

Penelope-Based User Friendly Fast Interface for Calculating Dose Distribution in Irradiated Products



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From good practices towards socioeconomic impact



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Overview

- ▶ A 2017 report by Fermilab¹, as well as a 2019 IAEA report², conclude that significant impediments remain for *device manufacturers* desiring to transition from gamma-ray and ethylene-oxide sterilization modalities to electron-beam or X-ray; and that these impediments include data and education gaps.
- ▶ The Office of Radiological Security (ORS) within the U.S. National Nuclear Security Administration (NNSA) asked Pacific Northwest National Laboratory (PNNL) to build a collaborative team that included major players in the medical device and biopharma production industries.
- ▶ The team was charged to focus on data, education and tool gaps, as identified by the Fermilab and IAEA reports, in order to help advance X-ray and electron beam technologies, and increase their use.
- ▶ This presentation covers a recently added task, which was to identify gaps in dose distribution modeling tools, and brainstorm ways in which to improve these software tools for use by non-experts.

1. FermiLab (2017). Accelerator-driven Medical Sterilization to Replace Co-60 Sources.
2. IAEA Consultancy Meeting on “Radiation effects on polymer materials” (2019) http://www-naweb.iaea.org/napc/iachem/working_materials/IAEA%20Consultancy%20Meeting%20Final%20Report%20polymer.pdf



Team Nablo – Active Members

- Pacific Northwest National Laboratory
- Becton-Dickinson
- Stryker
- Sartorius
- Texas A&M University
- Aix Marseille University
- Steri-Tek
- IBA
- Aerial CRT
- AAMI
- Boston Scientific
- Pall
- Bayer
- Millipore Sigma

stryker



SARTORIUS



**Boston
Scientific**



**Millipore
Sigma**



Current Approach Being Studied

- ▶ The main problem identified in our survey is that, due to its complexity and required labor, existing dose distribution software is out of reach for many potential users.
- ▶ As a result of the limitations of current commercial software identified by the survey, an approach is being pursued with the following features:
 - The flexibility to cover simple to moderately complex product geometries.
 - Wide range in input files – from images and photos, to CAD and CT scans.
 - Sufficient accuracy and precision of the dose distribution so the locations of the maximum and minimum dose can be determined.
 - Use by individuals who are novices at radiation modeling without the need for extensive computational resources.
 - Available to any user, and at little to no cost for license and training.



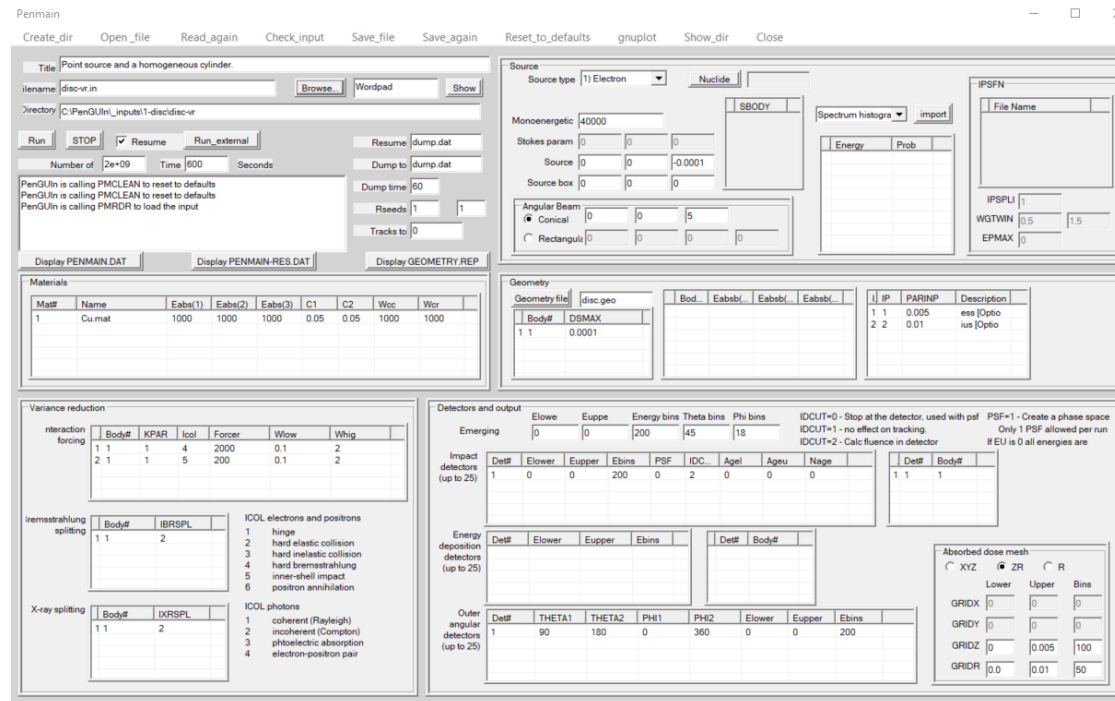
Proposed Software

- ▶ The software will use PENELOPE Monte Carlo code.
- ▶ PENELOPE will be called as an external program.
- ▶ The interface will create a voxel geometry of the product.
- ▶ A 2D interface will allow for the creation of simple configurations.
 - A single block of material
 - A simple image or photo.
 - Geometry drawn by mouse.
- ▶ More complex 3D geometry information can be imported.
 - From CAD files.
 - From other Monte Carlo codes.
 - From DICOM data.
- ▶ The current task and software is being referred to as PUFFIn – **P**enelope **U**ser **F**riendly **F**ast **I**nterface for electron and photon beam applications.



