

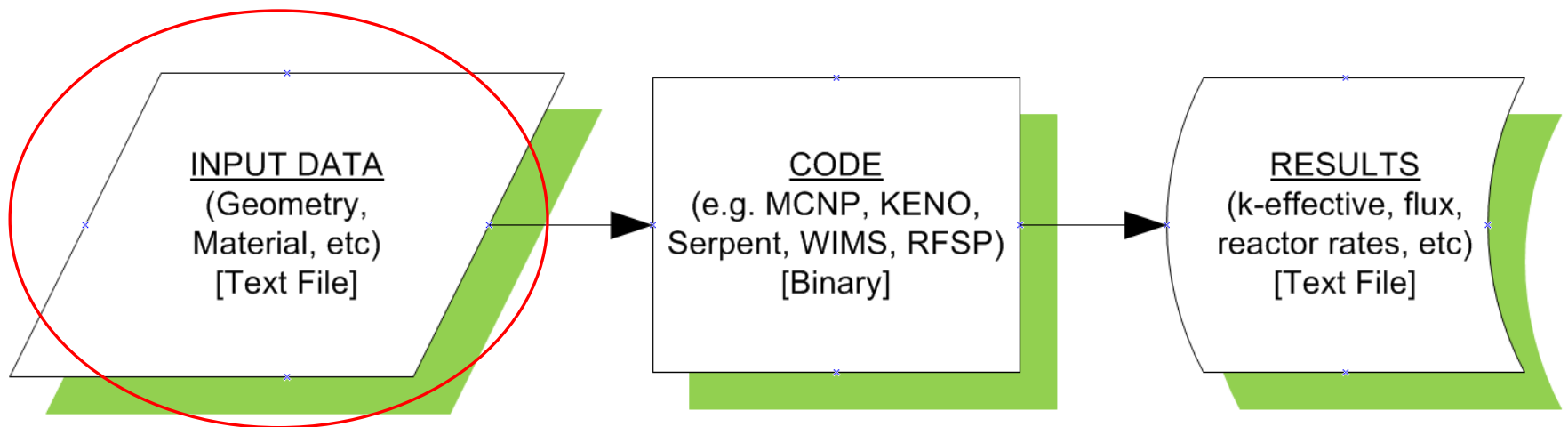
# **Modeling the ZED-2 Reactor w/ Serpent/MCNP/KENO**

**The 4th Annual Serpent Users' Group Meeting,  
17–19 September 2014  
Jesus College, Cambridge, UK**

J. C. Chow



# We are stuck!



# Survey

- How do you author input data files for simulations?
  1. Use a text editor.
  2. Use scripting languages such as Python, Perl, etc.

# Motivation

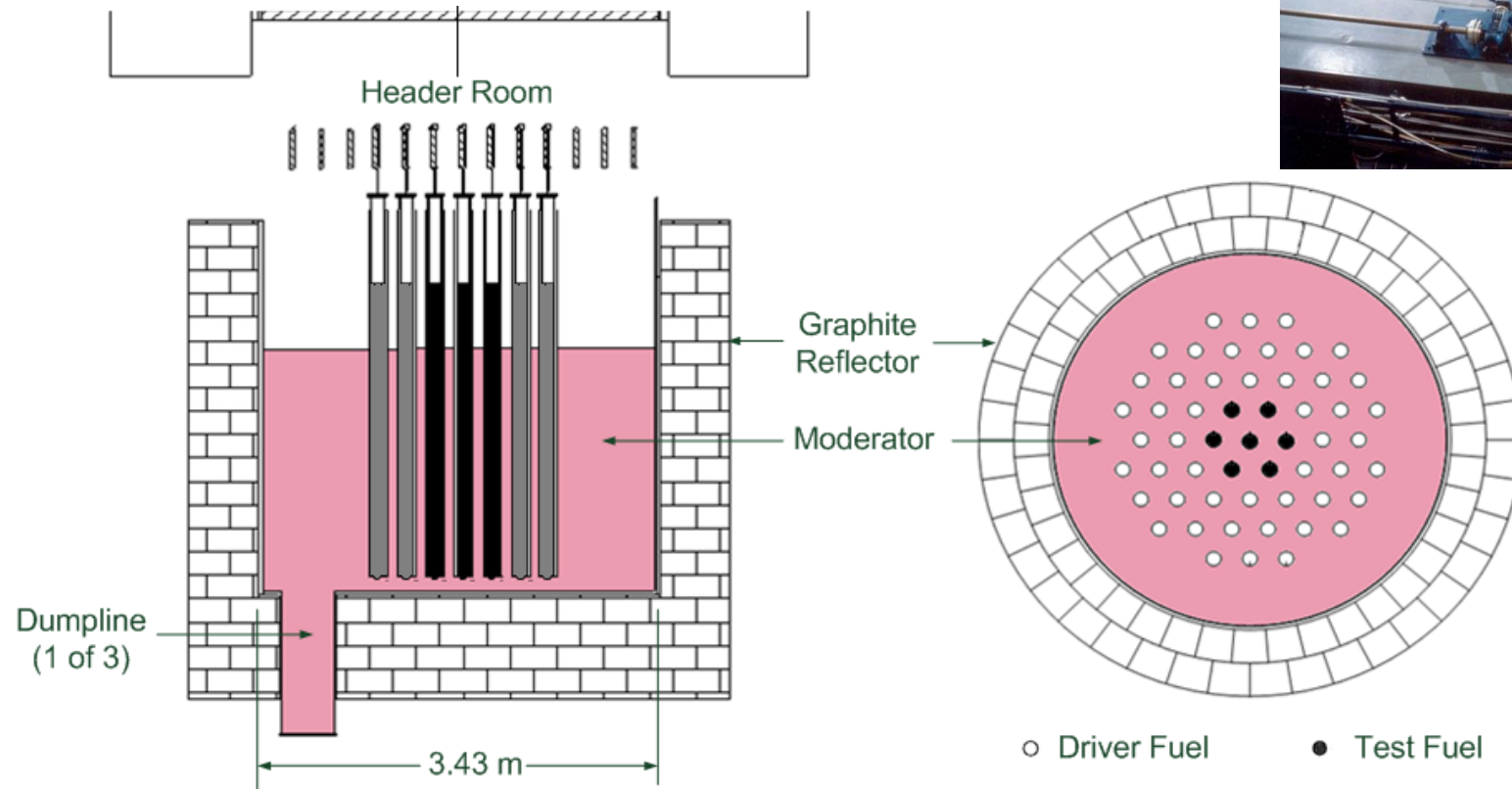
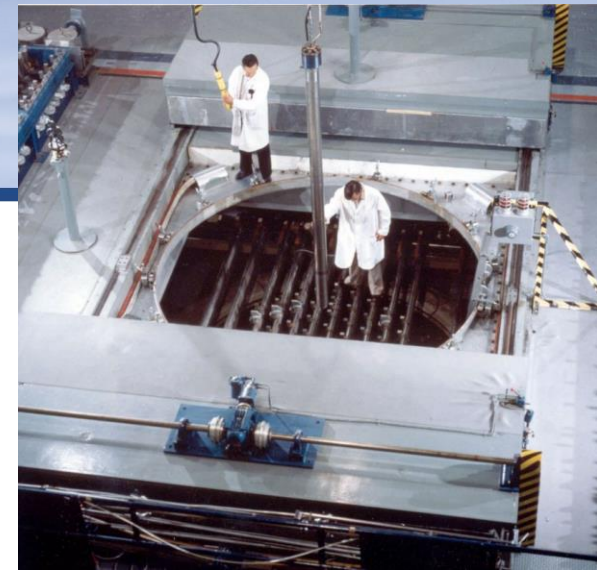
- Assignment: Validation of MCNP against ZED-2 data
- Requirement: Generate KENO models equivalent to existing ZED-2 MCNP models for analyses with TSUNAMI
- Task: use a text editor (and a pair of aging eyeballs) to author/edit ZED-2 models (thousands of lines / model)
- How can I guarantee consistency between MCNP and KENO models?
- Solve the problem programmatically... develop applications that share the same data source.

