



# **User Manual for EXODUS II Mesh Converter**

**Nuclear Engineering Division** 

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# **User Manual for EXODUS II Mesh Converter**

prepared by E. R. Shemon and C. W. Attaway Nuclear Engineering Division, Argonne National Laboratory

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#### ABSTRACT

A mesh conversion program has been developed to convert EXODUS II-formatted finite element meshes to the *ascii* format used by the PROTEUS-SN neutronics code developed at Argonne National Laboratory. This manual contains instructions, usage examples, and methodology for the mesh converter.

The PROTEUS-SN neutronics code requires a finite element mesh input file in one of several accepted formats (*ascii, nemesh, pntmesh,* or *bgpmesh*). None of these file formats are directly produced by conventional finite element file modeling codes, therefore format conversion is required. Currently, most finite element meshes are prepared using the Cubit program developed by Sandia National Laboratory. Cubit can export finite element meshes in a variety of formats including the portable EXODUS II format. EXODUS II files are binary files with NetCDF data storage structures designed to handle large object-oriented arrays. While a specialized EXODUS II application programming interface (API) exists to query EXODUS II data, the general NetCDF API can also be used for the same purpose.

The described program improves upon a previous tool which had limited flexibility and performance. Notably, the new converter successfully converts EXODUS II files generated with more recent versions of Cubit (version 13+) and has no limitation on mesh size (total number of vertices or elements). The converter queries data from the EXODUS II file using NetCDF API commands, reads the data in the file, reorganizes it, and writes it to the *ascii* file format used by PROTEUS-SN.

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## 1. Introduction

This chapter describes the basic functionality of the EXODUS II mesh converter program, whose purpose is to convert EXODUS II finite element meshes to the *ascii* format used by the PROTEUS transport code developed at Argonne National Laboratory. The program is written in C++ and depends on a C++-enabled NetCDF [3] library to access and interpret data collected from the input EXODUS II mesh.

## 1.1 Input File Summary

The program requires input in the form of one or more EXODUS II finite element meshes with proper extension type (".e" or ".exo"). The EXODUS II files must contain data following the EXODUS II naming conventions and must not be empty.

The Cubit meshing program [4] developed by Sandia National Laboratory is typically used to create meshes in EXODUS II format and has been routinely used to for PROTEUS-SN neutronics analysis. This converter program is compatible with EXODUS II meshes exported from Cubit versions 12+. Note that Cubit 13+ EXODUS II meshes have slightly different keywords for the vertex coordinates, and this difference is handled inside the converter automatically without user intervention.

## 1.2 Output File Summary

For each EXODUS II input mesh, two output files are produced: the *ascii*-formatted mesh for PROTEUS and an informative report file. Both files are generated in the same directory as the input EXODUS II mesh and follow a natural naming convention (input file Sample.e yields output files Sample.ascii and Sample\_REPORT.txt). The report file is provided as a user convenience to ensure accurate conversion and enable debugging – the conversion procedure is echoed in this file during the conversion process, including any errors encountered.

## 1.3 Quick Start Guide

The Makefile included with the distribution must be modified to properly compile the code. First, modify the NETCDF\_DIR variable to point to the local installation of NetCDF (version 4.0 or later, with C++/C support). The converter requires the NetCDF API to function – refer to Section 2.1 for NetCDF installation tips. For full verification capability, also modify the CUBIT\_12X, CUBIT\_13X, and PROTEUS\_X variables to point to the Cubit 12, Cubit 13, and PROTEUS-SN executables on the local machine. If any of these variables are left blank, the corresponding extended verification tests will not be performed, but the converter can still be compiled and tested. Figure 1 lists the variables in the Makefile which should be modified.

```
NETCDF_DIR=/software/netcdf-4.0.1/0-intel-11.1
CUBIT_12X=/usr/local/cubit-12.2/cubit
CUBIT_13X=/software/cubit-13.1/cubit
PROTEUS_X=/software/PROTEUS/sn2nd.x
```

#### Figure 1. Makefile variables to be modified for installing and testing converter.

Next, the code can be compiled using "make" to create the executable, and "make check" to test basic performance. Optional extended testing with Cubit and PROTEUS are available by typing "make verify" after also providing paths to Cubit and PROTEUS executable locations in CUBIT\_12X, CUBIT\_13X, and PROTEUS\_X variables as shown in the figure above.

