Instructions for using *EDM.exe*

To successfully run *EDM.exe* on a computer, one need to install a FORTRAN code compiler, Intel Visual FORTRAN or Intel oneAPI. If you haven't installed them, you can still proceed by locating certain dynamic link library files (on Windows system, these are files with suffix .dll) from other computers that have installed the compilers. The dynamic link library files are related to Intel Math Kernel Library (MKL) and OpenMP and could be found from the installation folders of the compilers mentioned above. For example, for Windows system with oneAPI, there are five related files that should be placed either in the same root directory as *EDM.exe* or in a path specified in the system environment variables. These files are *mkl_intel_thread.2.dll*, *libiomp5md.dll*, *libifcoremd.dll*, *mkl_core.2.dll*, and *mkl_def.2.dll*.

Next, running *EDM.exe* requires one or two input files. For solving mechanics problems considering thermal deformation effects, you need to provide the data file *EDM.inp* and the file *TEMPERATURE.dat* for description of temperature distribution. For other problems, the presence or absence of *TEMPERATURE.dat* does not affect the results. Typically, when solving heat conduction problems, a *TEMPERATURE.dat* file is generated alongside the results for possible thermal deformation analysis of the next step.

You can confirm a successful program run when the control window displays "Job terminated normally" or when the last line of the *EDM.log* file shows "Total computational time is...".

The program generates several output files, including:

- *EDM.out*: Contains the results from reading the input files and the computational results.
- *RESULTS.plt*: A contour plot file that can be opened using tecplot360.
- *INPUT_GEO.nas*: A file for drawing the input mesh, which can be opened using FEMAP.
- *EDM.log*: A file recording the elapsed time and status of the program run.

EDM.inp contains input data organized into various data blocks. Not all data blocks need to be present, and each group of data blocks is suggested to be written on a separate line. Different numbers within the data block are separated by at least one space. The superscript below means that a corresponding explanation is presented in the appendix at the end of this document.

Data block 1 (one row)

TITLE: Title should be the combination of letters and numbers and must satisfy 0< string length <=180.

Data block 2 (one row)

NDIM: The dimension of the problem, = 2 or 3. One-dimensional problems are not supported .

NDF: Number of the unknowns per node[1].

NSIG: The number of stress or heat flux components[2].

MNODE: Maximum number of nodes within the element[3].

NTP: Total number of nodes.

NTE: Total number of elements

MSOLVER: specifies the solver (= 1-7)[4]

Data block 3 (NTP rows, one row per node): Coordinates of all the nodes

I: Node number

CD(1,I): The x-coordinate of node I
CD(2,I): The y-coordinate of node I
CD(3,I): The z-coordinate of node I (can be negligible if two-dimensional)

Data block 4 (NTE rows, each element occupies one row): the information of all the elements
L: Element global number
IMAT: The corresponding material property group number of this element
NODE: The number of nodes in element L
LNDE(L,1): The global node number[5] of the first node of element L
LNDE(L,2): The global node number of the second node of element L
....
LNDE(L,NODE): The global node number of the last node of element L

Data block 5 (one row):
NTFACE: Total number of element face groups for given boundary conditions[6]:
Data block 6 (NTFACE rows, one row for each group of element face):
IEBGN: The starting element number for the boundary condition
IEEND: The end element number for the boundary condition
IESTEP: The element number step for the boundary condition
IFACE: Face number[7]
IGROUP: The group number of boundary conditions corresponding to this group of element face
IFLAG: The indicate of boundary condition type at each direction corresponding to this group of element faces[8]

Data block 7 (one row):
NBCV: The group number of specified boundary conditions[9]
Data block 8 (NBCV rows, one row for each group of specified boundary conditions):
IGRP: The group number of this boundary condition
LRET: Type of boundary condition (= 1 is the first type boundary condition or Dirichlet boundary condition, = 2 is the second type boundary condition or Von-Neumann boundary condition, = 3 is the heat convection boundary condition, = -2 when applying uniformed distribution pressure)
PRET: The correlation value 10 for this group of boundary conditions
If the surface tractions are trigonometric functions of time, which is usually for dynamics problem, then we need to enter them on the next two lines:
TEXT: Type of trigonometric function (SIN, COS, sin, or cos)
TEF: The time-close coefficient of the trigonometric function