The PENELOPE Monte Carlo Code

- ▶ Penetration and **ENERgy** Loss of **Positrons** and **Electrons**.
- ▶ Used for the transport of Gammas, Electrons, and Positrons.
- ▶ Developed by the University of Barcelona, Spain.
- ▶ Available from the Nuclear Energy Agency.
- ▶ Applications include Radiotherapy, Nuclear Medicine, Dosimetry and Detectors.
- ▶ PENELOPE can be run through the PENGUIn interface.

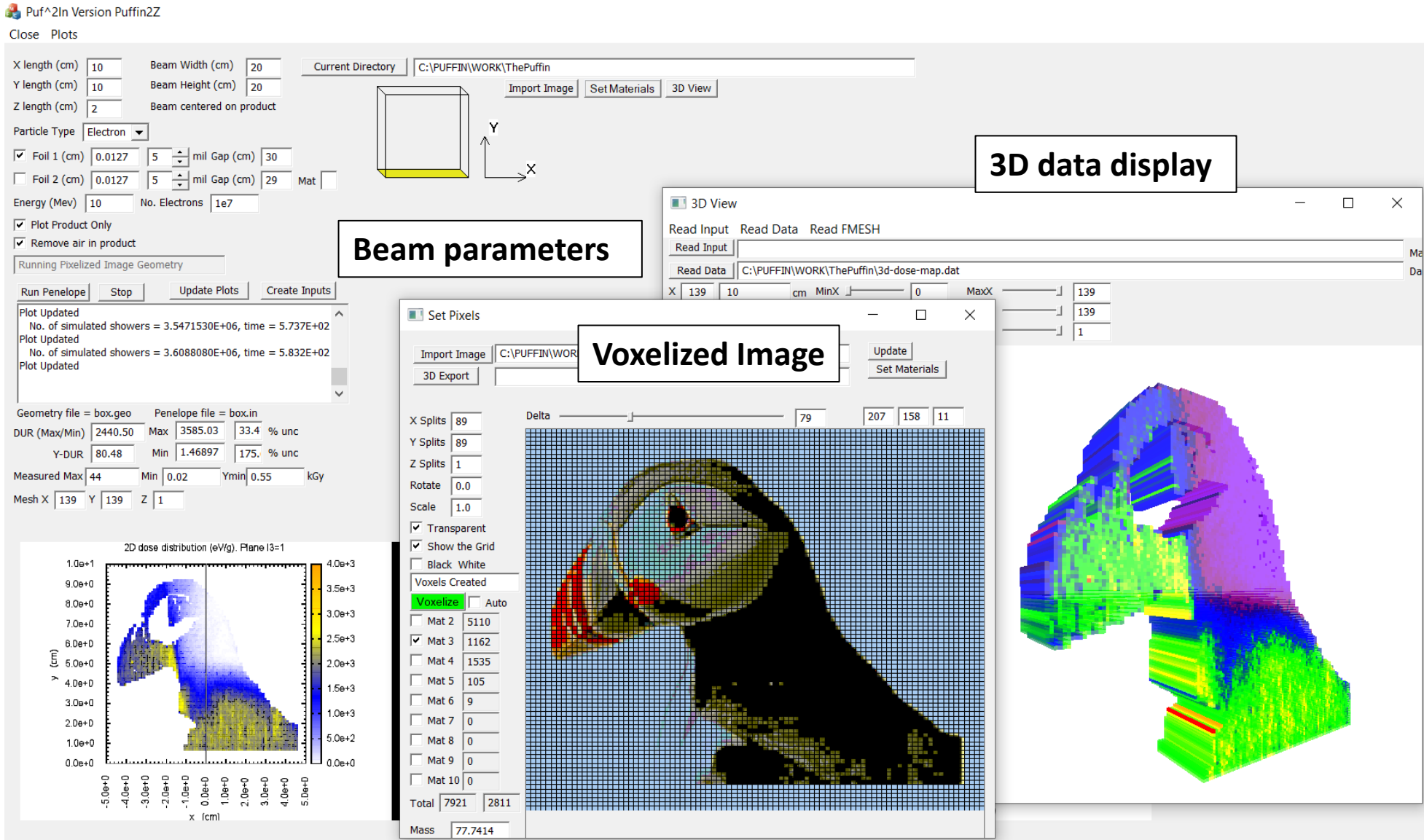


PENELOPE Capabilities

- ▶ **Simple** – The input files are concise compared to other Monte Carlo codes. The typical input file for this application is less than 50 lines. There is a separate geometry file that will vary in size depending on the geometry specifications.
- ▶ **Gnuplot** – Data files are displayed with Gnuplot, a world standard graphics package
- ▶ **Fast** – In comparison with other Monte Carlo codes for the same geometry – PENELOPE is shown to run substantially faster. The goal is for the calculation for a medium-complexity packaged product (for E-beam) to take less than 10 minutes with a single processor.
- ▶ **Minimal Size** – because the cross sections are part of the material definitions, it removes the need for a massive cross section data base. The complete PENELOPE distribution, including examples, tables and documentation is less than 1 GB.
- ▶ **Convenient distribution** – the PENELOPE code has already been incorporated in the GEANT4 code and the source code and executable can be distributed without additional restrictions with this software package.