\$> make
\$> make check
\$> make verify (only works if Cubit & PROTEUS are installed)
Figure 2. Commands to compile and test the converter.

To run a job, simply type "*ExodusConverter.x MyMesh.e*" where MyMesh.e is the name (or path) of any EXODUS II file you would like to convert. Upon successful conversion, MyMesh.ascii and MyMesh\_REPORT.txt appear in the same directory as MyMesh.e.

```
$> ExodusConverter.x MyMesh.e
$> ls
MyMesh.ascii MyMesh_REPORT.txt MyMesh.e
```

#### Figure 3. Example command line usage of the converter.

The file MyMesh\_REPORT.txt should be examined briefly for any errors. The file MyMesh.ascii can be directly used with PROTEUS if no errors were found.

## 2. Code Installation and Usage

This section describes how to install and use the EXODUS II finite element mesh converter.

#### 2.1 NetCDF Library Requirements

The EXODUS II mesh converter has a dependency on the NetCDF library. It uses the NetCDF API to query data from EXODUS II files which are actually specialized NetCDF data files. As mentioned in the previous section, the NETCDF\_DIR variable in the Makefile must point to a local installation of the NetCDF library, version 4.0+, with C and C++ capabilities enabled. The NetCDF library must be built with the same compiler that will be used for the EXODUS II Converter. The user is recommended to confirm the compiler version and C++ support by running the 'nc-config' utility with '—all' option located in the bin directory of the NetCDF installation. This command will list the NetCDF configuration information and capabilities as shown in Figure 4.

This netCDF 4	.0.1 has been built with the following features:
cc	-> icc
cflags	-> -I/software/netcdf-4.0.1/0-intel-11.1/include
libs	-> -L/software/netcdf-4.0.1/0-intel-11.1/lib -lnetcdf
cxx	-> icpc
has-c++	-> yes
fc	<pre>-&gt; ifort</pre>
fflags	-> -g -02 -I/software/netcdf-4.0.1/0-intel-11.1/include
flibs	-> -L/software/netcdf-4.0.1/0-intel-11.1/lib -lnetcdf
has-f77	-> yes
has-f90	-> yes
has-dap	-> no
has-nc2	-> yes
has-nc4	-> no
has-hdf5	-> no
prefix version	<pre>-&gt; /software/netcdf-4.0.1/0-intel-11.1 -&gt; netCDF 4.0.1</pre>

Figure 4. The NetCDF build specifications can be viewed running "nc-config –all" to display the current build information and the library flags.

The NetCDF package can be downloaded from the web (we recommend version 4.0.1, available at <u>www.unidata.ucar.edu/downloads/netcdf/ftp/netcdf-4.0.1.tar.gz</u>). Newer versions (4.2+) are available but require supplemental installations for C++ support. The recommended tarball contains everything needed by the converter in a single package. To configure, we recommend using the

options in Figure 5, where the compilers should be consistent with those you plan to use for the EXODUS II converter. The "--disable-netcdf-4 --disable-dap-remote-tests" options disable extended NetCDF functionalities that may require additional dependencies that are unnecessary for the converter.

\$> ./configure --prefix=/software/netcdf-4.0.1/0-intel-11.1 CC=icc F77=ifort
FC=ifort F90=ifort CXX=icpc --disable-netcdf-4 --disable-dap-remote-tests
\$> make check install

Figure 5. Recommended NetCDF configuration options for NetCDF 4.0 or 4.1 versions.

Table 1 lists the NetCDF function interfaces used by the converter (taken from NetCDF 4.0.1). If using a version of NetCDF past 4.0.1, check whether the function interfaces have changed as the converter will not work properly without updating the function interfaces to match the NetCDF API.

