MANUAL

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ADETS User Manual

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Contents

1 Introduction

ADETS (Automated DEpletion Transport System) calculates coupled neutronic/isotopic results for nuclear systems and produces a large number of criticality and burnup results based on various material feed/removal specifications, power(s), and time intervals. ADETS is a fully automated tool that links the LANL MCNP Monte Carlo transport code with the SCALE system, specifically ORIGEN-ARP (radioactive decay and burnup code). Additionally, ADETS can compute the dose at various distances of the reactor using a point gamma source, whose characteristics are computed by ORIGEN-ARP. In addition, ADETS is fully coupled with the Uncertanty Quantification, Probabilistic Risk Assessment, Parameter Optimization and Data Analysis code RAVEN (see [1], [2], [3]) (developed at the Idaho National Laboratory as well). RAVEN is released with ADETS but MCNP and SCALE (ORIGEN-ARP) are not included.

2 Manual Formats

In order to highlight some parts of the Manual having a particular meaning (e.g. input structure, examples, terminal commands, etc.), specific formats have been used. In this sections all the formats with a specific meaning are reported:

- ***XML input example:***

```
<MainXMLBlock>
  ...
  <anXMLnode name='anObjectName' anAttribute='aValue'>
     <aSubNode>body</aSubNode>
  </anXMLnode>
  ...
</MainXMLBlock>
```

- ***Bash Commands:***

```
cd trunk/raven/
./a_script.sh
cd ../../
```

3 Installation

3.1 Overview

The installation of the ADETS code is a straightforward procedure; depending on the usage purpose and machine architecture, the installation process slightly differs.

In the following sections, the recommended installation procedure is outlined. For alternatives, we encourage checking the ADETS wiki.

The installation process will involve two steps:

- Installing conda;
- Installing ADETS.

In order to install the software, begin with the installation of conda (section 3.2), and then with the one for ADETS (section 3.3).

3.2 Conda: Python Dependencies

The standard installation procedure for ADETS includes using Miniconda (often simply referred to as *conda*) to install the Python libraries required to run ADETS. If conda cannot be made available on an operating system, refer to the wiki (listed above) for alternatives. To install miniconda, follow the instructions for your operating system at `https://conda.io/miniconda.html`.

Once conda is installed, proceed to installing ADETS itself (section 3.3).

3.3 Installing ADETS

Once the ADETS dependencies have been installed and conda is present (see section 3.1), the rest of ADETS can be installed.

The installation of ADETS involves the following steps:

- Obtain the source code,
- Install the prerequisite Python libraries using conda

3.3.1 Obtaining ADETS Source Code

ADETS is hosted privately as a `Git` repo on INL `GitLab` and can be viewed at `https://hpcgitlab.hpc.inl.gov/alfoa/ADETS`. In general, using the git repository assures the most consistent usage and update process.

To clone ADETS, navigate in a terminal to the desired destination, for example `/projects`. Then run the commands

```
git clone git@hpcgitlab.hpc.inl.gov:alfoa/ADETS.git
cd ADETS
git submodule update --init
```

This will obtain ADETS as well as other submodules that ADETS uses. In the future, whenever we declare a path starting with `ADETS/`, we refer to the cloned directory.

3.3.2 Installing Python Libraries

ADETS depends heavily on Python (it is written in Python), and uses conda to maintain a separate environment to prevent conflicts with other Python library installations. This separate environment is called `adets_libraries`.

In order to establish this environment, navigate to `ADETS`, then

- **Any unix-based systems (e.g. Macintosh, Linux, etc.)**:

```
cd scripts
./establish_conda_env.sh --install
```

Assure that there are no errors in this process.

Note: If `conda` is not installed in the default location, then the path to the conda definitions needs to be provided, for example

- **Any unix-based systems (e.g. Macintosh, Linux, etc.)**:

```
cd scripts
./establish_conda_env.sh --install
   --conda-defs /path/to/miniconda3/etc/profile.d/conda.sh
```

replacing `/path/to` with the install path for `conda`.