PUFFIn Overview

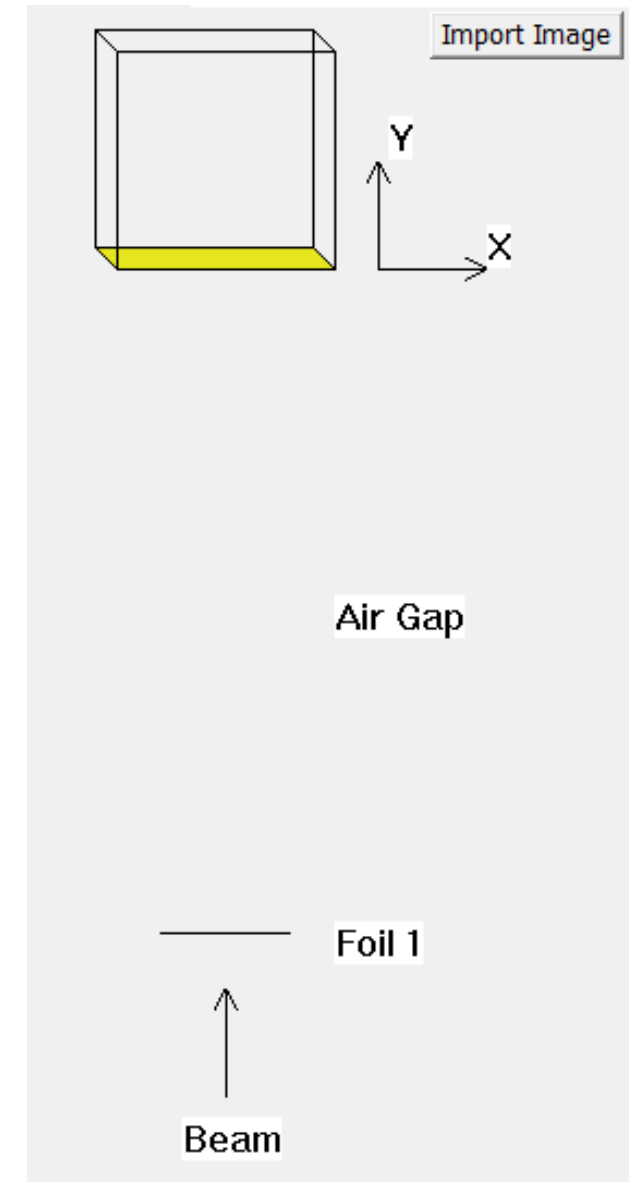


PUFFIn – Beam parameters

Input Parameters

- ▶ Product dimensions.
- ▶ Beam dimensions.
- ▶ Both Electron and Photon beams available.
- ▶ Foil position and thickness.
- ▶ Beam Energy.
- ▶ The beam comes from the Y direction.

X length (cm)	<input type="text" value="10"/>	Beam Width (cm)	<input type="text" value="20"/>
Y length (cm)	<input type="text" value="10"/>	Beam Height (cm)	<input type="text" value="20"/>
Z length (cm)	<input type="text" value="2"/>	Beam centered on product	<input type="checkbox"/>
Particle Type	<input type="text" value="Electron"/> ▼		
<input checked="" type="checkbox"/> Foil 1 (cm)	<input type="text" value="0.0127"/>	<input type="text" value="5"/> ▲ ▼	mil Gap (cm) <input type="text" value="30"/>
<input type="checkbox"/> Foil 2 (cm)	<input type="text" value="0.0127"/>	<input type="text" value="5"/> ▲ ▼	mil Gap (cm) <input type="text" value="29"/>
Energy (Mev)	<input type="text" value="10"/>	No. Electrons	<input type="text" value="1e7"/>
<input checked="" type="checkbox"/> Plot Product Only			
<input checked="" type="checkbox"/> Remove air in product			



PUFFIn – Materials

- ▶ A list of available materials is displayed.
- ▶ Materials for each region can be defined.
- ▶ A material and density is assigned to each color.
- ▶ The color of the material region in the plot can be changed.
- ▶ Standard PENELOPE materials are used.
- ▶ New materials can be created in PENELOPE.

Materials

silicon.mat 2.33 Create Material Same Mate

Save Load

Click to Set	Material Name	Density	Image Color	Plot Color
<input type="checkbox"/> Foil	Titanium.mat	4.54	Foil 1	
<input type="checkbox"/> Mat 2	Air.mat	0.00120479	Mat 2	
<input type="checkbox"/> Mat 3	PET50.mat	0.69	Mat 3	
<input type="checkbox"/> Mat 4	223-Mylar.mat	1.4	Mat 4	
<input type="checkbox"/> Mat 5	227-Polystyrene.mat	1.06	Mat 5	
<input type="checkbox"/> Mat 6	230-PolyVAcetate.m	1.19	Mat 6	
<input type="checkbox"/> Mat 7	220-PolyCarb.mat	1.2	Mat 7	
<input type="checkbox"/> Mat 8	232-PolyVButyral.ma	1.12	Mat 8	
<input checked="" type="checkbox"/> Mat 9	silicon.mat	2.33	Mat 9	
<input type="checkbox"/> Mat 10	224-Lucite.mat	1.19	Mat 10	

PUFFIn – Running PENELOPE

- ▶ The “Run PENELOPE” button will create an input and geometry file.
- ▶ PENELOPE is then run as a sub- process.
- ▶ PLOTS are displayed and updated while running.
- ▶ The total Dose Uniformity Ratio (DUR) and the DUR in the direction of the beam are calculated.