Function Interface	Purpose
<pre>nc_open(Filename, ReadWriteAccess, &amp;ncid)</pre>	Opens the EXODUS II file and gives it the handle <i>ncid</i>
<pre>nc_inq_dimid(ncid, const char name, &amp;id)</pre>	Returns the address ( <i>id</i> ) of a given dimension variable ( <i>name</i> )
<pre>nc_inq_dimname(ncid, id, &amp;characterarray)</pre>	Returns the name ( <i>characterarray</i> ) of a dimension variable, given its address ( <i>id</i> )
<pre>nc_inq_dimlen(ncid, id, &amp;length)</pre>	Returns the value of the dimension variable ( <i>length</i> ) given its address ( <i>id</i> )
<pre>nc_inq_varid(ncid, const char name, &amp;id)</pre>	Returns the address ( <i>id</i> ) of a variable, given its name ( <i>name</i> )
<pre>nc_inq_varname(ncid, id, &amp;characterarray)</pre>	Returns the name of a variable (characterarray), given its address (id )
<pre>nc_get_att_text(ncid, id, const char name, char * text[#] )</pre>	Returns the value ( <i>text</i> ) of an attribute ( <i>name</i> ) associated with a variable, given its address ( <i>id</i> )
<pre>nc_get_var_int(ncid, id, int * data [#])</pre>	Retrieve entire data array ( <i>data</i> ) from a variable data array, given its address ( <i>id</i> )

Table 1. NetCDF library functions used in the EXODUS II mesh converter (taken from NetCDF 4.0.1).

<pre>nc_get_var1_int(ncid,</pre>	id,	{0,0},	&datapt)	Retrieve a single data point (data) from a
				variable data array, given its address ( <i>id</i> )

#### 2.2 Building the Converter

In order to compile the converter tool, the user must first edit the NETCDF\_DIR variable in the Makefile to point to the local NetCDF installation location as in Figure 1. The other variables are optional to compile and perform basic tests with the converter, but required for the most rigorous verification tests.

Once the Makefile has been properly modified to point to the NetCDF installation, executing the command *"make"* will invoke compilation and produce the executable *"ExodusConverter.x"* in the current directory.

Next, the command "make check" should be issued to ask the converter to perform a series of benchmark tests. Each of these tests has a unique feature that will test all file variables that may be present in an EXODUS II mesh from CUBIT. After converting each of the provided EXODUS II files, the contents and size of the provided reference outputs and the new outputs are compared. Any differences denote a failed test and will be written to the command line immediately. Once all tests have been run and compared, the bench directories are cleaned of all files created during the testing.

Finally, the command "*make verify*" should be issued to generate meshes with different versions of Cubit, convert the meshes from EXODUS II to *ascii*, and test the meshes in PROTEUS-SN. This step can be skipped if no versions of Cubit are installed locally.

The command "make clean" removes the object file, executables, and any old verification test files.

### 2.3 Execution Syntax

After successfully building and testing, the program can be used to convert any EXODUS II mesh to the PROTEUS-SN *ascii* file format. Simply type the name of the program followed by the paths to as many inputs as needed as in Figure 6.

\$> ExodusConverter.x MyMesh.exo ThisMesh.e /path/to/ThatMesh.e

#### Figure 6. Example usage of converter with multiple input files.

The input files must have the correct EXODUS II file extension (".e" or ".exo") for proper conversion. Note that if paths to the input files are specified such as */path/to/my/Exodusmesh.e*, the resulting ascii file will be produced in the same directory, */path/to/my/Exodusmesh.ascii*.

#### 2.4 Limitations

The converter supports Cubit element types which are also supported by PROTEUS. Therefore, some element types available within Cubit are not valid element types for the converter and PROTEUS. When generating a mesh with Cubit, use only the following element types: BAR, BAR2, BAR3, TRI, TRI3, TRI6, QUAD, QUAD4, QUAD8, QUAD9, TETRA, TETRA4, TETRA10, HEX, HEX8, HEX10. In particular, ensure that the EXODUS II mesh does not contain SHELL or TRISHELL element types which are not supported by PROTEUS-SN or the converter. SHELL or TRISHELL element types are typically assigned by default if the user fails to specify an element type – thus the user should carefully check that they have assigned all element blocks properly.

## 3. Conversion Methodology

This chapter contains a description of the code methodology and is intended for an advanced user who wishes to modify the converter or understand exactly how the conversion is performed. We focus on describing EXODUS II finite element files created by Cubit 12+. EXODUS II files created by other software may have slightly different formats.

## 3.1 EXODUS II Overview

The EXODUS II file type is binary, portable, and cannot be read in a standard text editor. To read the contents of an EXODUS II file, the NetCDF utility "ncdump" can be used to dump the content to plain text. Each EXODUS II mesh file contains three important data sections: "dimensions", "variables", and "data".