# Conventional Approaches for Preparing Input Data

1. Direct typing using generic text editors: Notepad, Wordpad, Notepad++, vi, GEdit, Emacs, XEdit, ...
  2. Copy/paste pieces of data from existing models (text files) and spreadsheets.
  3. Modify existing models to obtain different configurations: (change in physical properties and/or geometry).
  4. Use extensive Excel® macros and/or other languages (e.g., Perl, Python, Fortran) to generate models.
- ❑ Using text editors (1-3) is always error-prone.
  - ❑ Using Excel® macros and/or other languages, etc, are preferable, but:
    - often tailored for personalized use
    - implemented in piecemeal fashions
    - little/no documentations
    - difficult to share with other colleagues.
  - ❑ Substantial effort is required for verification.

# The ZED-2 Reactor

Picture taken in the '60s



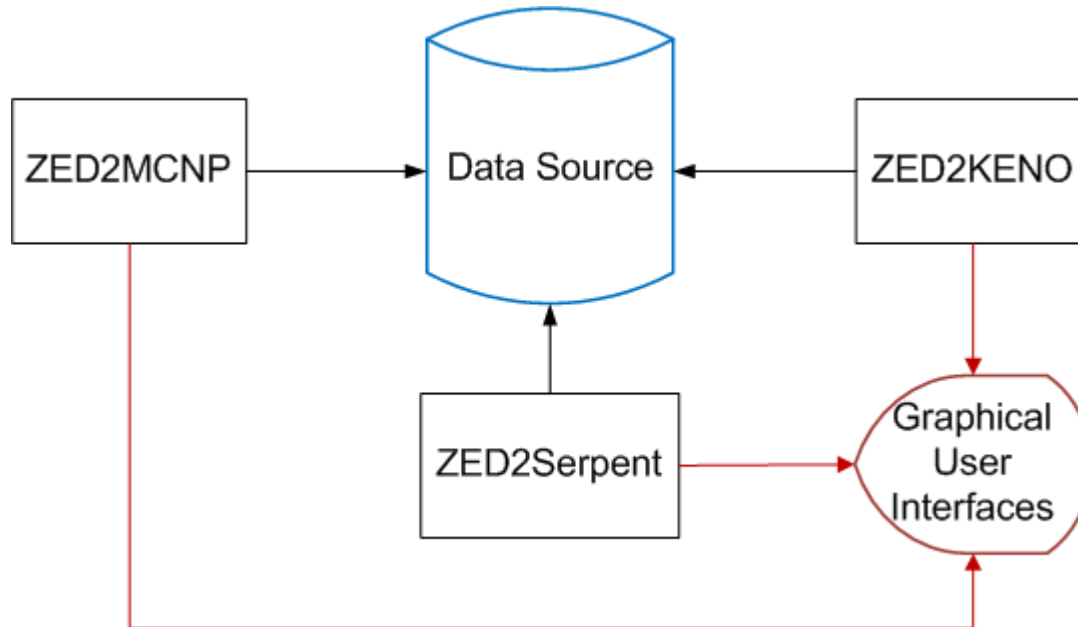


# A Typical ZED-2 MCNP Input File

- ~500 surfaces
- ~1,000 cells
- ~60 materials
- ~70 universes
- ~4,000 lines
- In order to modify the model for a specific configuration, we need to edit a few 10s to 100s lines of data.
- Many (personalized) tools have been developed, mostly in EXCEL, e.g., to define the heavy water composition or to convert material cards from ENDF-VI to VII.
- Ctrl+C ( from EXCEL) and Ctrl+V (to Notepad/Wordpad).



# ZED-2 Model Generators Development (1)

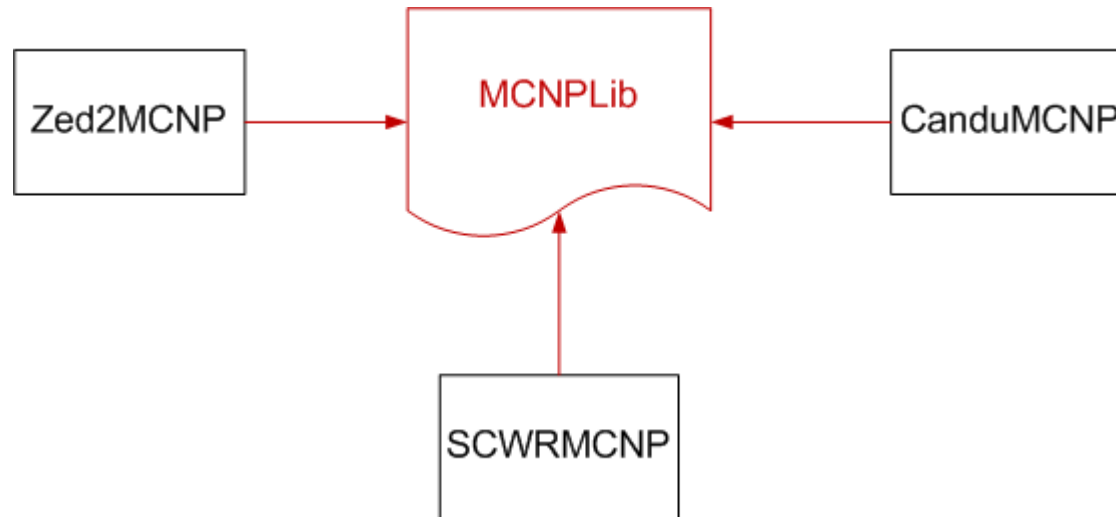


1. [Zed2MCNP](#) (2009) J.C. Chow
2. [Zed2KENO](#) (2009) J.C. Chow
3. [Zed2Serpent](#) (2013) G. Aversano (UOIT)

They all share the same Data Source and GUI's.