Data block 9 (one row):
NBODY: The number of types of body forces or source terms
Data block 10 (NBODY rows, one row per source term):
M: The group number of this source term
MBODY: This type of this source term[11]
IBODY: The number of input parameters for this source term
VBODY: Defines all the parameters required for this source term

Data block 11 (Specifies the element number in which the source term is applied, if NBODY=0, this block is absent).

NBDELEM: The amount of element groups that the source term is applied (one row)

When NBDELEM = 0, source term is applied to all the elements

When NBDELEM ≠ 0, NBDELEM is the amount of element groups that the source term is applied and NBDELEM row input should be given in the following form:

IEBEG, IEEND, IESTEP, IBDGRP

(IEBEG, IEEND and IESTEP are start and end element numbers and steps for the describe the elements where this source term is applied. IBDGRP is the corresponding group number of the source term)

Data block 12 (one row): specifies the number of property parameter type groups and the type of the problem.

NMATGRP: Number of material properties groups[12]

ISTRANS: Transient identification (=1 for transient heat conduction or structural dynamics; =0 is not)

ISNONLI: nonlinear identification (=1 means material nonlinear; =0 is not)

ISTM: Thermal stress identification (=1 is the mechanics problem considering thermal deformation, requires the file of *TEMPERATURE.dat*; =0 is not)

Data block 13 (NMATGRP rows): specifies parameters of material properties for linear problems (if ISNONLI =1, this data block is absent)

When NMATGRP>0, the material properties are based on elements:

IMAT: The group number of material properties.

When IMAT > 0, material properties are specified based on elements. The following parameters are entered in the same row as IMAT.

E0: Elastic modulus or thermal conductivity

PR: Poisson's ratio (not involved in the calculation for thermal conduction problem, can be any number and must be a number)

CT0: expansion coefficient in thermal deformation problems (not available for non-thermal deformation problems)

RHO: Material density in heat conduction or structural dynamics (not available for steady-state problems)

CP: constant pressure specific heat capacity in heat conduction or damping in structural dynamics (not available for steady-state problems)

MTYPE: Heterogeneous type[13]

N1: The number of parameters of heterogeneous material

MISOT: Anisotropic type[14]

N2: The number of parameters of anisotropic materials

C1(:): The parameters about heterogeneous material (absent if N1=0)[15]

C2(:): The parameters about anisotropic material (absent if N2=0)[16]

When IMAT< 0, the material must be heterogeneous, and the material properties are specified based on the nodes in each element (the same node can also have different properties in different elements), with one row for each node in the element and totally MNODE rows (each row is as

following).
E0: Elastic modulus or thermal conductivity
PR: Poisson's ratio (not involved in the calculation for thermal conduction problem, can be any number and must be a number)
CT0: expansion coefficient in thermal deformation problems (not available for non-thermal deformation problems)
RHO: Material density in heat conduction or structural dynamics (not available for steady-state problems)
CP: constant pressure specific heat capacity in heat conduction or damping in structural dynamics (not available for steady-state problems)
MISOT: Anisotropic type[14]
N2: The number of parameters of anisotropic materials
C2(:): The parameters about anisotropic material (absent if N2=0)[16]
When NMATGRP < 0, the materials must be heterogeneous, and the material properties are specified based on nodes one by one. The input is as follows (totally **-NMATGRP** rows):
MPBGN: The starting node number
MPEND: The end node number
MPSTEP: The node number step
E0: Elastic modulus or thermal conductivity
PR: Poisson's ratio (not involved in the calculation for thermal conduction problem, can be any number and must be a number)
CT0: expansion coefficient in thermal deformation problems (not available for non-thermal deformation problems)
RHO: Material density in heat conduction or structural dynamics (not available for steady-state problems)
CP: constant pressure specific heat capacity in heat conduction or damping in structural dynamics (not available for steady-state problems)
MTYPE: Heterogeneous type[13]
N1: The number of parameters of heterogeneous material
MISOT: Anisotropic type[14]
N2: The number of parameters of anisotropic materials
C1(:): The parameters about heterogeneous material (absent if N1=0)[15]
C2(:): The parameters about anisotropic material (absent if N2=0)[16]

