

AN INTERFACE PROGRAM FOR THE CONVERSION OF ANSYS TO MCNPX GEOMETRY

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Simulations gain in importance in physics and technical applications. While simulation codes cover many different areas of application, they have one common denominator: the geometry package. This package allows to describe the particular geometry setup using a meta-language which usually is not compatible between different simulation codes. In this short report a conversion program is introduced which converts the ANSYS meta-language to the MCNPX meta-language.

ABOUT THE SIMULATION SOFTWARE ANSYS

ANSYS is a general finite element modelling software package applicable to a wide variety of mechanical problems, involving acoustic, piezoelectric, thermal and thermoelectric analysis. These studies give help to a better understanding of how well a model reacts to common combinations of phenomena. Thanks to its set of linear and nonlinear elements ANSYS easily simulates even large and intricate structures which are separated into disjoint elements.

In the present case the geometric structure can be generated in ANSYS by decomposing it into small polyhedrons. The elements are numbered serially. The corners of each element are called nodes.

The command *ewrite* writes the selected elements to a file, where only elements having all of their nodes defined are written. The data are written in a ASCII format (FORTRAN format 14I6 or 14I8) with one element description per record for elements having eight nodes or less. For elements having more than eight nodes, nodes nine and above are written on a second record with the same format. In one record the node numbers are followed by attribute numbers characterising a particular element (one of which is the material number). The last item is the element number.

The command *nwrite* writes the selected nodes to a file. The data are again written in ASCII format (FORTRAN format I8, 6G20.13) with now one node description per record: The node number is followed by the x-, y-, and z-coordinate values of the global Cartesian system. The last three numbers, designating a local rotation, should be zero and hence this part is left blank.

ABOUT THE SIMULATION SOFTWARE MCNPX

MCNPX is a general purpose Monte Carlo particle transport code that extends the capabilities of the Los Alamos MCNP code. MCNPX supports 34 particle types and the ability to use physics models for energies where tabular data are not available.

The geometry of MCNPX treats an arbitrary three-

dimensional configuration of user-defined materials in geometric cells bounded by first- and second-degree surfaces of analytic geometry and fourth-degree elliptical tori. A complete specification of the geometry of a cell includes a list of signed surfaces bounding the cell, where the sign denotes the sense of the regions defined by the surfaces. The regions are combined with the Boolean intersection, union and complement operators.

Using several predefined geometrical bodies as in a combinatorial geometry scheme, MCNPX gives the user the added flexibility of defining geometrical regions. This macrobody capability is an alternative method of defining cells and surfaces. The macrobodies can be mixed with the standard cells and surfaces. The macrobody surface is decomposed accessible into surface equations and the facets are assigned individual numbers according to a predetermined sequence.

THE INTERFACE PROGRAM

It is of certain interest to carry out thermal and mechanical as well as Monte Carlo transport calculations on the same structure. At the moment it is necessary to specify the geometry in ANSYS and to set it up independently in MCNPX. Thus, an interface program which is implemented in C was developed to transform the geometry input in MCNPX based on the output files of ANSYS. As the Finite Element Technique is underlying the geometry input in ANSYS whereas the geometry input of MCNPX is not subject to these restrictions the direction of the transformation is reasonable.

In MCNPX Version 2.4.0 and higher there is an arbitrary polyhedron as a macrobody available which provides the possibility to build arbitrary tetrahedrons, hexahedrons, and triangular prisms. Therefore, the ANSYS-generated geometry should be restricted to these three bodies which are recognised by the Interface program from the node pattern in one record of the element file.

The application of the Interface program requires the existence of a file called *input.dat*; Fig. 1 displays the input form of this input file which has to contain at least twelve records. The data entries of each record are

separated by one or more blanks, while the format is free. Apart from record 11, which will not be read at all, only the last entry of each record is read by the Interface program, but not the preceding description.

#	Description	Entry
1	Input1:	elements.dat
2	Input2:	nodes.dat
3	Output:	mcnpix.dat
4	Scaling (Input2 to cm):	0.1
5	Void (yes/no):	yes
6	Voidnumber or blank:	99990
7	+F6 cellnumbers (yes/no):	yes
8	SD6 Record: volume (yes/no):	yes
9	SD6 Record: mass (yes/no):	yes
10	Display in Command-window (yes/no):	no
11	Materialnumber	density [g/cm ³]
12	1	8.933
:	2	0.777
:	3	0.23456

Fig. 1: Example for an input file "input.dat" of the Interface program.

The first three records concern the name of the two input files generated by ANSYS and the name of the output-file generated by the Interface program.

Record 4 declares the scaling factor to convert the units used in ANSYS for establishing the geometry to centimetre which is the unit used in MCNPX.

In MCNPX the whole universe has to be declared. Thus, the Interface program defines the outside world, which is the universe except for all elements on the element input file of ANSYS, if the entry on record 5 is "yes". The desired voidnumber has to be entered on record 6. Record 6 will not be read by the Interface program, if no void is desired on record 5. If a subdivision into an internal and an external void is desired, the user is required to do this, because the Interface program cannot distinguish the internal from the external void. As the Interface program makes use of the Boolean complement operator to generate the void, some problems may occur running MCNPX if there are too many cells. In this case the user is required to subdivide the void into two cells considering the geometry and to rerun MCNPX. Another possibility is to set this tool aside and to generate the void by intersection and union of the boundaries of the whole geometric structure.

Record 7 makes available a list of all cell numbers which can be useful if for instance the energy deposition averaged over the cell for cells is to be determined (tally F6).

On Records 8 and 9 some cell characteristics like volume and mass of each cell can be declared which

are required for some tallies in MCNPX. The Interface program calculates these cell characteristics and puts them to the output file in the order of the cell numbers.

Record 10 enables/disables the display of run-time information.

As mentioned before, record 11 will not be read by the Interface program. It just exemplifies the following records: ANSYS assigns a material number to each element. Elements consisting of the same material are assigned the same material number. These material numbers are to be found on the element output file of ANSYS and can be inherited by MCNPX as cell material numbers. In MCNPX each cell card requires the material number and the cell material density. Record 12 makes available the number of the material and the corresponding density in the claimed unit gram per cubic centimetre. If the whole geometric structure consists of more than one material, the mass density of each material has to be declared on the following records 13, 14 and so on. The number of records concerning the mass density should match the number of materials in the element file generated by ANSYS. In MCNPX the material is defined on a material card (M) that has the same material number. This is left to the user.

The subdivision of the physical space into cells is not necessarily governed only by the different material regions, but may be affected by problems of sampling and variance reduction techniques, the need to specify an unambiguous geometry, and the tally requirements. All these has to be taken into account when modelling a structure with ANSYS.

A very fine subdivision of a structure into cells by the Finite Element Technique Program ANSYS may cause problems in MCNPX but an accurate application of the Interface program facilitates the modeling of the geometry.

SUMMARY

The Interface program connects the two simulation codes ANSYS and MCNPX.

ACKNOWLEDGMENTS

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REFERENCES

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- [2] L. S. Waters et al., Version 2.4.o, User's Manual, LA-CP-02-408, Los Alamos National Laboratory, Los Alamos (2002); <http://mcnpix.lanl.gov>.