## ZED-2 Model Generators Development (2)



- Three applications for generating MCNP models for three physical systems: ZED-2, CANDU, and SCWR
- They all share the same MCNP class library (MCNPLib)
- Do we need a similar class library for Serpent?

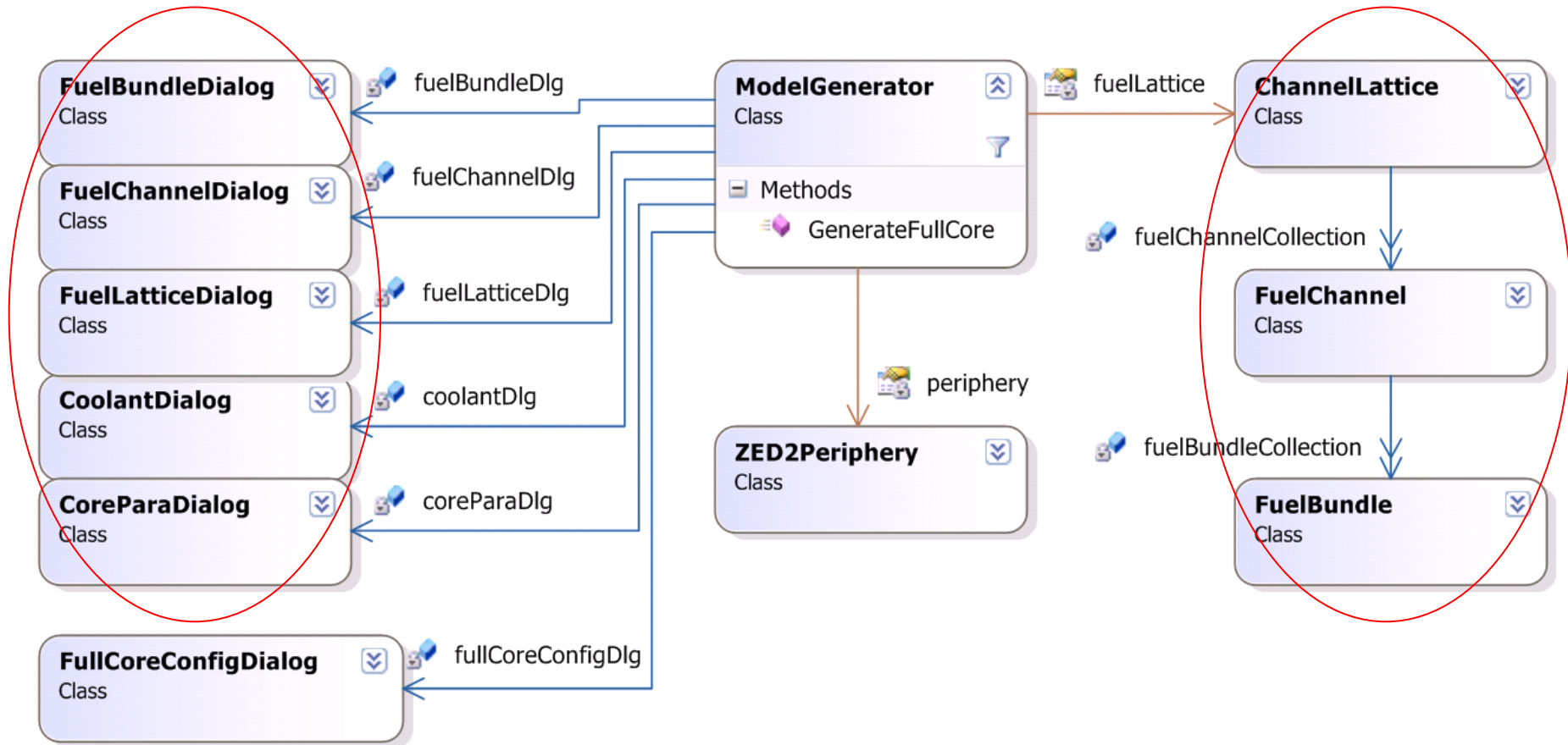
# About the ZED2- MCNP/KENO/Serpent Applications

- Written in C# 3.0 (syntactically very similar to C++)
- Integrated Development Environment (IDE) Visual Studio 2008 IDE (Microsoft).
- Takes advantage of the rich Windows GUI features provided by .Net (dot-net) Framework Library 3.5 (Microsoft).
- Truly object-oriented (OOP) implementation.
- Requires a static set of input files (prerequisites):
  - Shifting the focus of managing a single (huge) data file to a set of files, each of which serves a specific purpose.
  - Analogous to the OOP; *a problem is decomposed into a number of objects (methods and data are built around the objects to solve the problem).*
- Once the set of files is ready, a full-core model can be generated with a few clicks of the mouse.

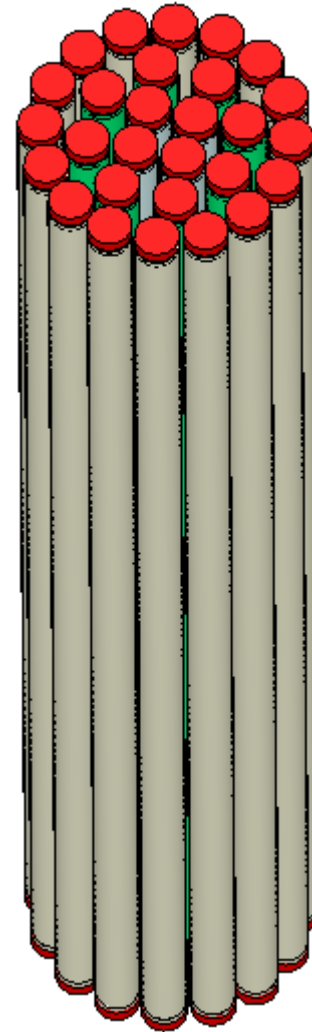
# Model Prerequisites

1. Fuel Bundles: 28-el NU, 37-el MOX, CANFLEX-LEU...
  2. Fuel Channels: fuel bundles contained in pressure/calandria tube
  3. Coolants: D<sub>2</sub>O, H<sub>2</sub>O, Air, CO<sub>2</sub>...
  4. Fuel Lattice: fuel channels contained in core configuration (square or hexagonal)
  5. Core Parameters: critical height, moderator purity, lattice pitch, etc
- ❑ Each prerequisite is associated with a GUI (Graphical User Interface)
  - ❑ Data entered for each prerequisite are saved in an XML file.
  - ❑ All the (interdependent) prerequisites for a particular experimental run are assembled into a single configuration.