Data block 14: Material parameters for nonlinear problems (ISNONLI=0 this data block is absent)
IMAT: (one row) Material property group number. (Must be greater than 0)

METYPE, NE0, CE0(NE0) occupy one row
METYPE: Function type of elastic modulus or thermal conductivity with respect of temperature or displacement[17].
NE0: The number of parameters required for the function mentioned in METYPE.
CE0(NE0): Parameters required for the function mentioned in METYPE.

MPTYPE, NPR, CPR(NPR) occupy one row (only when NDF > 1, it is required.)

MPTYPE: Function type of Poisson's ratio with respect of displacement[17].
NPR: The number of parameters required for the function mentioned in MPTYPE
CPR(NPR): Parameters required for the function mentioned in MPTYPE.

MCTTYPE, NCT, CCT(NCT) occupy one row (only when NDF > 1 and ISMT = 1, it is required.)
MCTTYPE: Function type of expansion coefficient with respect of displacement[17].
NCT: The number of parameters required for the function mentioned in MCTTYPE.
CCT(NCT): Parameters required for the function mentioned in MCTTYPE.

MRTYPE, NRH, CRH(NRH) occupy one row (only when ISTRANS=1, it is required.)
MRTYPE: Function type of density with respect of temperature[17].
NRH: The number of parameters required for the function mentioned in MRTYPE.
CRH(NRH): Parameters required for the function mentioned in MRTYPE.

MCPTYPE, NCP, CCP(NCP) occupy one row (only when ISTRANS=1, it is required.)
MCPTYPE: Function type of specific heat with respect of temperature[17].
NCP: The number of parameters required for the function mentioned in MCPTYPE.
CCP(NCP): Parameters required for the function mentioned in MCPTYPE.

Data block 15: (one row) parameters for nonlinear problem (if ISNONLI=0, this data block is absent)
OMG: nonlinear iterative relaxation factor, generally = 1, the desirable range is 0.7~1.
TOLN: convergence judgment tolerance or maximum iteration steps for material nonlinear problems (tolerance < 1, steps >= 1 and must be integer)

Data block 16: (one row) parameters for transient problem (if ISTRANS=0, this data block is absent)
THETA: θ of the transient problem ($0 < \theta <= 1$, fully implicit when $\theta = 1$)
DELTAT: time step Δt
TOLT: judging tolerance to reach steady state or maximum time step for transient heat conduction problem (tolerance <1, step >=1 and must be integer)

Data block 17: (one row) if ISTRANS=0 and ISNONLI=0, this data block is absent
NINIT: The total group number of initial conditions

Data block 18: (NINIT rows, one row for each group of nodes) if ISTRANS=0 and ISNONLI=0, this data block is absent
IPBGN: start node number
IPEND: end node number
IPSTEP: node number step
SPU: the initial temperature or initial velocities and displacements of the node. For heat conduction problem, total number is 1; for dynamics, total number is 2*NDF.

Appendix:

(1) NDF: For heat conduction problem, NDF = 1; For mechanics problems, NDF = NDIM (problem dimension)

(2) NSIG: For mechanics problems, = 3, plane stress problem, = 4, plane strain problem, = 6, three-dimensional problem. For the heat conduction problem, whatever the value is, it is set to NDIM in program.

(3) NODE:

2D problem: = 7 is a quadratic triangular element; = 9 is a quadrilateral element;

= 16 is a cubic quadrilateral element; = 25 is a quartic quadrilateral element;

3D problem: = 11 is a quadratic tetrahedral element; 21 or 27 are quadratic hexahedral elements;

= 64 is a cubic hexahedral element; = 125 is a quartic hexahedral element.