### 3.1.1 Dimensions Section

The "dimensions" section of an EXODUS II file defines values for the following "dimension" variables. These dimensions are used to declare arrays appearing later in the file.

EXODUS II Dimension	Definition
len_string	Max length of a string
num_dim	Number of dimensions in the mesh 1, 2, 3
num_nodes	Total number of nodes (vertices) in the mesh
num_elem	Total number of elements in the mesh
num_el_blk	Total number of element blocks in the mesh
<pre>num_side_sets</pre>	Total number of sidesets in the mesh
num_side_ss1	Number of elements that have a surface belonging to sideset 1 (etc.)
num_el_in_blk1	Number of elements in block 1 (etc.)
num_nod_per_el1	Number of nodes per element in block 1 (etc.)

Table 2.	EXODUS	Π	dimensions	given	in	mesh	file.
I able 2	LICDUD	**	unitensions	SITCH		meon	me.

### 3.1.2 Variables Section

The "variables" section of an EXODUS II file contains the *declaration* of data arrays including their dimensions and their "attributes". Note the dimensions of each of the variables were defined in the "dimensions" section. The only data contained in this section is the element type of each block, and it is given as an attribute of the connectivity array for each block.

EXODUS II Variable	Definition
<pre>char coor_names(num_dim, len_string)</pre>	character array holding the names of the dimensions
<pre>int ss_prop1(num_side_sets)     ss_prop1:name = "ID"</pre>	Integer array holding the "prop1" attribute for all the sidesets. "prop1" in this case is defined as the "ID", so the array ss_prop1 holds the "ID" for each sideset.
<pre>int elem_ss1(num_side_ss1)</pre>	Integer array defining the elements which have a surface in sideset 1 (etc.)
<pre>int side_ss1(num_side_ss1)</pre>	Integer array defining the reference surface on each element belong to sideset 1 (etc.)
<pre>int eb_prop1(num_el_blk)     eb_prop1:name = "ID"</pre>	Integer holding the "prop1" attribute for the element blocks. "prop1" in this case is defined as "ID", so the array eb_prop1 holds the "ID" for each element block.
<pre>int connect1(num_el_in_blk1, num_nod_per_el1)</pre>	Integer array holding the connectivity for element block 1 (etc.). The element block has the attribute "elem_type" which in this example is "QUAD8".
[Cubit 12 and earlier convention] double coord(num_dim, num_nodes)	Real array holding the coordinates of the vertices, in order of all X, all Y, and all Z.
<pre>[Cubit 13+ convention] double coordx(num_nodes) double coordy(num_nodes) (2D/3D only) double coordz(num_nodes) (3D only)</pre>	Real arrays holding the X, Y, and Z coordinates of the vertices, if applicable.

Table 3.	EXODUS	Π	variables	declared	in	file.

Cubit 13 introduced a new convention to the EXODUS II file which includes different ordering of variables in the files, different variable names. Files written by Cubit 12 lump the vertex coordinates together into one large variable named "coord". Files written by Cubit 13 separate the vertex coordinates into different coordinate variables depending on the number of dimensions present in the mesh: "coordx", "coordy", and "coordz". The converter tool internally checks how many coordinate variables are present in the file so that the coordinates are handled correctly.

#### 3.1.3 Data Section

The "data" section contains the values of the arrays declared in the "variables" section of the file. The naming convention is identical to that in Table 3.

## 3.2 Conversion Process

The following pseudo-code describes the conversion process. The procedure is further described in the following sections.

## Check input arguments

-Makes sure the file exist and have proper extension (.e, .exo) -Creates the output and report files

#### **Open EXODUS II file as a NetCDF data library**

- 'nc\_open' command opens an existing EXODUS II file

#### **Retrieve general information about the mesh**

-'nc\_inq' with no data section attached returns the length of each section

#### **Retrieve dimensions**

-'nc\_inq\_dimid' returns the ID of a dimension listing

-'nc\_inq\_dimname' is used to make sure the proper variable is being queried

-'nc\_ing\_dimlen' returns the value stored at a known ID

#### **Retrieve Variable IDs**

-Based on the dimensional values retrieved, the converter loops through variables