3.3.3 Updating ADETS

ADETS updates frequently, and new features are added while bugs are fixed on a regular basis. To update ADETS, navigate to `ADETS`, then run the commands

- **Any unix-based systems (e.g. Macintosh, Linux, etc.)**:

```
git pull
./scripts/establish_conda_env.sh --install
./build_raven
```

4 Running ADETS

The ADETS code is a Python software. The entry point resides on the Python side and is accessible via a command line interface. After following the instructions in the previous Section, ADETS is ready to be used. The `adets_run` script is in the ADETS folder. To run ADETS, open a terminal and use the following command (replace `<inputFileName.xml>` with your ADETS input file):

```
./adets_run <inputFileName.xml>
```

Using `adets_run` is the recommended way to run ADETS. In the event bypassing the typical environment loading and checks is desired, it can also be run via the `main.py` script using python, with the input file as argument. However, this is not recommended, as it will use whatever default versions of Python and other libraries are discovered, rather than the matching libraries set up during installation.

5 ADETS Input Structure

ADETS input (XML format) is organized in different XML blocks, each with a different functionality. The main input blocks are as follows:

- **<Simulation>**: The root node containing the entire input, all of the following blocks fit inside the *Simulation* block.
- **<run_info>**: Specifies the calculation settings (number of parallel simulations, etc.).
- **<title>**: Specifies the name of the simulation (title of the analysis)
- **<time_control>**: Defines the settings of the time evolution of the simulation
- **<burn_info>**: Sets up the burning strategy for MCNP and SCALE
- **<shielding_info>**: Sets up shielding calculation.

Each of these blocks are explained in dedicated sections in the following chapters.

5.1 Comments

Comments may be included in the ADETS input using standard XML comments, using <!-- and --> as shown in the example below.

```
<Simulation>
  ...
  <!-- An Example Comment -->
  <burn_info>
  ...
```

Comments may be placed anywhere *except* before the **<Simulation>** node or after the **</Simulation>** node. Comments outside the root node will cause errors in maintaining input file compatibility. Additionally, comments must completely surround any nodes they comment out. Comments are intended to completely remove blocks of code, or to add readability. For instance, the following is INCORRECT usage:

```
  <!--<burn_info> -->
  <!--</burn_info> -->
```

and the following is compatible usage for a code block:

```
<!--<burn_info>
  <isotopes_file>
    ...
  </isotopes_file>
  ...
</burn_info> -->
```

6 Input Keywords and Settings

6.1 title

In the **<title>** block, the user specifies the name of the analysis

6.2 run_info

In the **run_info** block, the user specifies how the overall computation should be run and the location of the executables. In the following subsections, we explain all the keywords and how to use them in detail.

6.2.1 run_info: Executables

This sub-section contains the information regarding the XML nodes used to define the location of the executables (MCNP and SCALE):

- **<mcnp_executable>**, ***string, required field***, specifies the absolute or relative (with respect to the location where the ADETS is run) path to the executable of MCNP
  Default: None
- **<scale_executable>**, ***string, required field***, specifies the absolute or relative (with respect to the location where the ADETS is run) path to the executable of SCALE (i.e. scalerte)

  Default: None

6.2.2 run_info: Execution

This sub-section contains the information regarding the XML nodes used to define how the software needs to be run.

- **<n_processors>**, ***int, optional field***, specifies the number of processors that need to be used for each MCNP and SCALE calculation
  Default: 1
- **<enviroment_bash>**, ***string, optional field***, specifies the absolute or relative (with respect to the location where the ADETS is run) path to the location of the enviroment bash

file. If not provided, no special environment will be loaded.
Default: None

- **<screen_log>**, ***string, optional field***, If "true" or "t" the screen output of the MCNP runs will be exposed on ADETS screen. If "false" or "f" the MCNP run screen output will be redirected in a log file.
Default: false

6.2.3 run_info: MCNP files

This sub-section contains the information regarding the XML nodes used to define the MCNP needed files.