(4) MSOLVER: Solver identifier

= 1 The sparse LU factorization solver PARDISO_UNSYM from INTEL MKL library is used.

= 2 The solver DGESV for fully populated matrix from INTEL MKL library is used and is not available for transient and nonlinear problems.

= 3 The LU factorization solver CMLIB_LUD for fully populated matrix from the LINPACK library is used and is not available for transient and nonlinear problems.

= 4 Sparse LU factorization solver from INTEL MKL library, DSS_UNSYM is used.

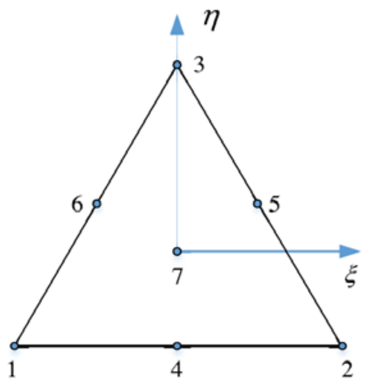
= 5 Sparse iterative solver with ILU0 pre-conditioned from INTEL MKL library, FGMRES_ILU0 is used.

= 6 The sparse equation iterative solver with ILUT pre- conditioned in INTEL MKL library, FGMRES_ILUT, is used.

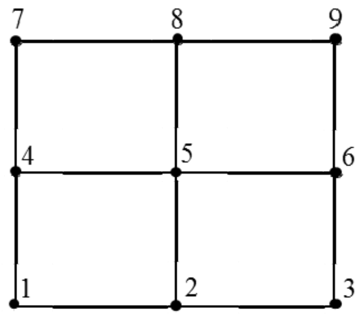
(Note: MSOLVER>0, directly solve the equation; MSOLVER<0, only available for sparse solvers 1,4,5,6, further compress the non-zero elements of the coefficient matrix and solve.)

(5) LNDE: The node number order of the element nodes is shown in the following figure:

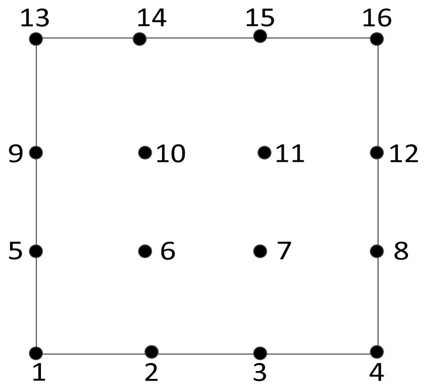
Element for 2D problem:



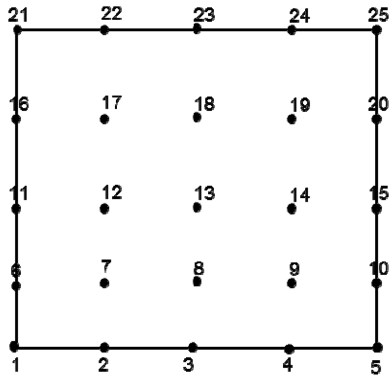
NODE=7



NODE=9

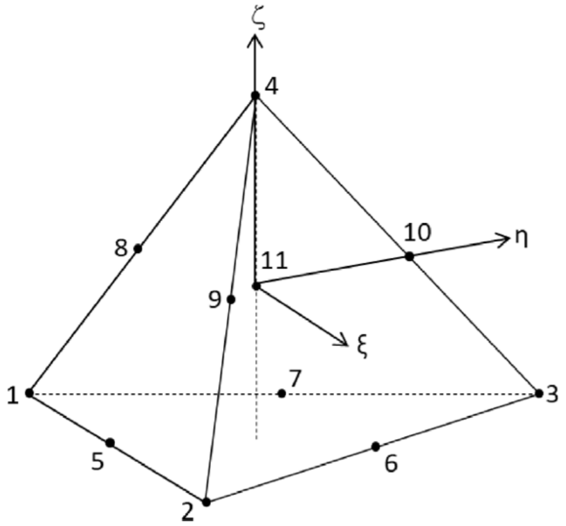


NODE=16

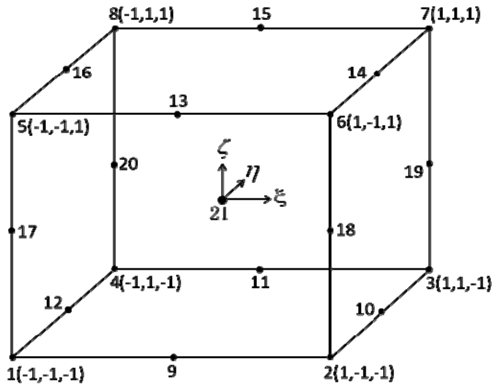


NODE=25

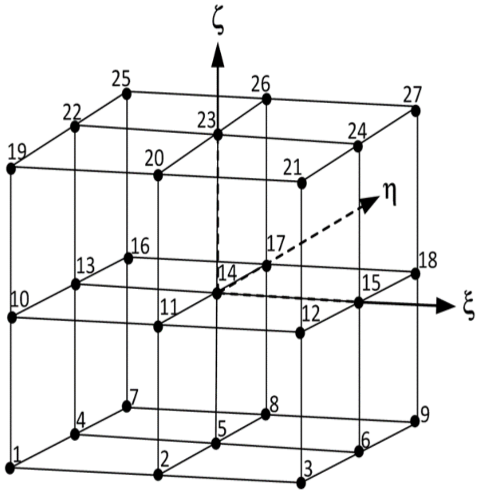
Element for 2D problem:



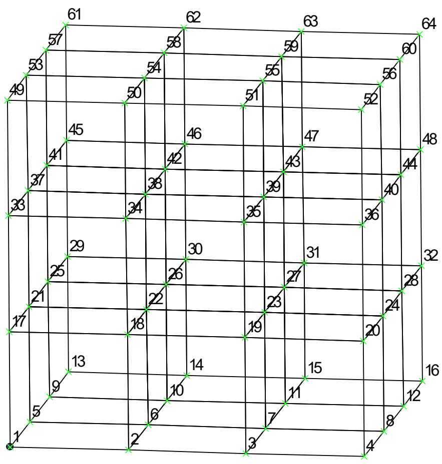
NODE=11



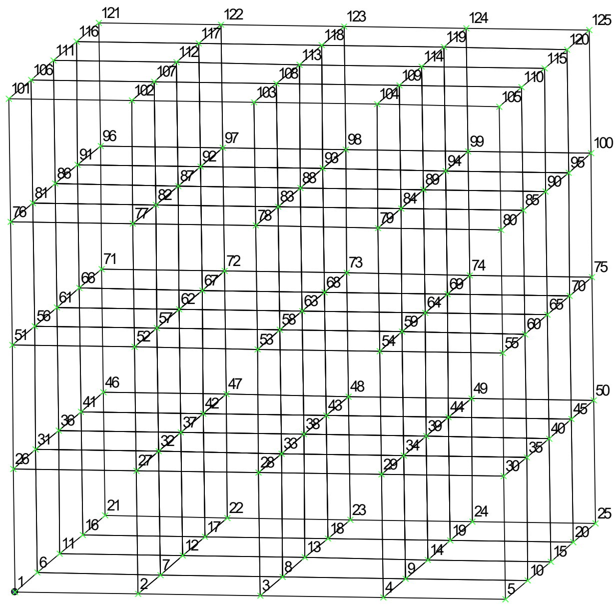
NODE=21



NODE=27



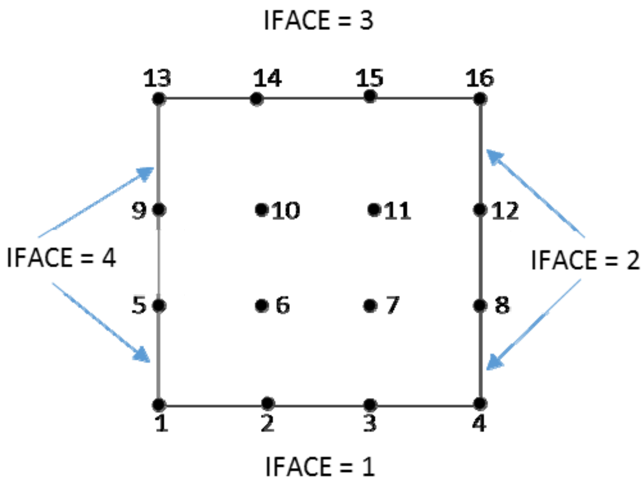
NODE=64



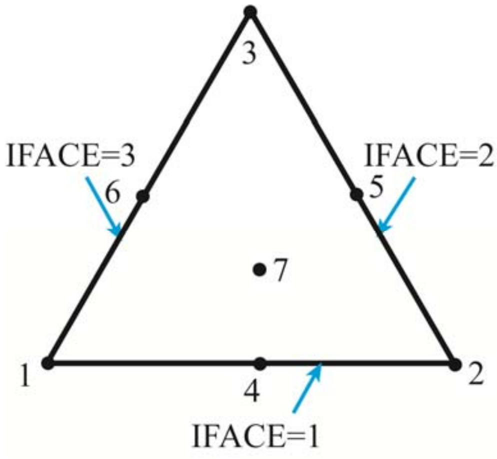
NODE=125

(6) NTFACE: The number of faces in 2D elements is 4, and that in 3D elements is 6.

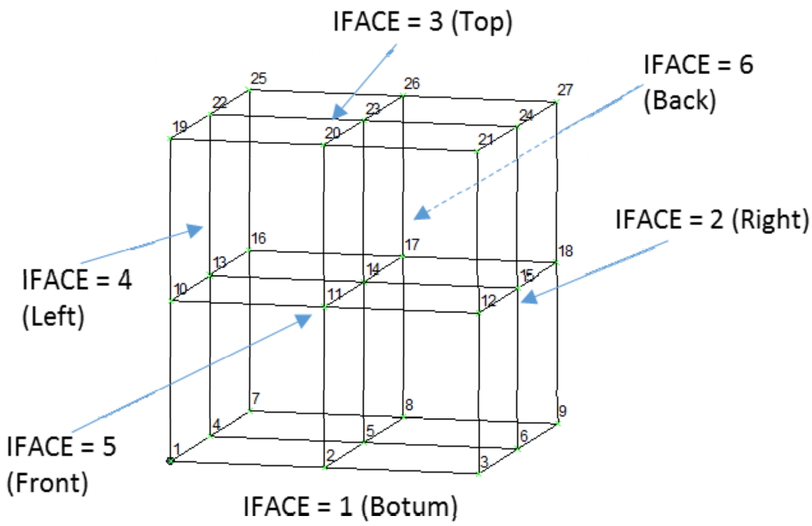
(7) IFACE: The face number of boundary conditions, and the face number in 2D or 3D element is shown as follows:



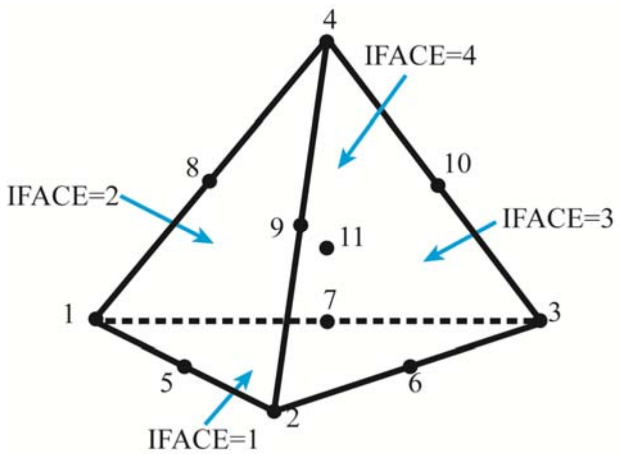
2D rectangular elements



2D triangular elements



3D hexahedron elements



3D tetrahedral elements

(8) The number of digits of the IFLAG is the same as NDF, and the heat conduction problem has only one digit, which indicates the boundary condition type for this group of faces; Mechanics problems may have 2 or 3 bits, representing the (x, y) and (x, y, z) directions, respectively, to

indicate the boundary condition type for each direction. No boundary condition (represents adiabatic in heat conduction problems, surface free for mechanics problems) can be written as 0. when the value of this digit is not the same as the boundary condition type (refer to LRET), the corresponding direction will not be treated.