Run Penelope Stop Update Plots Create Inputs

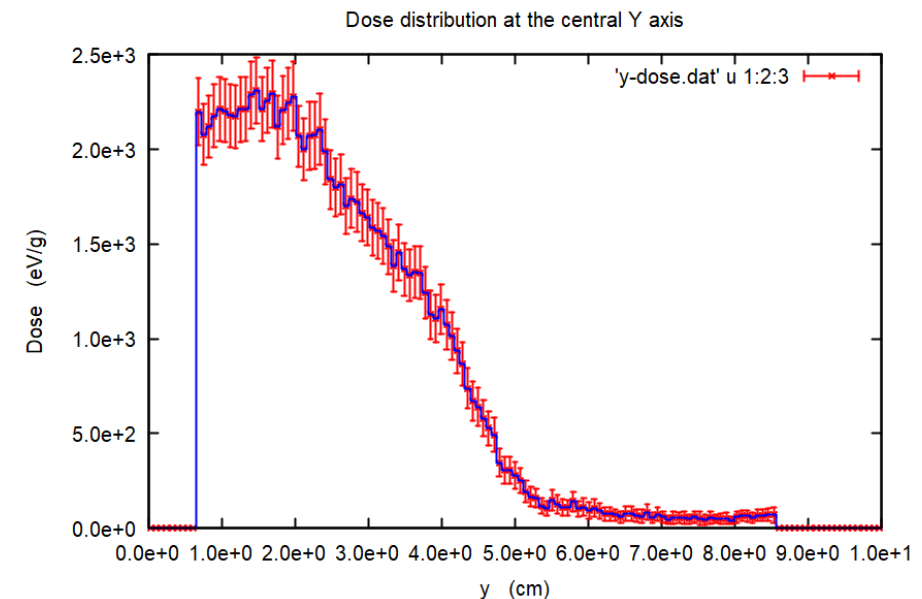
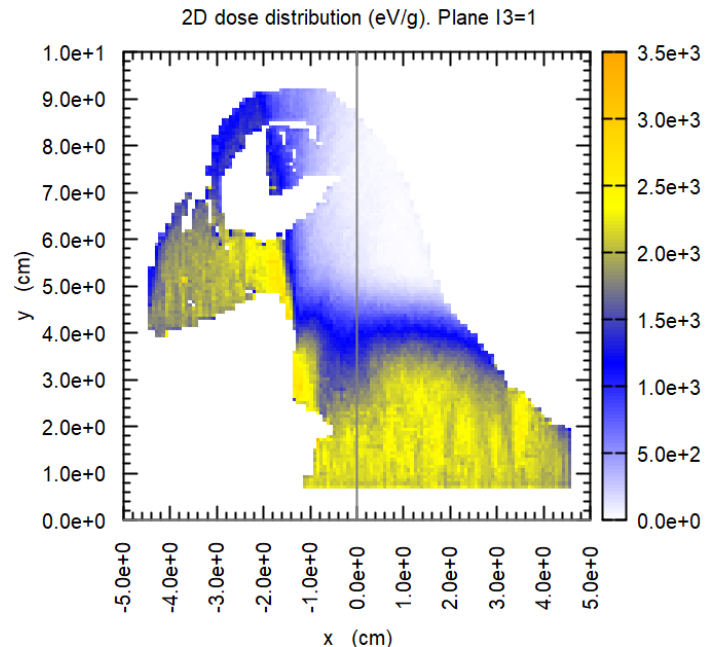
No. of simulated showers = 9.9641030E+06, time = 1.603E+03
No. of simulated showers = 1.0000000E+07, time = 1.608E+03
*** END ***

Plot Updated
Plot Updated
===Penelope Run Finished.