- **<xsdir_file>**, ***string, required field***, specifies the absolute or relative (with respect to the location where the ADETS is run) path to MCNP XSDIR file
Default: None
- **<mcnp_input>**, ***string, required field***, specifies the absolute or relative (with respect to the location where the ADETS is run) path to MCNP reference input file that will be used for the simulation
Default: None

6.2.4 run_info: Examples

Here we present a few examples using different components of the RunInfo node:

```
<run_info>
    <mcnp_executable>~/MCNP/MCNP_CODE/bin/mcnp6</mcnp_executable>
    <scale_executable>~/SCALE/bin/scalerte</scale_executable>
    <n_processors>2</n_processors>
    <xsdir_file>~/MCNP/MCNP_DATA/xsdir_endfb-7.0</xsdir_file>
    <mcnp_input>./test_program/mcnp_input_file.ip</mcnp_input>
</run_info>
```

6.3 time_control

In the **time_control** block, the user specifies the settings of the burning and depletion calculation, in terms of time steps and power history.

This XML node allows the following attributes:

- **units**, ***optional string attribute***, time units. The user can choose among the following options
  - days
  - hours
  - seconds

  Default: days

The **<time_control>** XML block allows for several XML sub-nodes. In the following subsections, we explain all the keywords and how to use them in detail.

- **<n_bu_steps>**, ***int, required field***, number of burn up steps (MCNP calculations).
  Default: None
- **<power_history>**, ***float array, required field***, specifies the power history in p.u. (i.e. values between 0 and 1). A number of entries equal to the number of burn up steps (**<n_bu_steps>**) must be inputted.
  Default: None
- **<time_steps>**, ***int array, required field***, specifies the number of time steps (in SCALE) to be used for each burn up step. A number of entries equal to the number of burn up steps (**<n_bu_steps>**) must be inputted.
  Default: None
- **<time_bounds>**, ***float array, required field***, specifies the time bounds (units=**units**) characterizing each burn up step. A number of entries equal to the number of burn up steps plus one (**<n_bu_steps>**+1) must be inputted.
  Default: None

6.3.1 time_control: Example

Here we present an example of the **<time_control>** XML block :

```
<time_control units="hours">
  <n_bu_steps>6</n_bu_steps>
  <power_history>1.0 1.0 1.0 0.0 0.0 0.0</power_history>
  <time_steps>2 3 1 3 3 3</time_steps>
  <time_bounds> 0.0 10.0 12.0 15.0 16 18 24.0</time_bounds>
</time_control>
```

6.4 burn_info

In the **burn_info** block, the user specifies the burn up settings in terms of cells to be depleted, power, etc. The **<burn_info>** XML block allows for several XML sub-nodes. In the following subsections, we explain all the keywords and how to use them in detail.

- **<power>**, ***float, required field***, the reactor power in Watts
  Default: None
- **<cells>**, ***int array, required field***, list of all the MCNP cells that need to be burned
  Default: None
- **<volumes>**, ***float array, required field***, list of all the volumes of the MCNP cells that will be burned. **Note:** the number of entries must match the number of entries in the **<cells>** XML node.
  Default: None
- **<isotopes_file>**, ***string, required field***, specifies the absolute or relative (with respect to the location where the ADETS is run) path to the file containing the list of isotopes that will be considered in the burning stages (for which new cross sections will be computed to transfer to SCALE). **Note:** the isotope file is just a list of isotopes. For example:

```
U-235
U-238
PU238
PU239
PU241
PU242
AM243
Ge-76
Se-79
Se-80
Xe135
```

  Default: None **Note:** The format is case insensitive and it neglets the dashes (e.g. u235, U235, U-235, etc.)

6.4.1 burn_info: Example

Here we present an example of the **<burn_info>** XML block :

```
<burn_info>
    <power>5.5E8</power>
     <cells>
        483 968 1453 1938 2423 2908 3393 3878
        4363 4848 5333 5818 6303 6788 7273
        7758 8243 8728 9213 9698 10183
    </cells>
    <volumes>
       3.83884286E+03  3.83884286E+03 3.83884286E+03
       3.83884286E+03  3.83884286E+03 3.83884286E+03
       3.83884286E+03  3.83884286E+03 3.83884286E+03
       3.83884286E+03  3.83884286E+03 3.83884286E+03
       3.83884286E+03  3.83884286E+03 3.83884286E+03
       3.83884286E+03  3.83884286E+03 3.83884286E+03
       3.83884286E+03  3.83884286E+03 3.83884286E+03
    </volumes>
  <isotopes_file>./test_program/isotope_list.txt</isotopes_file>
</burn_info>
```