(9) NBCV: total number of surface traction groups. If the faces have the same face number and have the same boundary conditions, the faces belong to the same boundary condition group.

(10) LRET:

If it is the first type of boundary condition for heat conduction problems, LRET= 1, the temperature value is given.

If it is the second type of boundary condition for heat conduction problems, LRET= 2, the heat flux value is given.

If it is the third type of boundary condition for heat conduction, LRET= 3, the heat convection coefficient and the far-field temperature value are given.

If it is the first type of boundary condition for mechanics, LRET= 1, the displacement values in all directions are given.

If it is the second kind of boundary condition for mechanics, LRET= 2, the surface traction value in all directions are given; and LRET= -2, the pressure value is given, positive for pressure and negative for pull.

(11) MBODY: The source term type

$$1\text{：}\quad f_i = c_i \quad \left(i = 1 \sim \text{NDF}\right) \qquad \text{(constants)}$$

$$2\text{:}\quad f_i = c_i + d_j x_j \quad \left(i, j = 1 \sim \text{NDF}\right) \qquad \text{(linear)}$$

$$3\text{:}\quad Q = \frac{x}{100}\left(1 - \frac{x}{100}\right)$$

$$4\text{:}\quad Q = \frac{\left(0.1 - \sqrt{x^2 + y^2}\right)\left(0.3 - z\right)}{0.03 * 0.01}$$

$$5\text{:}\quad Q = cx\left(6 - x\right)$$

Any function of coordinates can be developed through codes

(12) When NMATGRP > 0, the material property parameters are given based on element; When NMATGRP < 0, the material property parameters are specified based on nodes, and different material property parameters can be assigned to different nodes through different groups.

(13) MTYPE: The type of heterogeneous material:

0: Homogeneous property

$$1\text{:}\quad \mu = \mu_0 e^{\sum c_i x_i}$$

$$2\text{:}\quad \mu = \mu_0 + \sum_{i=1}^{D} c_i x_i \qquad D = \text{NDIM}$$

3: $\mu = \mu_0 + \sum_{i=1}^{D} c_i x_i + \sum_{i=1}^{D}\sum_{j=i}^{D} c_{ij} x_i x_j$

4: $\mu = \mu_0 + br$ in which $r = \sqrt{\sum_{i=1}^{D} c_i (x_i - d_i)^2}$

5: $\mu = \mu_0 + br^2$

6: $\mu = \mu_0 e^{br}$

7: $\mu = \mu_0 e^{br^2}$

8: $\mu = \left(1 + \frac{x}{100}\right)^3$

9: $\mu = \mu_0 e^{b(\sqrt{x^2+y^2}-4)}$

10: $\mu = \mu_0 e^{1/15ay}$

(14) MISOT: The type of anisotropic material: (New type or function with heterogeneity are to be developed.)
0: Isotropic problem
1: Nine engineering constants E_1, E_2, E_3, ν_{12}, ν_{13}, ν_{23}, G_{12}, G_{13}, G_{23} are input into C2 in order.
(15) C1(:): the array of material property parameters used to define heterogeneous material.
(16) C2(:): the array of material property parameter used to define anisotropic materials.
(17) METYPE, MPTYPE, MCTTYPE, MRTYPE and MCPTYPE: The types of nonlinear material properties that vary with temperature or displacement (represented by T).
0: homogeneous problem: a constant C_(1)
1: Linear: C_(1)+ C_(2)*T
2: Quadratic: C_(1)+ C_(2)*T+ C_(3)*T^2