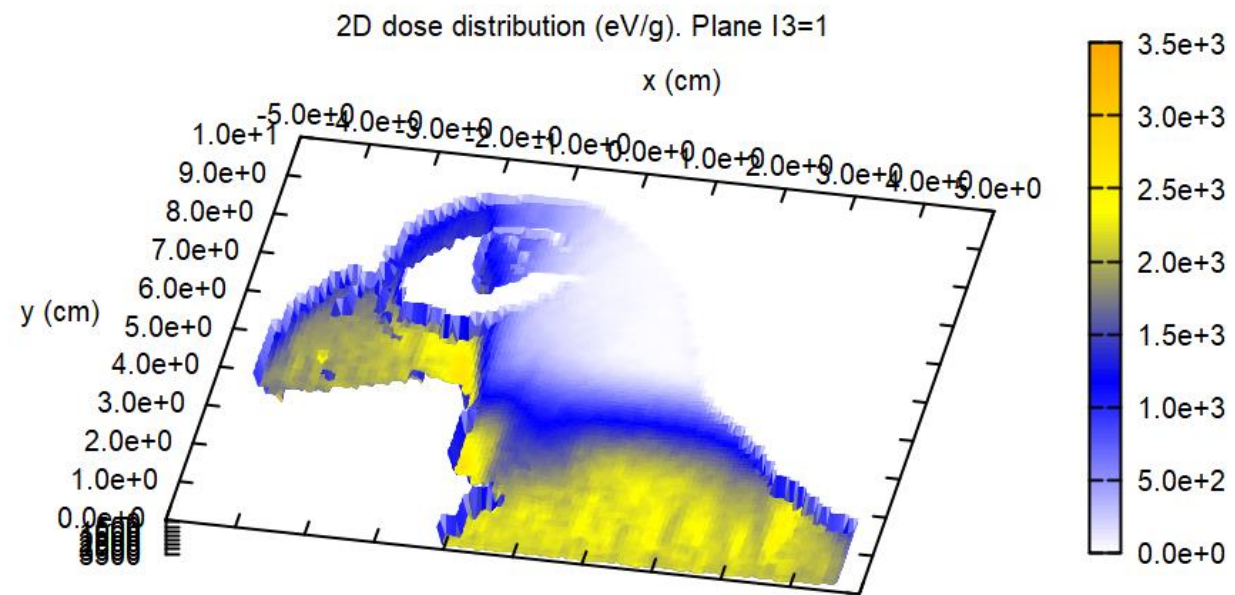
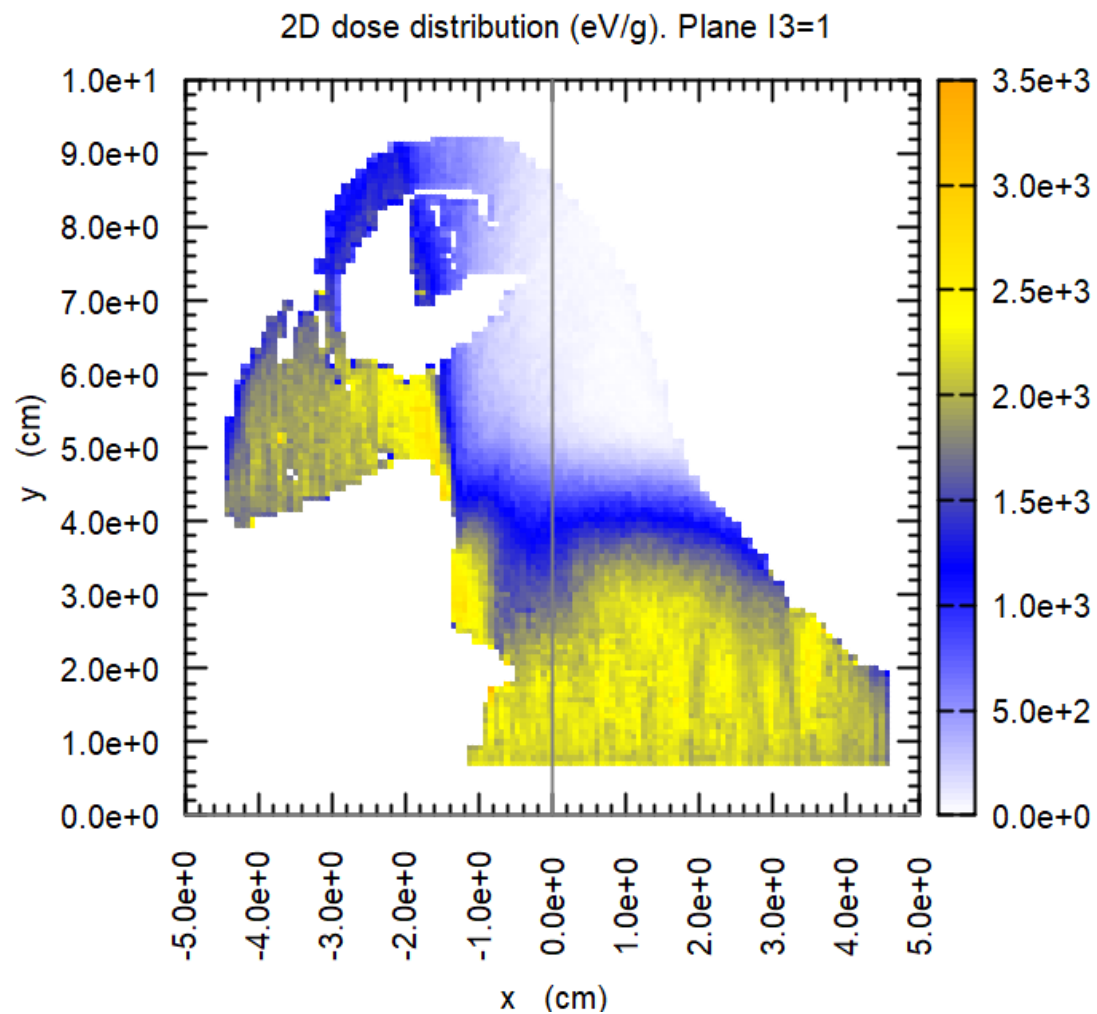
Geometry file = box.geo Penelope file = box.in