-Finds all needed variable ID's that will be used to retrieve data

-'nc\_inq-varid' gives the variable ID

-'nc\_inq\_varname' is used to check that the proper variable is being queried

#### Write Coordinates

-In order to save memory, the coordinate array is written to the output file

-'nc\_get\_var1\_double' is used to pull out one data pt. of type 'double'

-Uses Variable IDs and dimension values to pull out individual data points

-Data is stored in arrays with lengths found in the dimension section

-'nc\_get\_var1\_int' is used to pull out one data pt. of type 'int'

#### Write Other Info to Output

-Once all data points have been retrieved and tested for boundary conditions the points are accessed once again in order to write them to the output

#### **Remap Connectivity**

-While only necessary for some element types, a remapping function is called. This second function changes the order that the nodes of each element are written to the output file.

#### **Boundary Information**

-Since the individual data pts. already have been checked for boundary conditions the number of bounds is already known along with all required information.

#### Figure 7. Description of the conversion process

## 3.2.1 Command Line Input and Output File Creation

The converter reads the command line argument(s) to check that valid EXODUS II inputs exist and have the correct file extension (.e or .exo). It also creates the file handles for the final *ascii* mesh and the report summary. The name of both of these documents is based on the EXODUS II input file prefix. Given any input file name, the converter names the output files by reading the character string of the input name, removing the EXODUS II file extension, and replacing it with ".ascii" or "\_REPORT.txt". The

converter can process files outside of the current working directory, but output files are created in the same directory as the input file, not the current working directory.

#### 3.2.2 Reading the Dimensions

The converter opens the EXODUS II file as a NetCDF data library using the nc\_open command. The converter uses NetCDF commands (see **Error! Reference source not found.**) to parse through the dimension section and retrieve the information needed to initialize array and set loop variables later on for the variable section. The key information queried here is the number of dimensions, number of element blocks in the mesh, total number of nodes, number of sidesets, number of elements held in each block, and the number of nodes per element in each block. These values are written to the *ascii* file.

### 3.2.3 Reading the Variables

Using the dimensions retrieved from the dimension section, the converter sets loops to collect the IDs of each block, sideset, and connectivity variable. An ID is essentially an "address" in the file. In order to ensure the correct variable is read, a variable name check is implemented in each major variable retrieval loop.

### 3.2.4 Writing Coordinates and Basic Block Information

At this point, the location and size of important data has been determined. The converter begins process the vertex array point by point rather than as a whole. This point-by-point method takes more time than processing everything at once, but removes any size limitations on the input file. At this stage the vertex coordinates are all written to the output file.

Next, the basic block information is written to the output file: the number of elements in the block, number of boundary elements in the block, number of nodes per element in the block and the equation and interpolation orders of the elements. Each EXODUS II element type is then mapped to a PROTEUS-SN element type, and the PROTEUS-SN element type is written to file along with the block Region ID and the connectivity array.

### 3.2.5 Connectivity Remapping

The connectivity of each element given in the EXODUS II file format is based on EXODUS II element type ordering [1], shown in Figure 8. However, each EXODUS II element type must be mapped via the converter to a PROTEUS-SN element type as shown in Table 4. For element types with different vertex ordering, the connectivity array is changed in order to follow the PROTEUS-SN convention.

Note that CIRCLE, SPHERE and SHELL(3D) EXODUS II element types are not supported as they are not realistic for neutronics simulations. WEDGE may be added in the future although it is not currently supported. Appendix B contains figures that define the element types and node ordering supported by PROTEUS.

## 3.2.6 Boundary Information

During the data retrieval stage, each element was tested to see if it contained a boundary surface. These elements are then written out to the output file followed by the array of sideset IDs to which each element belongs. Finally, the converter prints a list sideset IDs corresponding to the boundary elements, as well as the element number within the block and the reference surface number containing the boundary surface.



Node Ordering for Standard Element Types

Figure 8. EXODUS II element types and node ordering, courtesy Ref [1].

Table 4. Listing of supported Cubit/EXODUS II element types and node remapping to PROTEUS element type.

