index, umag and scale are read in and passed to user_plot. The append setting is respected. Additional user-specified input can be read in after append if desired. More information on user_plot is available in Section 2.11.5.

- filepref : (character(len=80), default = 'qcplot') The prefix which will be used to produce the name of the output file. The plot command builds a unique filename for each plot produced using four components: the user-defined filepref, a letter code identifying the file type, a unique, automatically incremented 3-digit number and the .plt file extension. The key-specific letter codes are:
  - '_D': Displacement (disp) plot.
  - '_B': Boundary Condition (bcon) plot.
  - '_e': Strain (stra) plot.
  - '_s': Stress (stre) plot.
  - '_E': Energy (ener) plot.

  - '_G': Ghost Force (ghos) plot.
  - '_P': Patched (patc) plot.
  - '_R': Repatom (repa) plot.
  - '_A': Atoms (atom) plot.
  - '_t': Atom Types (type) plot.
  - '_U': User-specified (user) plot.

  For example, if filepref=qcplot, and the key=disp, the filenames generated would be qcplot_D001.plt, qcplot_D002.plt, qcplot_D003.plt etc. each time a disp plot is generated.

- index : (integer, default=0) A switch modifying the behavior of each of the key options. The effects of index for each key are detailed above.

- umag : (double precision, default=0.0) used with key='disp', 'bcon', 'stre', 'stra', 'ener', 'ghos', 'patc' and 'user'. Sets the magnification factor for the displacements added to the nodal reference positions. If umag=0.0, plot will be in the reference configuration. If umag=1.0, plot will be in the deformed configuration. Other values of umag will appropriately exaggerate or reduce the current displacement field.

- polyfile : (character(len=80), default='poly.dat') Only used by key='atom'. Filename of the file with the coordinates of the polygon vertices defining the region where atoms should be plotted.

- scale : (double precision, default=1.0) Used with key='disp', 'bcon', 'stre', 'stra', 'ener', 'ghos' and 'user'. Sets the magnification factor for the output variable.

- append : (integer, default=0) If append is set to 1, the code will attempt to append the output to an existing file of the same name, rather than writing each output to a

new file. In `append` mode, the code searches the home directory for the most recently written file with the same `filepref` and 2-character letter code as discussed above, and appends to that file. If no comparable file has been previously written, a new file is created.

The `append` option is available for all `plot` types. Note that in order for it to be correctly read, all previous data for the command must be present, even if the default values are to be used or the data is not relevant to that plot type. Said another way, the code expects `append` to be the fifth datum after the `key` on the command line. So, for example, setting `append` mode for a `repatom` plot type requires the command

```
plot,repa,filepref, , , ,1
```

to be used.

Because `append` is the last datum and it is defaulted to `0`, it can be omitted if the append option is not desired[16].

4.14 Macro 'prop' : define proportional load table

Loading is incremented in the QC method by variable referred to as the `time`, despite the static nature of QC simulations. This `time` variable is further used to compute a proportional load variable `prop`. The `prop` command is used to define the dependence of the `prop` variable on the `time` variable. This dependence is read in as a set of ordered pairs, between which QC will linearly interpolate to obtain a piecewise linear function of `prop` vs `time`. The prop versus time curve may contain step functions (i.e. two prop values that have the same time value). See Section 2.11.2 for an explanation how `prop` is used in the application of boundary conditions.

calling format: `prop,,npld,[fileprefix],[time(1),pload(1),time(2),pload(2),...]`

Description of input variables:

- `npld` : (integer) Number of points in proportionality graph.

[16]The possible exception to this rule is a `user` plot, where there may be additional `data` following `append`.

- `fileprefix` : (character(len=80)) Prefix of file containing graph data. The program will try to open a file called `fileprefix.prp` from which to read the data. If the `fileprefix` is absent, graph data is read from argument list.
- `time(i)` : (double precision) `time` coordinates of a set of points on a piecewise linear time-proportionality graph.
- `pload(i)` : (double precision) `prop` coordinates of a set of points on a piecewise linear time-proportionality graph.

Note that there is no `key` required for this command, and so the double-comma is required to denote an empty `key` field. Note also that if the values are to be read from the argument list rather than from a file, a second double-comma must explicitly appear to ensure that `fileprefix` is interpreted as an empty string.

4.15 Macro 'prot' : protect existing nodes from being deleted by coarsening

If the user plans to take advantage of the mesh coarsening features in the adaptive meshing algorithm, it is usually necessary to define a set of "protected" nodes that will not be removed by coarsening and hence prevent the essential features of the mesh geometry from being lost. The `prot` command provides a simple means to this end by allowing the user to protect either all existing nodes or all existing boundary nodes in the current mesh.

calling format: `prot[,key]`

- `key` :
  - `'  '` : protect all nodes in the model.
  - `'boun'` : protect all nodes on the model boundaries.