# UML Class Diagram of a Model Generator



# Fuel Bundle Geometry



Model

# Fuel Bundle Configuration

Verify Parameter VALUES

Bundle Name: **nu-28-BM** Length: **49.67**

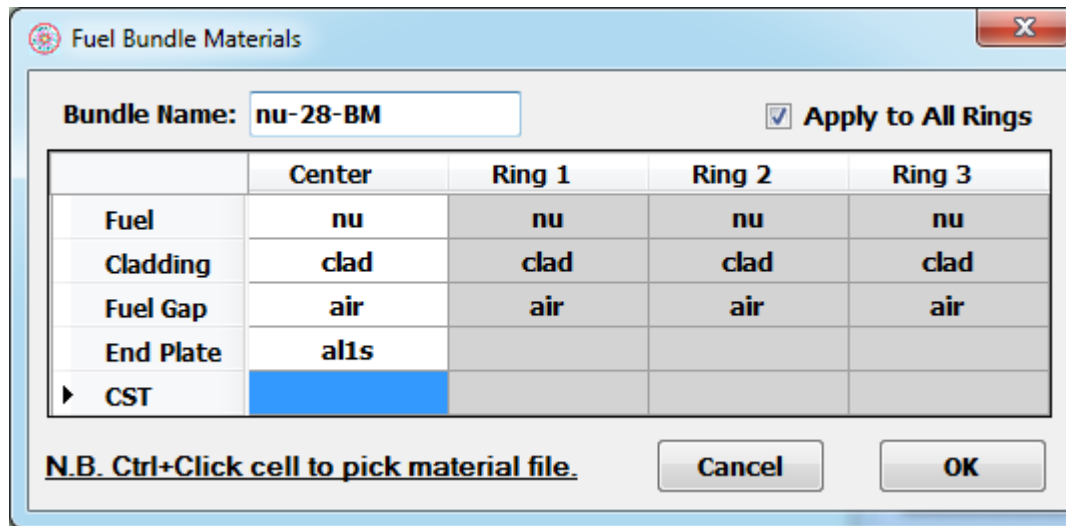
Description: **28-element bundle with NU fuel in Zr-2 sheath (BM)**

Dimensions in cm. Total Pin Counts:  ☐ Apply to All Rings

	Center	Ring 1	Ring 2	Ring 3
▶ Fuel Radius	0	0.7105	0.7105	0.7105
Fuel Stack Length	0	47.73	47.73	47.73
Clad IR	0	0.7155	0.7155	0.7155
Clad OR	0	0.7609	0.7609	0.7609
Top Plenum	0	0.2084	0.2084	0.2084
Bottom Plenum	0	0	0	0
Top Cap	0	0.1694	0.1694	0.1694
Bottom Cap	0	0.1952	0.1952	0.1952
Endplate Thickness	0	0.4432	0.4432	0.4432
Half Coolant Thickness	0	0.2403	0.2403	0.2403
Pin Count	0	4	8	16
Encompassing Zone #	0	0	0	1
Pitch Circle Radius	0	1.163	2.652	4.206
First Pin Offset (deg)	0	45	22.5	11.25

Materials Misc. Verify Save Clear Exit

# Fuel Bundle Material

A screenshot of a software dialog box titled "Fuel Bundle Materials". It features a "Bundle Name" field with the text "nu-28-BM" and a checked checkbox labeled "Apply to All Rings". Below these is a table with five columns: "Center", "Ring 1", "Ring 2", and "Ring 3". The rows represent different components: "Fuel", "Cladding", "Fuel Gap", "End Plate", and "CST". The "CST" row is currently selected, highlighted in blue. At the bottom of the dialog, there is a note: "N.B. Ctrl+Click cell to pick material file.", and two buttons labeled "Cancel" and "OK".

**Fuel Bundle Materials**

Bundle Name:  ☒ Apply to All Rings

	Center	Ring 1	Ring 2	Ring 3
Fuel	nu	nu	nu	nu
Cladding	clad	clad	clad	clad
Fuel Gap	air	air	air	air
End Plate	al1s			
▶ CST				

N.B. Ctrl+Click cell to pick material file.

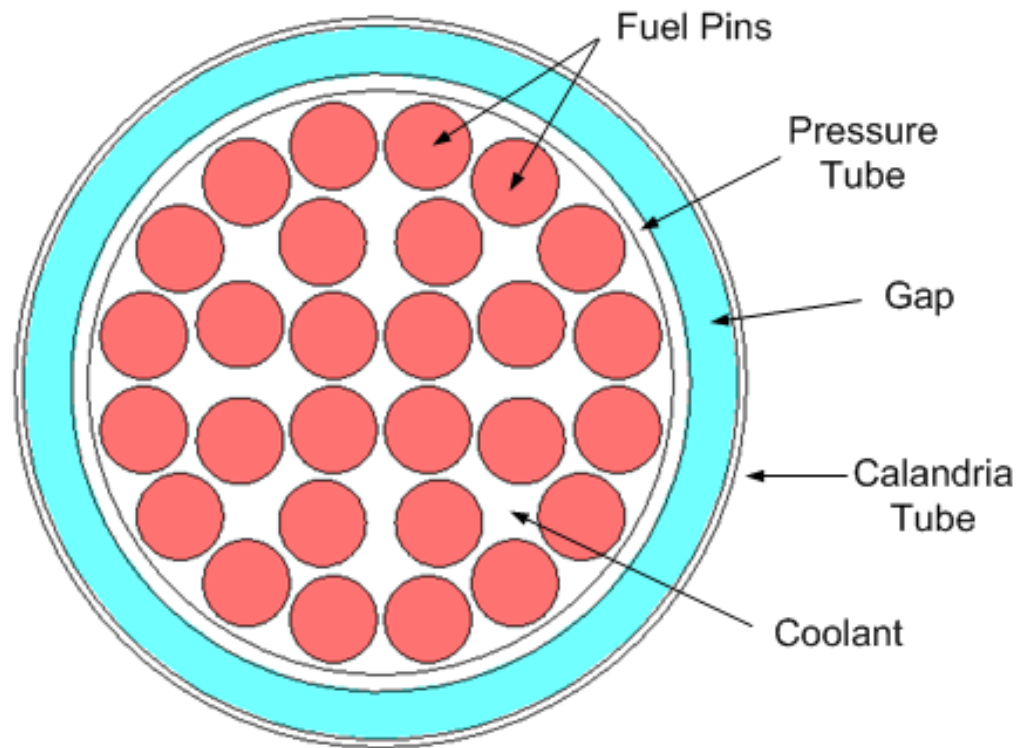
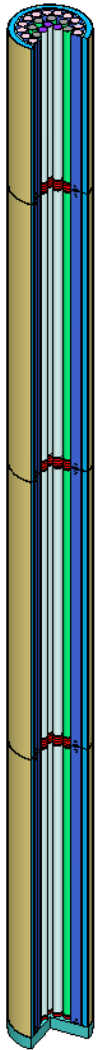
Cancel OK