Cubit EXOD Element Elen Type Ty	US II ent Oe EXODUS II to Ascii Node Remapping (Order of EXODUS II Nodes listed in Ascii format)	PROTEUS Element Type	Element Order
---------------------------------------	--	-------------------------	------------------

Cubit Element Type	EXODUS II Element Type	EXODUS II to Ascii Node Remapping (Order of EXODUS II Nodes listed in Ascii format)	PROTEUS Element Type	Element Order
BAR	TRUSS/BEAM	No remapping	BAR	1
BAR2	TRUSS/BEAM	No remapping	LAGRANGE BAR	1
BAR3	TRUSS/BEAM	[1,3,2]	LAGRANGE BAR	2
TRI / TRI3	TRIANGLE	No remapping	LAGRANGE TRI* (or TRIANGLE)	1
TRI6	TRIANGLE	[1,4,2,6,5,3]	LAGRANGE TRI	2
QUAD	QUAD	[1,2,4,3]	LAGRANGE QUAD	1
QUAD4	QUAD	[1,2,4,3]	LAGRANGE QUAD	1
QUAD8	QUAD	[1,5,2,6,3,7,4,8]	QUADRILATERAL	2
QUAD9	QUAD	[1,5,2,8,9,6,4,7,3]	LAGRANGE QUAD	2
TETRA / TETRA4	TETRA	No remapping	TETRAHEDRON* (or LAGRANGE TET)	1
TETRA10	TETRA	[1,5,2,6,3,7,8,9,10,4]	TETRAHEDRON	2
HEX	HEX	[1,2,4,3,5,6,8,7]	LAGRANGE BRICK* (or BRICK)	1
HEX8	HEX	No remapping	BRICK* (or LAGRANGE BRICK)	1
HEX20	HEX	[1,9,2,10,3,11,4,12,13,14,15, 16,5,17,6,18,7,19,8,20]	BRICK	2

\*An asterisk indicates that the PROTEUS-SN serendipity and Lagrange linear elements are equivalent for this case (identical node ordering).

## 3.3 Output File Descriptions

### 3.3.1 ASCII File Format

The file format for the *ascii* file is located in Appendix A. The *ascii* file contains the data found in the EXODUS II file only reordered and reformatted. This new format consists of three sections –

information regarding the mesh as a whole, the entire coordinate table listing, and the individual block data.

The general mesh information is always located on the first line and states the total number of vertices in the mesh, the number of dimension, the total number of blocks that are present in the mesh, and lastly an unused integer set to zero for later use.

The second section is a list of all coordinates in the mesh ordered by dimension with all X dimension coordinates being listed first, then the Y's, and lastly the Z's. Only the coordinates listed in the EXODUS II file are printed to the ascii file, for example, in 2D, X and Y vertices only are printed.

The final section holds information regarding each element block. The first line for each block holds the number of elements in the block, the number of boundary conditions, and how many nodes are attached to each element, an unused integer, the order of interpolation, and the equation order. Following this line is a listing of the element type of the entire block and the region name. The connectivity arrays that hold the node ordering are then listed. The connectivity of a given element type may or may not be reordered from the EXODUS II depending on the element type and interpolation order found during the conversion process. The final pieces of information for this section are the sidesets that correspond to the boundary elements found in the side sets, the boundary elements (numbered by element number within the specific element block ), and lastly the boundary surface associated with each boundary element.

#### 3.3.2 Report File

For each conversion performed, a report file is written to show the success or failure of each step in the conversion process. While it is easy to read the error immediately from the command line, the report allows for review later on if needed.

CONVERSION REPORT
EXODUSII FILE OPENED
INPUT DATA
Number of Dimensional Variables: 14
Number of Variables: 13
Number of Dimensions in Mesh: 2
Number of Blocks in Mesh: 1
Number of Elements in Mesh: 4
Number of Nodes in Mesh: 25
Beginning Data Scavenging
Found All Block Element Types
BLOCK: 1 REGION: 1: QUAD9
Retrieving Coordinates
Successfully Retrieved Coordinates
Setting Block Orders
All Blocks Successfully Mapped
Writing to Output
Writing Connectivity for Block: 1
Conversion Successful
End

#### Figure 9. Example of a successful report file.

As shown in Figure 9, the report file echoes the key mesh information as well as each successful step performed in the conversion process. If the conversion process ends early due to an error, the report file can be referenced to see the step where the conversion failed. If an error results from trying to convert an unsupported element type, an incomplete listing of variables in the file, or an error in the node mapping, a clear error message is written in the report file that lists the error encountered and any other information that can help identify the problem. For example, if there is an unknown element type listed in the mesh, then the report announces that there was an unknown element type on a specific block.