DUR (Max/Min) 553.99 Max 3292 20.3 % unc
Y-DUR 56.31 Min 5.9424 118. % unc

Measured Max 44 Min 0.08 Ymin 0.78 kGy



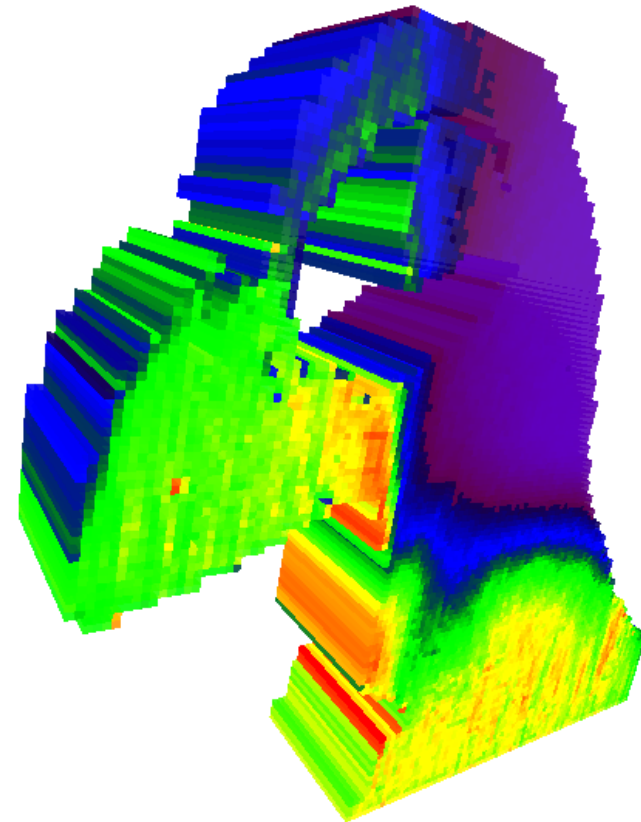
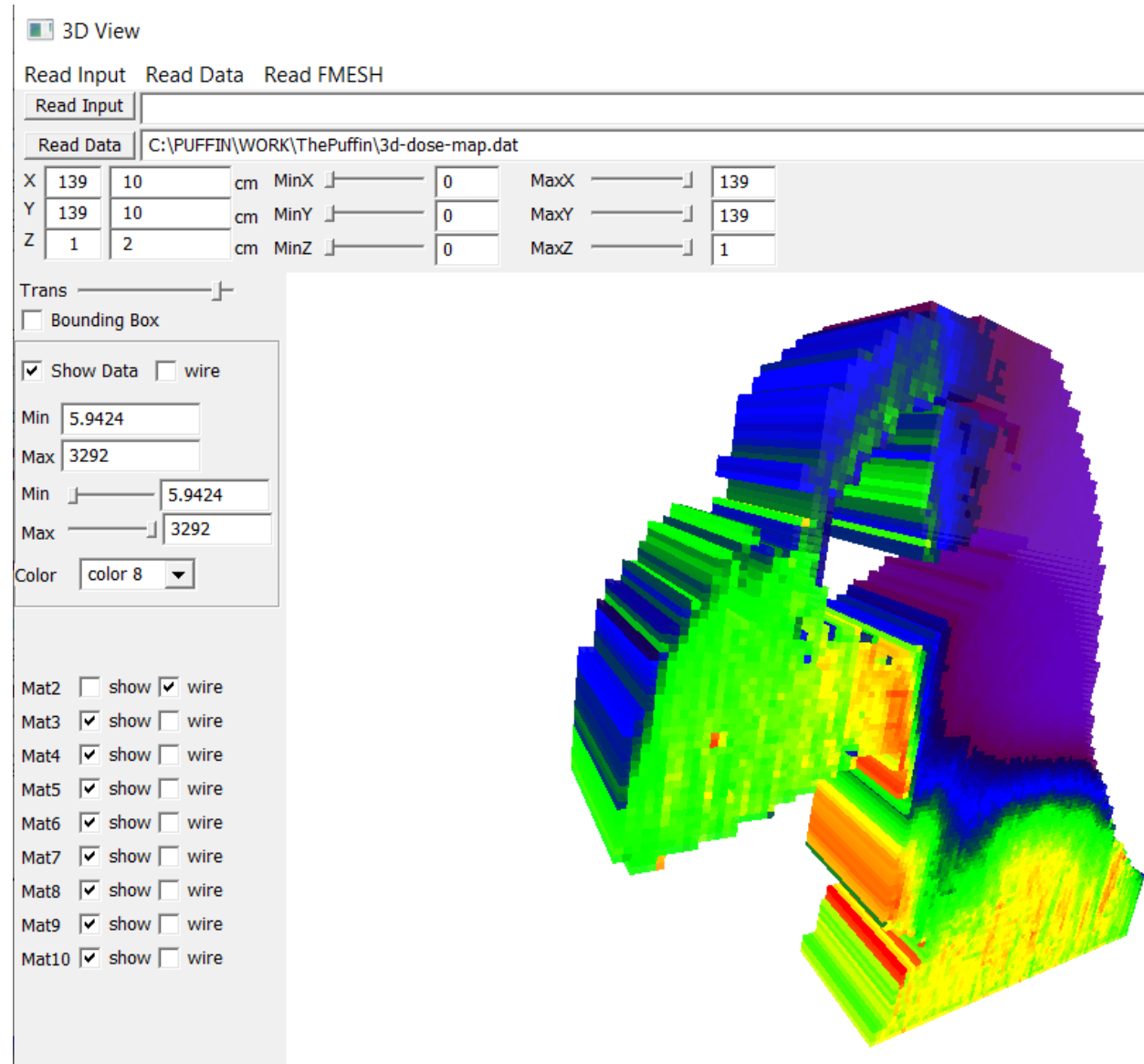
PUFFIn – Plots



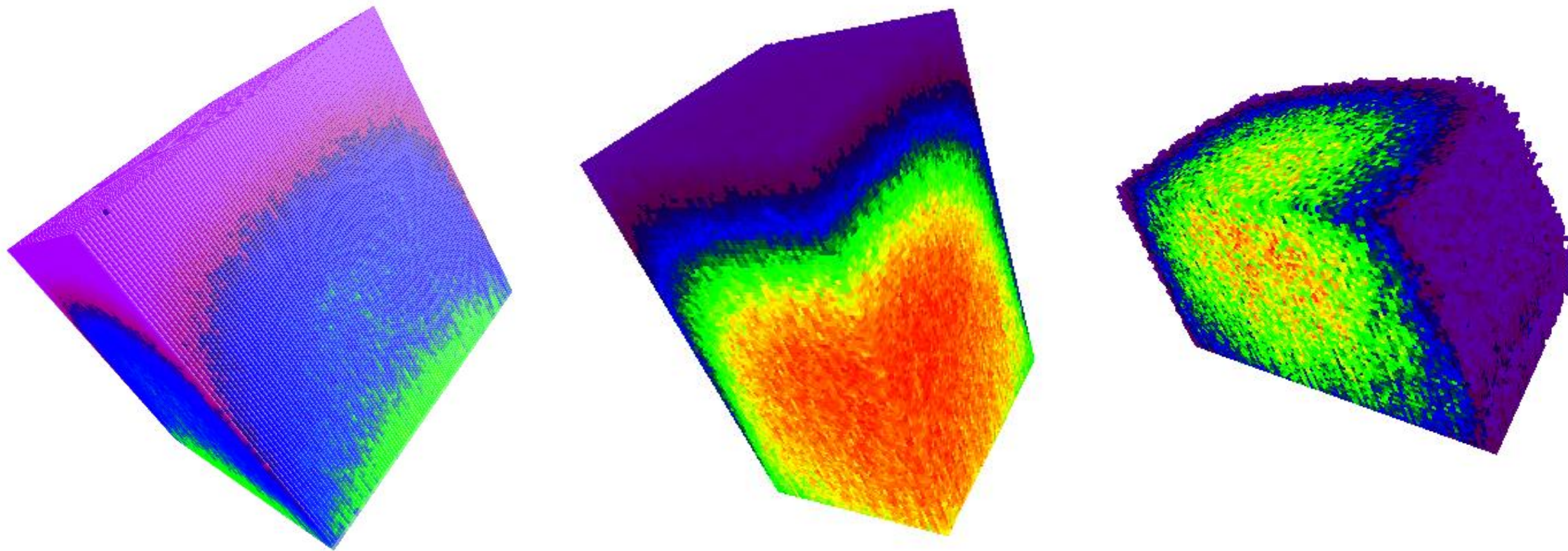
PUFFIn – 3D Data Display

Options:

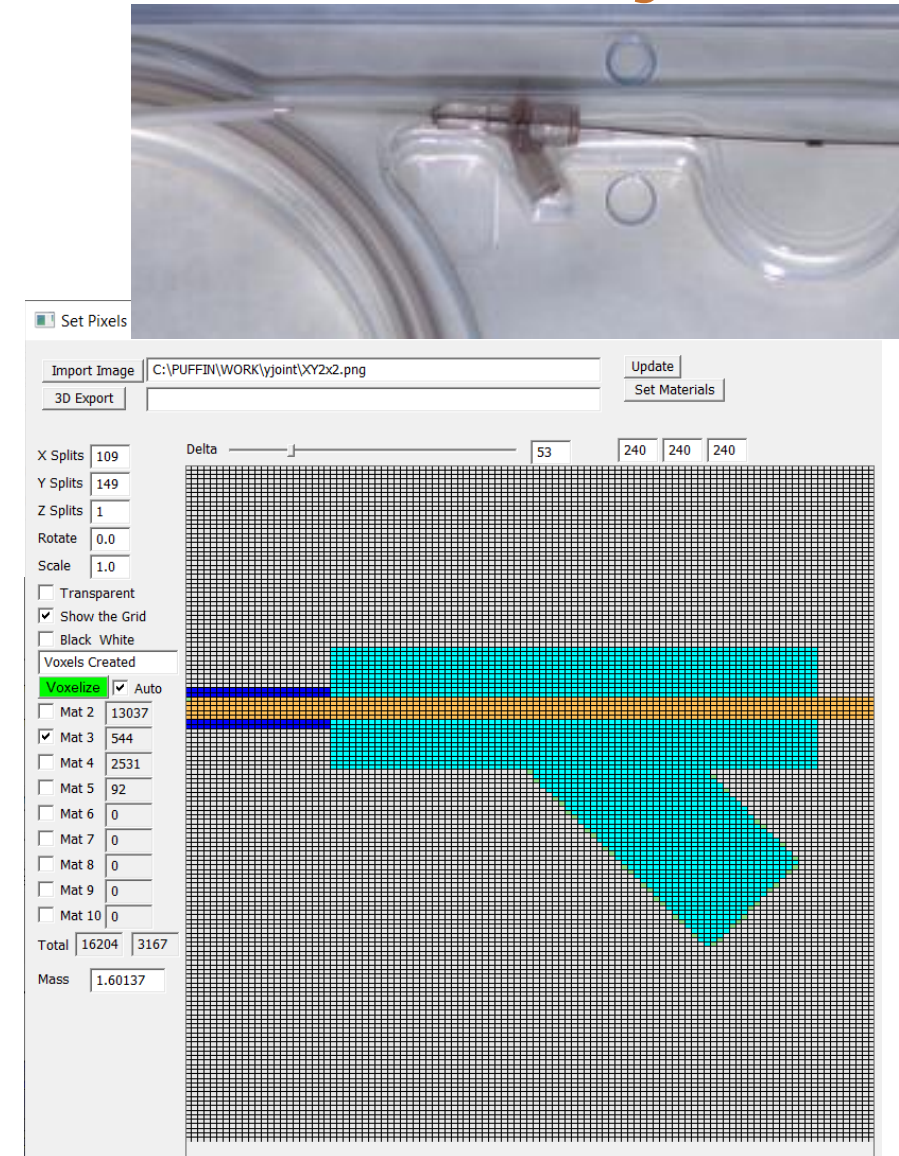
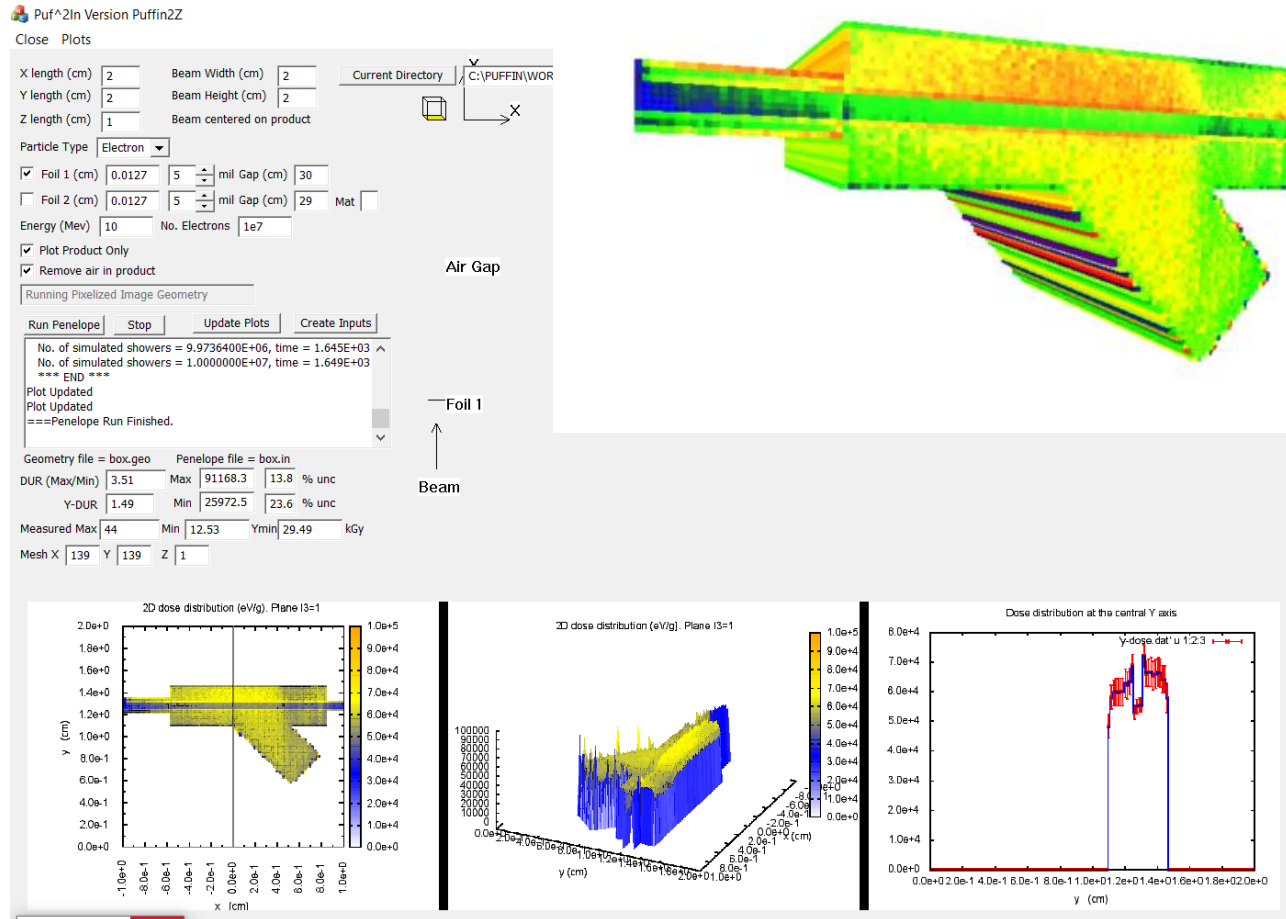
- ▶ Color Map.
- ▶ Transparency.
- ▶ Min and max data to display.
- ▶ Min and max X values.
- ▶ Min and max Y values.
- ▶ Min and max Z values.