# Bundle Data Saved as XML

```
<?xml version="1.0" encoding="UTF-8"?>
<BundleParameter Description="28-element bundle with NU fuel in Zr-2 sheath (BM)">
  <BundleName>nu-28-BM</BundleName>
    <!--Logical length that defines a bundle-->
  <bundleLength>49.67</bundleLength>
  <fuel>
    <fuelRadius>0, 0.7105, 0.7105, 0.7105</fuelRadius>
    <fuelStackLength>0, 47.73, 47.73, 47.73</fuelStackLength>
    <material>nu, nu, nu, nu</material>
  </fuel>
  <clad>
    <cladIR>0, 0.7155, 0.7155, 0.7155</cladIR>
    <cladOR>0, 0.7609, 0.7609, 0.7609</cladOR>
    <!--endcap thicknesses-->
    <topCap>0, 0.1694, 0.1694, 0.1694</topCap>
    <bottomCap>0, 0.1952, 0.1952, 0.1952</bottomCap>
    <material>clad, clad, clad, clad</material>
  </clad>
  <plenum>
    <!--void gap between fuel and endcap-->
    <topPlenum>0, 0.2084, 0.2084, 0.2084</topPlenum>
    <bottomPlenum>0, 0, 0, 0</bottomPlenum>
    <material>air, air, air, air</material>
  </plenum>
</endplate>
```

# Fuel Channel



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# Fuel Channel Configuration

ZED-2 Fuel Channel Configuration

**Fuel Bundles:**

- 37-element-NU
- Blank
- NPD-7
- nu-28-BM
- nu-37-production
- nu\_37
- um-19
- zeeprod
- zeeprodImpure

**Fuel Channel:** BM-plugged

**Description:** 5 x nu-28 bundles in Al-1S channel w/ plug [BM

	Bundle Type	Elevation
▶ Bundle 6		262.4713
Bundle 5	nu-28-BM	212.8013
Bundle 4	nu-28-BM	163.1313
Bundle 3	nu-28-BM	113.4613
Bundle 2	nu-28-BM	63.7913
Bundle 1	nu-28-BM	14.1213

N.B. Bundle #1 is at the bottom (Dimensions in cm)

	IR	OR	Material
▶ PT	5.0965	5.3925	pt
CT	6.230	6.369	ct
Gap			air

N.B. Ctrl+Click cell to pick material. Cell Width [cm]:

**Top:** generic-pt-ct-top-Alcap **Bottom:** nu-28-bottom-plugged

Clear Save Exit

# Coolant Property

Coolant Properties

Coolant Property Name:  
BM28el-coolant

Coolant

Type: d2o

Purity (%): 99.816

Temperature [°C]: 23.61

Density (g/cm3): 1.10444282

Cover Gas Type: air

Gas Den (g/cm3): 0.00119

Save

Clear

Exit

# Core Layout

ZED-2 Fuel Lattice Configuration

Fuel Lattice Name: HexU233Test

Description: 5 x th-u233 in hot channel + 48 nu-28 (unplugged)

Available Fuel Channels

- 56. testFSR
- 57. th-pu-hot
- 58. th-u233
- 59. th-u233-hot
- 60. th\_u235-19
- 61. um-19
- 62. um-37
- 63. zeeprod