## 4. Benchmark Problems

A series of benchmark tests are provided to make sure that the converter is installed correctly and that the produced *ascii* meshes are fully compatible with PROTEUS-SN. These tests are separated into two subdirectories under the "verification" directory.

The first directory, "verification/benchmarks" contains several reference EXODUS II and ascii meshes to test whether the source code is working as intended. Invoking the command "make check" runs a script to converts the benchmark meshes and compares the results to reliable reference files. A shell script checks the outputs against the reference files for size and content and writes any differences to the standard output. A description of the benchmark test meshes is given in Table 5. The tests are intended to cover meshes containing various element types, sizes, and also test different Cubit versions.

Bench #	File Extension	Cubit Version	# of Nodes	# of Element Blocks	Element Type(s)
00	.e	12	1198	4	QUAD8
01	.e	12	1080	3	TRI3 & QUAD4
02	.e	13	231600	38	TRI3 & QUAD4
03	.e	12	535279	70	HEX
04	.e	13	13198	12	TRI3 & QUAD4
05	.e	13	25	1	QUAD9
06	.e	13	81	1	HEX20
07	.e	13	141	1	TRI6
08	.e	13	158	1	TETRA10
09	.exo	12	115494	8	HEX

 Table 5. Benchmark test descriptions "verification/benchmarks" directory.

The second test folder, "verification/PROTEUS\_Benchmarks", is an optional, extended test-suite to test the compatibility of converter with various versions of Cubit as well as PROTEUS. A series of scripts are invoked that (1) create various EXODUS II meshes with Cubit, (2) convert each mesh to *ascii*, and (3) test the mesh with PROTEUS-SN. These tests are invoked by the command "*make verify*". Remember that to be able to run these tests the variables CUBIT\_12X, CUBIT\_13X and PROTEUS\_X must be correctly defined in the Makefile prior to typing the command.

CUBIT Journal File Name	Elements tested
generate_TRI.jou	TRI
	TRI3
	TRI6
generate_TETRA.jou	TETRA
	TETRA4
	TETRA10
generate_QUAD.jou	QUAD
	QUAD4
	QUAD8
	QUAD9
generate_HEX.jou	HEX
	HEX8
	HEX20

 Table 6. List of Cubit journal files and the elements types to be generated on-the-fly for testing converter compatibility with Cubit and PROTEUS. Each journal file leads to the creation of multiple files used in testing the converter.

## 5. Summary

A new EXODUS II finite element mesh converter has been developed to convert EXODUS II meshes (typically created by Cubit) to PROTEUS-SN *ascii* mesh format. The conversion program replaces an old converter which had limitations on mesh size and compatibility issues with Cubit. The new program works with different versions of Cubit (any version 12+) and has no limitation on EXODUS II file size. Error checking, error reporting and usage syntax have also been greatly improved. The converter is limited to element types supported by PROTEUS-SN (a subset of those produced by Cubit).

For questions, assistance, or to obtain the converter, please contact <u>nera-software@anl.gov</u>.

## 6. References

- 1. Schoof, Larry A. and Yarberry, Victor R., "EXODUS II: A Finite Element Data Model" Sandia National Laboratories, Computational Mechanics and Visualization Department, November, 1995.
- 2. Shemon, E. R., M. A. Smith, C.H. Lee, and A. Marin-Lafleche, "PROTEUS-SN User Manual", ANL/NE-14/6, Argonne National Laboratory, June 30, 2014.
- 3. Russ Rew, Glenn Davis, Steve Emmerson, Harvey Davies, Ed Hartnett, Dennis Heimbigner and Ward Fisher, "NetCDF Documentation" UCAR & UCP, Unidata, 2008.
- 4. Ted Blacker, Randy Morris, "Cubit 13.1 User Documentation", Sandia National Laboratories, Albuquerque, NM, 2012.