Example of isotope list file:

```
U-234
U-235
U-236
U-238
NP237
NP238
PU236
PU238
PU239
PU240
PU241
PU242
AM241
AM242M
AM243
CM242
CM243
CM244
CM245
CM246
CM247
```

CM248
BK249
CF249
CF250
CF251
CF252
He-4
Ge-76
Se-77
Se-78
Se-79
Se-80
Br-81
Se-82
Kr-82
Kr-83
Kr-84
Kr-85
Rb-85
Kr-86
Rb-87
Sr-87
Sr-88
Y-89
Sr-90
Zr-90
Zr-91
Zr-92
Zr-93
Nb-93
Zr-94
Mo-94
Zr-95
Nb-95
Mo-95
Zr-96
Mo-96
Mo-97
Mo-98
Tc-99
Mo100
Ru100

Ru101
Ru102
Rh103
Ru104
Pd104
Pd105
Ru106
Pd106
Pd107
Ag107
Pd108
Ag109
Pd110
Cd110
Cd111
Cd112
Cd113
In113
Cd114
Sn114
In115
Sn115
Cd116
Sn116
Sn117
Sn118
Sn119
Sn120
Sb121
Sn122
Te122
Sb123
Te123
Sn124
Te124
Sb125
Te125
Sn126
Te126
I-127
Te128
Xe128

I-129
Xe129
Te130
Xe130
Xe131
Xe132
Cs133
Xe134
Cs134
Ba134
I-135
Xe135
Cs135
Ba135
Xe136
Ba136
Cs137
Ba137
Ba138
La139
Ce140
Pr141
Ce142
Nd142
Nd143
Ce144
Nd144
Nd145
Nd146
Pm147
Sm147
Nd148
Sm148
Sm149
Nd150
Sm150
Sm151
Eu151
Sm152
Eu152
Gd152
Eu153

```
Gd153
Sm154
Eu154
Gd154
Eu155
Gd155
Gd156
Gd157
Gd158
Tb159
Gd160
Dy160
Dy161
Dy162
Dy163
Dy164
Ho165
Er166
Er167
Er168
Er170
```

6.5 shielding_info

In the **shielding_info** block, the user specifies the settings for performing the shielding (point source) computation. This block is **OPTIONAL** and if not provided, no SHIELDING will be performed.

This XML node allows the following attributes:

- **nps**, ***optional integer attribute***, number of histories to be used in the MCNP shielding calculation.
  Default: 1e5

The **<shielding_info>** XML block allows for several XML sub-nodes. In the following subsections, we explain all the keywords and how to use them in detail.

- **<steps_to_analyze>**, ***integer array, required field***, list of burn up steps (integer ids) at the end of which a shielding calculation is performed
  Default: None

- **<materials>**, ***XML node, required field***, list of all the materials needed to perform the shielding calculation. Within the **<materials>** XML block as many **<mat>** as needed can be inputed. The **<mat>** XML node requires the following attributes:

  - **name**, ***required string attribute***, the name of the material (e.g. concrete)
    Default: None
  - **rho**, ***required float attribute***, the density of the material (g/cm3)
    Default: None

  In the body of the node the isotopes IDs (MCNP nomenclature) and weighting fractions or density fractions need to be inputted in pairs. For example:

```
<mat name="air" rho="1.200E-3">
      1001    2.07864E-06
      7014    4.10358E-05
      8016    1.09303E-05
      18000  2.33750E-07
</mat>
```

- **<layers>**, ***float array, required field***, specifies the radius (in centimeters) of all the layers that bounds the cell strata. For each entry, a **so** surface will be created and filled with the material specified in the **<filler>** XML block. For example, if **<layers>** is 100200300, 3 so surfaces will be created with 100, 200 and 300 cm radius. Consequentially, 3 cells (4 considering the "all world") will be created.
  Default: None

- **<filler>**, ***string array, required field***, specifies the materials that constitute the strata determined by the **<layers>** XML block. **Note:** The number of entries in this XML block must match the number of entries in the **<layers>** block. For example, if **<filler>** is $airconcreteair$, 3 cells will be created containing air, concrete and air with bounds defined by the surfaces created based on the **<layers>** XML node.
  Default: None