Pitch Type

☐ Square ☒ Hexagonal

☐ Closed Center

Record KENO Special Cells

Start List Clear

Save Clear Exit

-12 -10 -8 -6 -4 -2 2 4 6 8 10 12

Q

P

O

N

M

L

K

J

I

H

G

F

E

# Core Parameters

ZED-2 Core Parameters

Configuration Name:  
BM1

Run No. : 1

Moderator Height [cm] 191.002

Moderator Purity [wt%] : 99.821

Moderator Temperature [°C] : 23.61

Moderator Density [g/cm3] : 1.105058

Air Density [g/cm3] : 0.0012

Gd Poison Conc. [ppm] : 0.00

Boron Poison Conc. [ppm] : 0.00

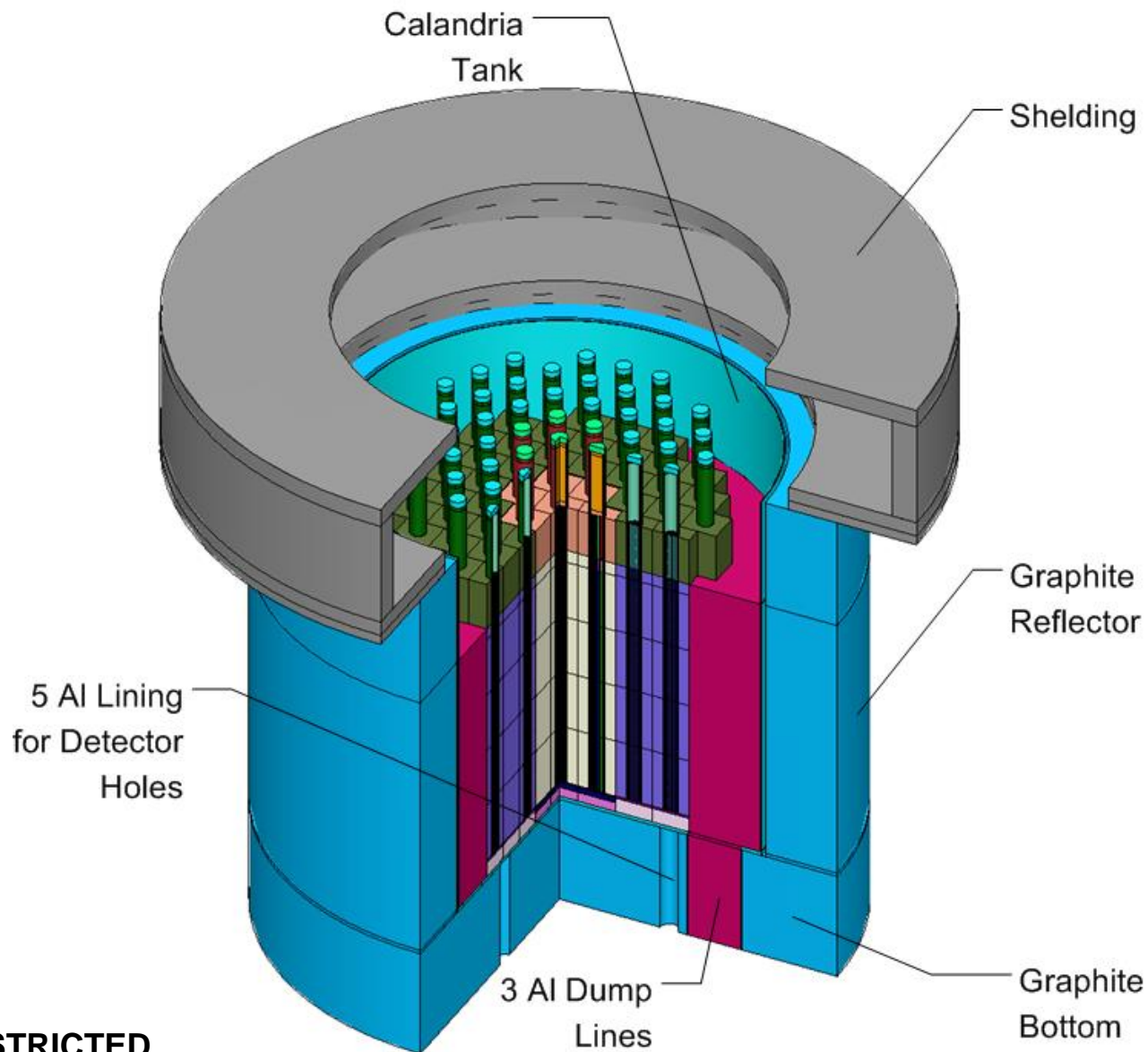
Pitch [cm] : 31.0

Bare / Infinite Lattice  
☐ Enabled

Set Parameters

Save Clear Exit

# ZED-2 Core Periphery – Anything other than the Core



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# Full Core Configuration

ZED-2 Full Core Configuration [2\_BM28el.xml]

Configuration Name: 2\_BM28el

Stringer File Name:

Core Parameters:  Fuel Lattice:

Fuel Channel:   Coolant:

# Zed2Serpent

ZED-2 Serpent (v1.0 - August 2013) [BM2]

File Prerequisites Make Full Core (F5) Tools Settings Help

```
% Coolant density : 1.10444282 [g/cm3]
% Cover gas type : air
% Cover gas density : 0.00119 [g/cm3]
% Containing bundles : nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM
% Bundle elevations : 14.1213, 63.7913, 113.4613, 163.1313, 212.8013 [cm]
% Pressure tube IR/OR : 5.0965, 5.3925 [cm]
% Calandria tube IR/OR : 6.23, 6.369 [cm]
%-----
% CELLS
%-----
% The universe outside of ZED-2

cell 1 0 outside 32
cell 2 0 outside -10
cell 3 0 outside 33

% Reactor top n shields

cell 4 0 std-bglne003 25 -33 7 -26
cell 5 0 std-air002 3 -25 7 -26
cell 6 0 std-air002 -3 34 -26
cell 7 0 std-bglne003 27 -33 26 -28
cell 8 0 std-air002 -27 26 -28
cell 9 0 std-bglne003 29 -33 28 -30
cell 10 0 std-air002 -29 28 -30
cell 11 0 std-air002 -33 30 -31
cell 12 0 std-bcem004 -33 31 -32

% Calandria tank and graphite reflector

cell 13 0 std-als005 3 -4 8 -7
cell 14 0 std-als005 -4 9 -8 11 12 13
cell 15 0 std-air002 4 -5 9 -7
cell 16 0 std-grpt006 5 -6 9 -7
cell 17 0 std-air002 6 -33 10 -7

% Detector holes

cell 18 0 std-air002 -20 10 -9
cell 19 0 std-air002 -21 10 -9
cell 20 0 std-air002 -22 10 -9
cell 21 0 std-air002 -23 10 -9
cell 22 0 std-air002 -24 10 -9

% Dump lines

cell 23 0 moderator000 -11 10 -8
cell 24 0 std-als005 11 -14 10 -9
cell 25 0 std-air002 14 -17 10 -9
cell 26 0 moderator000 -12 10 -8
cell 27 0 std-als005 12 -15 10 -9
cell 28 0 std-air002 15 -18 10 -9
cell 29 0 moderator000 -13 10 -8
cell 30 0 std-als005 13 -16 10 -9
cell 31 0 std-air002 16 -19 10 -9
cell 32 0 std-grpt006 -6 17 18 19 20 21 22 23
24 10 -9

% Bundle (nu-28-BM)

set title "ZED-2 Model: 2_BM28el"
% 54xBM1-plugged[air]
% 1xBM-plugged[d2o]
%-----
% Generated by Zed2SerpentWriter.exe [ZED-2 Serpent (v1.0 - August 2013)]
% Date: [18-Jul-2014 14:01]
% User login name: CHOWJ
% Target Nuclear Data Library: XS_70MT
%-----
% ZED-2 Core Parameters
%-----
% Run number : 2
% Moderator height : 191.619 [cm]
% Moderator purity : 99.821 [wt%]
% Moderator temperature : 296.76 K [23.61°C] [2.55728E-8 MeV]
% Moderator density : 1.105058 [g/cm3]
% Air density : 0.0012 [g/cm3]
% Pitch : 31.0 (hexagonal) [cm]
% Al floor thickness : 2.69 [cm]
%-----
% Fuel bundle: [nu-28-BM]
%-----
% Bundle length : 49.67 [cm]
% Fuel pellet radius : 0, 0.7105, 0.7105, 0.7105 [cm]
% Fuel stack length : 0, 47.73, 47.73, 47.73 [cm]
% Total fuel mass : 22.1485 [kg]
% Fuel density : 10.45, 10.45, 10.45, 10.45 [g/cm3]
% Fuel temperature : 296.76, 296.76, 296.76, 296.76 [K]
% Total clad mass : 1.976 [kg]
% Clad density : 6.56, 6.56, 6.56, 6.56 [g/cm3]
% Total enplate mass : 0.1216 [kg]
% Endplate density : 2.694 [g/cm3]
% Total bundle mass : 24.2461 [kg]
% Clad IR : 0, 0.7155, 0.7155, 0.7155 [cm]
% Clad OR : 0, 0.7609, 0.7609, 0.7609 [cm]
% Fuel top plenum : 0, 0.2084, 0.2084, 0.2084 [cm]
% Fuel bottom plenum : 0 [cm]
% Top cap thickness : 0, 0.1694, 0.1694, 0.1694 [cm]
% Bottom cap thickness : 0, 0.1952, 0.1952, 0.1952 [cm]
% End plate thickness : 0, 0.4432, 0.4432, 0.4432 [cm]
% Pin count in rings : 0, 4, 8, 16 (28 pins total)
% Pitch circle radius : 0, 1.163, 2.652, 4.206 [cm]
% Pin elevation : 0, 45, 22.5, 11.25 [deg]
%-----
% ZED-2 fuel channel: [BM1-plugged]
%-----
% Coolant type : air
% Coolant temperature : 296.76 K [23.61°C] [2.55728E-8 MeV]
% Coolant density : 0.00119 [g/cm3]
% Containing bundles : nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM
% Bundle elevations : 14.1213, 63.7913, 113.4613, 163.1313, 212.8013 [cm]
% Pressure tube IR/OR : 5.0965, 5.3925 [cm]
% Calandria tube IR/OR : 6.23, 6.369 [cm]
%-----
% Fuel bundle: [nu-28-BM]
%-----
% Bundle length : 49.67 [cm]
% Fuel pellet radius : 0, 0.7105, 0.7105, 0.7105 [cm]
% Fuel stack length : 0, 47.73, 47.73, 47.73 [cm]
% Total fuel mass : 22.1485 [kg]
```