4.16 Macro 'repo' : print out current energy and out-of-balance forces

calling format: `repo`

This command prints a brief report to the output stream including the current value of the energy and out-of-balance force norm. The latter quantity is of particular interest since it should be zero (to within some tolerance) for a converged solution.

4.17 Macro 'rest' : read/write restart files

calling format: `rest,key,fileprefix`

- `key` :
  - `'read'` : read stored simulation from a previously written binary restart file.
  - `'writ'` or `'  '` : write simulation data to binary restart file.
  - `'txrd'` : read stored simulation from a previously written ASCII text restart file.
  - `'txwt'` or `'  '` : write simulation data to ASCII text restart file.
- `fileprefix` : (character(len=80), default=`'qc'`) Prefix of the restart file name. The program will automatically append the `.res` extension to create the filename for binary restart files or the `.trs` extension for ASCII text restart files.

Restart files can be used to prevent loss of simulation results in the event that a QC simulation is terminated unexpectedly, for example due to a power failure. Restart files can also be used to re-start a run with different simulation parameters. ASCII text and binary restart files perform the identical function, but text restarts are typically about 3 times as large as their binary equivalent. The text version should only be used if portability of the restart file across different platforms is not possible with the binary format.

Each time a `restart` command is used to write a restart file, the code checks for the existence of a file `fileprefix.res` (or `fileprefix.trs`, as appropriate) in the working directory. If such a file exists, it is moved to a file `fileprefix_LAST.res` before the new file is written. In this way, there are up to two restart files saved at a time. Upon a third attempt to write a restart file with the same name, the same procedure is followed and the old copy of `fileprefix_LAST.res` is lost.

The only important data not stored in the restart file is the stiffness matrix in order to avoid unnecessarily large files. The stiffness matrix can easily be recomputed after reading a restart file using the `tang` command.

A restart file can be read at any point in the `macros` stage of the simulation, but are typically read in as the first `macros` command. Re-starting from a previously written restart file is best done by using a new input file with a very similar list of commands in the `head` stage. Some changes to the commands in the `head` are possible, others must be used with caution, and others will not lead to a successful restart.

Some examples of changes to the `head` stage that are permissible:

1. Changes to some of the `fact` settings or `flag` settings.

2. Changes to the constitutive information (using a different interatomic potential), provided that the lattice parameter of the new potential is identical to that of the original one.

3. Changes or additions to the no-adaption zones.

4. Increasing the allocated storage for repatoms (`maxnp`) or elements (`maxel`), see Section 3 of the *QC Tutorial Guide* for more details.

Some examples of changes that must be used with caution:

1. Any changes to the mesh generator will be completely ineffectual, as the `rest` command will read in the entire mesh from the restart file and overwrite the generated mesh.

2. Changes to the active/inactive status of any grain boundary segments must be accompanied by the appropriate adaptive remeshing after the restart file is read in, since the newly activated grain boundary may be in a region of coarse mesh and cause nonlocal atoms to represent large volumes of the material. This will lead to an energy functional that is a very poor approximation to the correct one.

Some examples of changes that will not lead to a successful restart:

1. Changes to the grain definitions. Modifying the orientation or shape of the grains will generally not lead to a successful restart. Repatoms in the restart file data will no longer fall on Bravais lattice sites, as required by the simulation, or elements may fall entirely outside of the newly shaped grains.

2. Changes to the material definitions. Modifying the Bravais lattice will have a similar effect to that of modifying the grain orientations.

4.18 Macro 'setp' : store current resultant for comparison in conv,pdel

calling format: setp

The command setp computes and stores the current value of the user-defined applied force (using the same user_pdel routine described in Section 2.11.3. Each subsequent call to conv,pdel will compare the current value of the force to that stored at the last call to setp to decide if convergence has been achieved.

4.19 Macro 'solv' : call solver routine

The two solvers available in the QC method are a Newton-Raphson (NR) method and the Conjugate Gradient (CG) method. Both are called from the same command by using different key options.

calling format: solv,key,dsmax,maxfn,iprint

Description of input variables:

- key :
  - 'nr ' : Newton-Raphson solver
  - 'cg ' : Conjugate Gradient solver

- `dsmax` : (double precision, default=1.5) Maximum allowed change in a dof in a single step, units of length.
- `maxfn` : (integer, default=10000), limit on simulation.
  - `maxfn>0` : maximum allowed evaluations of the energy and out-of-balance forces is maxfn.
  - `maxfn<0` : maximum number of CG iterations is |`maxfn`|.
- `iprint` : (integer, default = 0) The number of interactions between CG outputs. *E.g.*, if `iprint=3` output is written every third CG iteration. If `iprint=0`, no output is generated.