#### **APPENDIX A**

```
Figure A1. PROTEUS-SN ascii file format.
```

```
_____
01 BASIC MESH INFO
02 VERTEX POSITION DATA
03 BLOCK DATA
SECTION 01: BASIC MESH INFO
_____
LINE NUMBER: 1
FORMAT(4110): <NumVertices> <NumDimensions> <NumBlocks> <unused integer>
DESCRIPTION:
                : (I10)...Number of nodes (vertices) in the mesh
<NumVertices>
<NumDimensions> : (I10)...Number of dimension (1,2,3)
<NumBlocks> : (I10)...Number of blocks (block=group of elements with common type and
material)
<unused integer> : (I10)...0
_____
SECTION TYPE 02: VERTEX POSITION DATA
_____
LINE NUMBERS: 2+, number of lines = ceil{NumVertices*NumDimensions/8}
FORMAT(8(1PE15.8)): <X Vert Array> <Y Vert Array> <Z Vert Array>
                      -These arrays will break over multiple lines in groups of 8.
DESCRIPTION:
<X Vert Array> : Reals.... X value of each vertex in the mesh
<Y Vert Array> : Reals.... Y value of each vertex in the mesh
                     -(present only for 2D and 3D problems)
<Z Vert Array> : Reals.... Z value of each vertez in the mesh
                  -(present only for 3D problems)
_____
SECTION TYPE 03: BLOCK DATA
_____
LINE NUMBERS: immediately following last SECTION type 02 data
DESCRIPTION:
*** The following lines are repeated for each block in NumBlocks:***
SECTION SUBTYPE 3A, FORMAT( 6110): <NumElementsInBlock> <NumBoundarySurfacesInBlock>
<NodesPerElement> <unused integer> <Order Interp> <Order Equat>
SECTION SUBTYPE 3B, FORMAT( 2A16): <ElementType> <RegionName>
SECTION SUBTYPE 3C, FORMAT(12I10): { <ConnectivityArray> }; repeat for each element in block
SECTION SUBTYPE 3D, FORMAT( 7A16): { <SurfaceBCTag> }; repeat for each surface element in block
SECTION SUBTYPE 3E, FORMAT(12I10): { <ElementNumber> <ReferenceSurface> } repeat for each
boundary surface in block
<NumElementsInBlock> : Integer....Number of elements in this block
<NumBoundarySurfInBlock> : Integer....Number of boundary surfaces in this block
<NodesPerElement> : Integer....Number of boundary suffaces in this break
<unused integer> : Integer....Number of nodes on an element
<unused integer> : 0 (reserved for future use)
<Order_Interp> : Integer....Order of the spatial interpolation for elements in this

                                    block
<Order_Equat> : Integer...Order of the spatial equations
<ElementType> : Character... The element type for all elements in a block
<RegionName> : Character... The assigned region name for the current
                                     block of elements, ex. REGION 00000001
<ConnectivityArray> : CONNECTIVITY(J),J=1,NodesPerElement lists the global indices of
                         nodes on the element.
: Integer.... Reference element surface number corresponding to this
                                     boundary surface
_____
END OF FILE FORMAT DESCRIPTION
```

## **APPENDIX B**

The following figures depict the various element types supported by PROTEUS-SN, including their node ordering. Cyan color indicates the reference surface numbering for each element.



Figure B.1. PROTEUS 1-D Finite Element Vertex Layout.



Figure B.2. PROTEUS 2-D Triangular Serendipity Finite Element Vertex Layout.



Figure B.3. PROTEUS 2-D Triangular LaGrange Finite Element Vertex Layout.



Figure B.4. PROTEUS 2-D Quadrilateral Serendipity Finite Element Vertex Layout.



Figure B.5. PROTEUS 2-D Quadrilateral LaGrange Finite Element Vertex Layout.



Figure B.6. PROTEUS 3-D Tetrahedral Serendipity Finite Element Vertex Layout.



Figure B.7. PROTEUS 3-D Tetrahedral LaGrange Finite Element Vertex Layout.



Figure B.9. PROTEUS 3-D Wedge (Prism) LaGrange Finite Element Vertex Layout.



Figure B.10. PROTEUS 3-D Hexahedral Serendipity Finite Element Vertex Layout.



PROTEUS 3-D Hexahedral LaGrange Finite Element Vertex Layout.



# **Nuclear Engineering Division**

Argonne National Laboratory 9700 South Cass Avenue, Bldg. 208 Argonne, IL 60439-4842

www.anl.gov



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