Goto #  
Goto Surface  
Goto Cell  
Goto Lattice  
Goto Transformation  
Goto Run Options  
Goto Source  
Goto Material  
Goto Tally

Statistics: cell(90) surface(87) material(27) universe(0) lines(0) comments(0)

In(27) col(47) Nucl. Data Lib: xs\_70mt - Dataset: BM28el

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# Zed2MCNP

ZED-2 MCNP (v1.1 - May 2014) [2\_BM28e1]

File Prerequisites Make Full Core (F5) Tools Settings Help

```

C Coolant density      : 1.10444282 [g/cm3]
C Cover gas type      : air
C Cover gas density   : 0.00119 [g/cm3]
C Containing bundles  : nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM
C Bundle elevations   : 14.1213, 63.7913, 113.4613, 163.1313, 212.8013 [cm]
C Pressure tube IR/OR : 5.0965, 5.3925 [cm]
C Calandria tube IR/OR : 6.23, 6.369 [cm]
C
C CELLS
C
C The universe outside of ZED-2
C
1 0 +31:-9:+32 IMP:N=0
C
C Reactor top n shields
C
2 3 -1.28034597 +24 -32 +6 -25 IMP:N=1 TMP=2.55728E-8 $ n shield right
3 2 -0.0012 +2 -24 +6 -25 IMP:N=1 TMP=2.55728E-8 $ air right above
4 2 -0.0012 -2 +33 -25 IMP:N=1 TMP=2.55728E-8 $ air in top of
5 3 -1.28034597 +26 -32 +25 -27 IMP:N=1 TMP=2.55728E-8 $ n shield radia
6 2 -0.0012 -26 +25 -27 IMP:N=1 TMP=2.55728E-8 $ air in main he
7 3 -1.28034597 +28 -32 +27 -29 IMP:N=1 TMP=2.55728E-8 $ n shield above
8 2 -0.0012 -28 +27 -29 IMP:N=1 TMP=2.55728E-8 $ air at top of
9 2 -0.0012 -32 +29 -30 IMP:N=1 TMP=2.55728E-8 $ concrete (as a
10 4 -0.95011917 -32 +30 -31 IMP:N=1 TMP=2.55728E-8 $ n shield on ro
C
C Calandria tank and graphite reflector
C
11 5 -2.699 +2 -3 +7 -6:-3 +8 -7 +10 +11
C
12 2 -0.0012 +3 -4 +8 -6
13 6 -1.63 +4 -5 +8 -6
14 2 -0.0012 +5 -32 +9 -6
C
C Detector holes
C
15 2 -0.0012 -19 +9 -8
16 2 -0.0012 -20 +9 -8
17 2 -0.0012 -21 +9 -8
18 2 -0.0012 -22 +9 -8
19 2 -0.0012 -23 +9 -8
C
C Dump lines
C
20 1 -1.105058 -10 +9 -7 IMP:N=1 TMP=2.55728E-8 $ dump line #1 (
21 5 -2.699 +10 -13 +9 -8 IMP:N=1 TMP=2.55728E-8 $ dump line #1 (
22 2 -0.0012 +13 -16 +9 -8 IMP:N=1 TMP=2.55728E-8 $ dump line #1 (
23 1 -1.105058 -11 +9 -7 IMP:N=1 TMP=2.55728E-8 $ dump line #2 (
24 5 -2.699 +11 -14 +9 -8 IMP:N=1 TMP=2.55728E-8 $ dump line #2 (
25 2 -0.0012 +14 -17 +9 -8 IMP:N=1 TMP=2.55728E-8 $ dump line #2 (
26 1 -1.105058 -12 +9 -7 IMP:N=1 TMP=2.55728E-8 $ dump line #3 (
27 5 -2.699 +12 -15 +9 -8 IMP:N=1 TMP=2.55728E-8 $ dump line #3 (
28 2 -0.0012 +15 -18 +9 -8 IMP:N=1 TMP=2.55728E-8 $ dump line #3 (
29 6 -1.63 -5 +16 +17 +18 +19 +20 +21 +22 +23 +9 -8 IMP:N=1 TMP=2.55728E-8 $ bottom graphit
C
C Bundle [nu-28-BM]
C