- **<tally_location>**, ***int array, required field***, specifies the surface (layer) for which a tally for the dose calculation needs to be created. For example, if **<tally_location>** is 345, 3 $F2$ tallies will be created for the third, forth and fifth layer specified in the **<layers>** XML block.
  Default: None

- **<dose_conversion>**, ***XML node, required field***, This node is used to define the flux-to-dose conversion factors to be used in the tally calculation (see MCNP manual section 11.2 "FLUX-TO-DOSE CONVERSION FACTORS). Within the **<dose_conversion>** XML block two XML nodes must be inputted:

  - **<energy>**, ***float array, required field***, Energy bins in MeV

– **<factors>**, ***float array, required field***, Corresponding DF factors in $(rem/hr)/(p/cm2-s)$

6.5.1 shielding_info: Example

Here we present an example of the **<shielding_info>** XML block :

```
<shielding_info nps="6e6">
    <!-- this is optional -->
    <!-- steps to analyze (of the previous burn up steps-->
    <steps_to_analyze>3 4 5 6</steps_to_analyze>
    <!-- set the materials to be used -->
    <materials>
      <mat name="concrete" rho="3.68">
          1001    -0.00600
          8016    -0.50000
          11023  -0.01700
          13027  -0.04800
          14028  -0.28940
          14029  -0.01518
          14030  -0.01042
          19000  -0.01900
          20000  -0.08300
          26054  -0.00068
          26056  -0.01106
          26057  -0.00026
      </mat>
      <mat name="b_water" rho="1.0">
          1001  1.11706E-01
          5010  3.69219E-04
          5011  1.63115E-03
          8016  8.86294E-01
      </mat>
      <mat name="air" rho="1.200E-3">
          1001   2.07864E-06
          7014   4.10358E-05
          8016   1.09303E-05
          18000  2.33750E-07
      </mat>
    </materials>
    <dose_conversion>
        <!-- taken from MCNP manual -->
```

```
        <energy>
           0.01 0.015 0.02 0.03 0.04 0.05
           0.06 0.08 0.1 0.15 0.2 0.3 0.4
           0.5 0.6 0.8 1 1.5 2 3 4 5 6 8 10
           11 13 15
        </energy>
        <factors>
           2.78E-06  1.11E-06 5.88E-07 2.56E-07
           1.56E-07 1.20E-07 1.11E-07  1.20E-07
           1.47E-07 2.38E-07 3.45E-07 5.56E-07
            7.69E-07 9.09E-07  1.14E-06 1.47E-06
            1.79E-06 2.44E-06 3.03E-06 4.00E-06
            4.76E-06 5.56E-06 6.25E-06 7.69E-06
            9.09E-06 1.03E-05 1.18E-05 1.33E-05
        </factors>
    </dose_conversion>
    <layers>100  200      250    1000 2000 </layers>
    <filler>air b_water concrete  air  air </filler>
    <tally_location> 2 3 4 5</tally_location>

</shielding_info>
```

7 RESULTS

At end of the ADETS calculation, several results will be exported in Comma Separated Value files. The results will be stored in a folder named “RESULTS”. The following RESULTS will be generated:

- Curies, Gamma Power (Watts), Grams, Power and Gamma Spectra for each cell and burn up step
- Total Curies, Gamma Power (Watts), Grams, Power and Gamma Spectra for each burn up step
- Shielding CSV with doses as function of distances for each burn up step that has been requested to analyze

Document Version Information

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References

[1] C. Rabiti, A. Alfonsi, J. Cogliati, D. Mandelli, R. Kinoshita, S. Sen, C. Wang, P. W. Talbot, and Daniel, "Raven user manual," tech. rep., Idaho National Laboratory, INL/EXT-15-34123, 2015.

[2] A. Alfonsi, C. Rabiti, D. Mandelli, C. W. Joshua Cogliati, P. W. Talbot, D. P. Maljovec, C. Smith, and J. Zhoul, "Raven user guide," tech. rep., Idaho National Laboratory, INL/EXT-18-44465, 2018.

[3] A. Alfonsi, C. Rabiti, D. Mandelli, C. W. Joshua Cogliati, P. W. Talbot, D. P. Maljovec, and C. Smith, "Raven theory manual," tech. rep., Idaho National Laboratory, INL/EXT-16-38178, 2016.


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