Note that parameters `maxfn` and `iprint` are only used in the CG routine, but they must be specified for both solver options. This is because the NR routine includes a error trap that will attempt to use the CG solver in the event of a NR failure.

4.20 Macro 'stat' : Recompute local/nonlocal representative atom status

The `stat` command should be called whenever there is need to check that current repatom nonlocal/local status is consistent with the nonlocality criterion. However, it can be a slow process and must be used judiciously to avoid excessive computational time.

A repatom can be given nonlocal status for one of two reasons. First, if it is within `PROXFACT*rcut` of any active surface or grain boundary, it will be made nonlocal. Secondly, it will be made nonlocal if it is in a region of the crystal that is experiencing significant variation in the deformation gradient on the atomic scale. Details of this criterion can be found in [3, 19], and is discussed in more detail in Section 3.2 of the *QC Tutorial Guide*.

The status command also serves to check that the neighbor lists for the current set of nonlocal repatoms is up-to-date. This is invoked using `stat,update` as described below. In

this case, the status is only re-calculated if it is deemed that the deformation since the last neighbor-list computation is such that neighbor lists may have changed.

calling format: `stat[,key]`

- `key` :
  - `'  '` : compute status of all representative atoms in the model and set up auxiliary arrays, such as neighbor lists, to speed execution.
  - `'upda'` : check whether stored auxiliary arrays are up-to-date, and whether the displacements since the last status calculation are too large, making it necessary to recompute the lists. Note that this key option does not technically check whether the `status`, *per se*, needs to be updated. Rather, this option ensures that repatoms which currently have nonlocal status also have up-to-date neighbor lists. The criterion for neighbor list updates is not the same as the criterion for local/nonlocal status.

    Interatomic potentials typically have a distance `rcut` beyond which it is assumed that atoms do not interact. The QC code computes and stores a list of all neighbors within `CUTFACT*rcut` of each atom for the current nodal displacements, and thus there is a cushion of `rpad=(CUTFACT-1)*rcut` in the neighbor list. As long as no other atom moves more than `rpad` closer to the atom of interest, the neighbor list will include at least all of the neighbors required for a correct energy calculation.

    The `'upda'` option checks the displacement of all atoms since the last neighbor list update, and triggers a new list computation if the sum of the two largest displacements (of all the atoms) exceeds `rpad`. This is a conservative criterion, ensuring that necessary neighbors are never missing from the lists, but significantly reducing the computational time spend on neighbor searches.

Additional discussion of the functions of the `status` command can be found in Section 4.3 of the *QC Tutorial Guide*.

4.21 Macro 'stpr' : print state variables (stress, strain other elemental quantities)

Writes elemental data to the log file `qc.log`.

calling format: `stpr,[key],[n1],[n2]`

Description of input variables:

- `key`:
  - `'  '` or `' stre'` : print stresses.
  - `'stra'` : print strains.
  - `'inte'` : print internal element variables. See the comments in `Code/mod_global.f` for a detailed list of these variables (`IEPT`, `IFPT`, `ILPT`, `IGPT`).
- `n1` : (integer, default=1) Lower limit of element range to be printed.
- `n2` : (integer, default = number of elements) Upper limit of element range to be printed.

4.22 Macro 'syst' : compute system matrix and right-hand side concurrently

calling format: `syst`

The `syst` command updates the out-of-balance force vector and the stiffness matrix for the current repatoms, statuses and displacements.

4.23 Macro 'tang' : form tangent stiffness

calling format: `tang`

The `tang` command is like the `syst` command, except that it only updates the stiffness matrix and not the out-of-balance forces.

4.24 Macro 'time' : increment time

calling format: `time,[key],[dtstep | varstp],[tmax]`

- `key`:
  - `'  '` : normal time increment. If `dtstep` is defined this will be the timestep, otherwise, time will be incremented by `dt`, set by macro `'dtim'`.
  - `'vari'` : timestep will equal the fraction (`varstp`) of the maximum possible timestep that would cause the first element in the mesh to become inverted.
- `dtstep` : (double precision) Constant timestep (for `key='  '`)
- `varstp` : (double precision) Variable timestep factor (for `key='vari'`)
- `tmax` : (double precision) Maximum time, simulation will be terminated when this time is reached.

4.25 Macro 'tole' : set solution tolerance

calling format: `tole,,globaltol`

Note that there is no `key` required for this command, and so the double-comma is required to denote an empty `key` field.

Description of input variables:

- `globaltol`: (double precision, default=1.e-9_dp) Tolerance used for solver and convergence checks.

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