```

ZED-2 Model 2\_BM28e1

```

C
C Generated by Zed2MCNFWriter.exe
C Date: [18-Jul-2014 14:06]
C User login name: CHOWJ
C Target Nuclear Data Library: XS_70MT
C
C ZED-2 Core Parameters
C
C Run number      : 2
C Moderator height : 191.619 [cm]
C Moderator purity : 99.821 [wt%]
C Moderator temperature : 296.76 K [23.61°C] [2.55728E-8 MeV]
C Moderator density : 1.105058 [g/cm3]
C Air density      : 0.0012 [g/cm3]
C Pitch           : 31.0 (hexagonal) [cm]
C Al floor thickness : 2.69 [cm]
C Submerged Element Mass : 3842.69 [kg] (A>=90 only)
C
C Fuel Bundles
C
C nu-28-BM
C
C Fuel Channels
C
C 54 * BM1-plugged[air]
C 1 * BM-plugged[d2o]
C
C Fuel bundle: [nu-28-BM]
C
C Bundle length      : 49.67 [cm]
C Fuel pellet radius  : 0, 0.7105, 0.7105, 0.7105 [cm]
C Fuel stack length   : 0, 47.73, 47.73, 47.73 [cm]
C Total fuel mass     : 22.1485 [kg]
C Total heavy elements : 19.5244 [kg]
C Fuel density        : 10.45, 10.45, 10.45, 10.45 [g/cm3]
C Fuel temperature    : 296.76, 296.76, 296.76, 296.76 [K]
C Total clad mass     : 1.976 [kg]
C Clad density        : 6.56, 6.56, 6.56, 6.56 [g/cm3]
C Total enplate mass  : 0.1216 [kg]
C Endplate density    : 2.694 [g/cm3]
C Total bundle mass   : 24.2461 [kg]
C Clad IR             : 0, 0.7155, 0.7155, 0.7155 [cm]
C Clad OR             : 0, 0.7609, 0.7609, 0.7609 [cm]
C Fuel top plenum     : 0, 0.2084, 0.2084, 0.2084 [cm]
C Fuel bottom plenum  : 0 [cm]
C Top cap thickness   : 0, 0.1694, 0.1694, 0.1694 [cm]
C Bottom cap thickness : 0, 0.1952, 0.1952, 0.1952 [cm]
C End plate thickness : 0, 0.4432, 0.4432, 0.4432 [cm]
C Pin count in rings  : 0, 4, 8, 16 (28 pins total)
C Pitch circle radius  : 0, 1.163, 2.652, 4.206 [cm]
C Pin elevation        : 0, 45, 22.5, 11.25 [deg]
C
C ZED-2 fuel channel: [BM1-plugged]
C
C Coolant type      : air
C Coolant temperature : 296.76 K [23.61°C] [2.55728E-8 MeV]
C Coolant density   : 0.00119 [g/cm3]
C Containing bundles : nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM, nu-28-BM
C Bundle elevations  : 14.1213, 63.7913, 113.4613, 163.1313, 212.8013 [cm]

```

Statistics: cell(173) surface(86) material(24) universe(18) tally(0) lines(1561) comments(481)

In(24) col(15) Nuc. Data Lib: xs\_70mt - Dataset: BM28e1

UNRESTRICTED

# Final Remarks

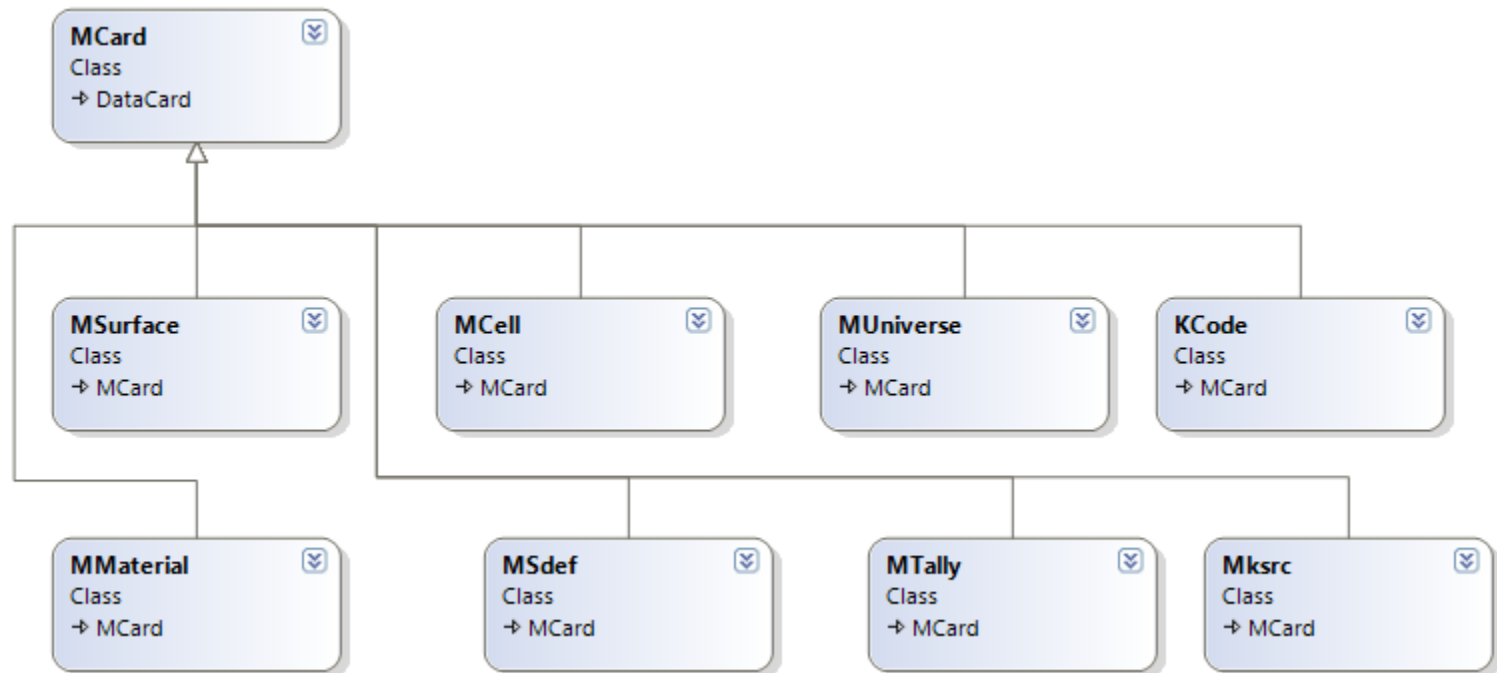
My personal claim:

*This approach of generating input data for simulation can be generalized to apply to any type of simulations, of any physical systems, with any complexity, and using any code.*

*Will a Serpent Class Library be useful?*



# MCNP Class Library



# KENO Class Library