PUFFIn – 3D Data Display 10 MeV Electrons in Water



PUFFIn – Boston Scientific Wallstent Yjoint



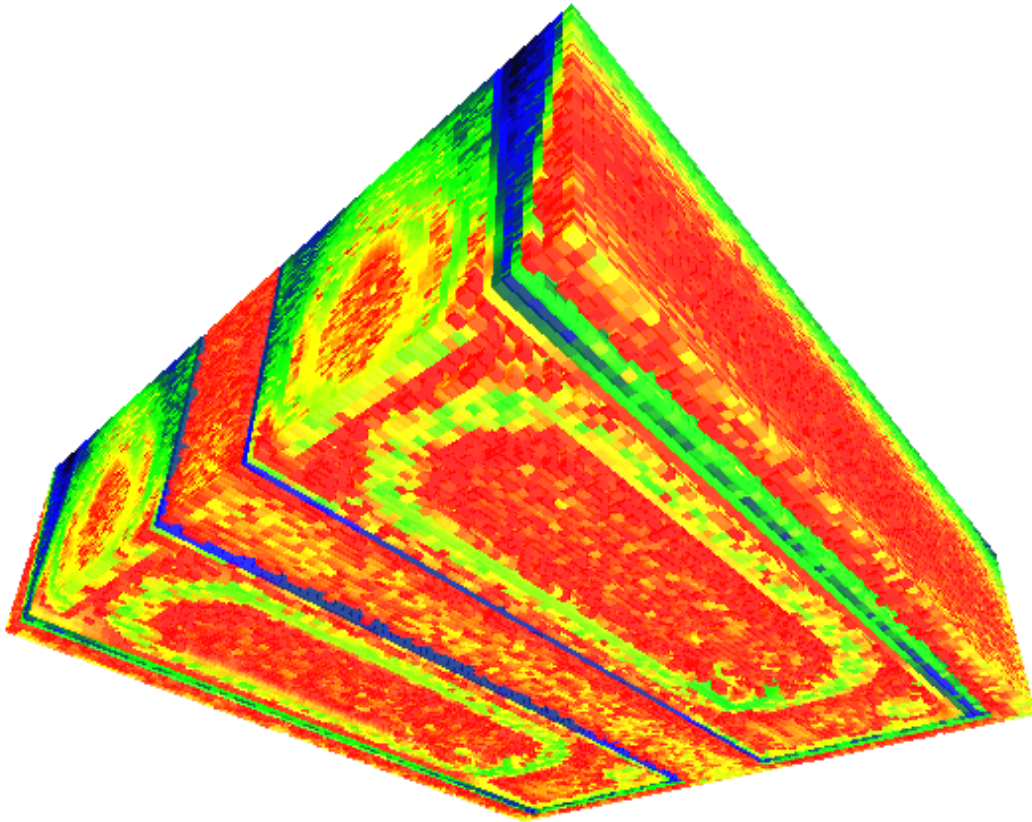
PUFFIn 3D Geometry – Bayer Stellant

- ▶ 3D geometries can be created from multiple 3D data sets.
- ▶ In this case a mesh tally file is used to transfer data from an existing code to a format that can be read by PUFFIn.
- ▶ A voxel version of PENELOPE is being tested that can run this input.

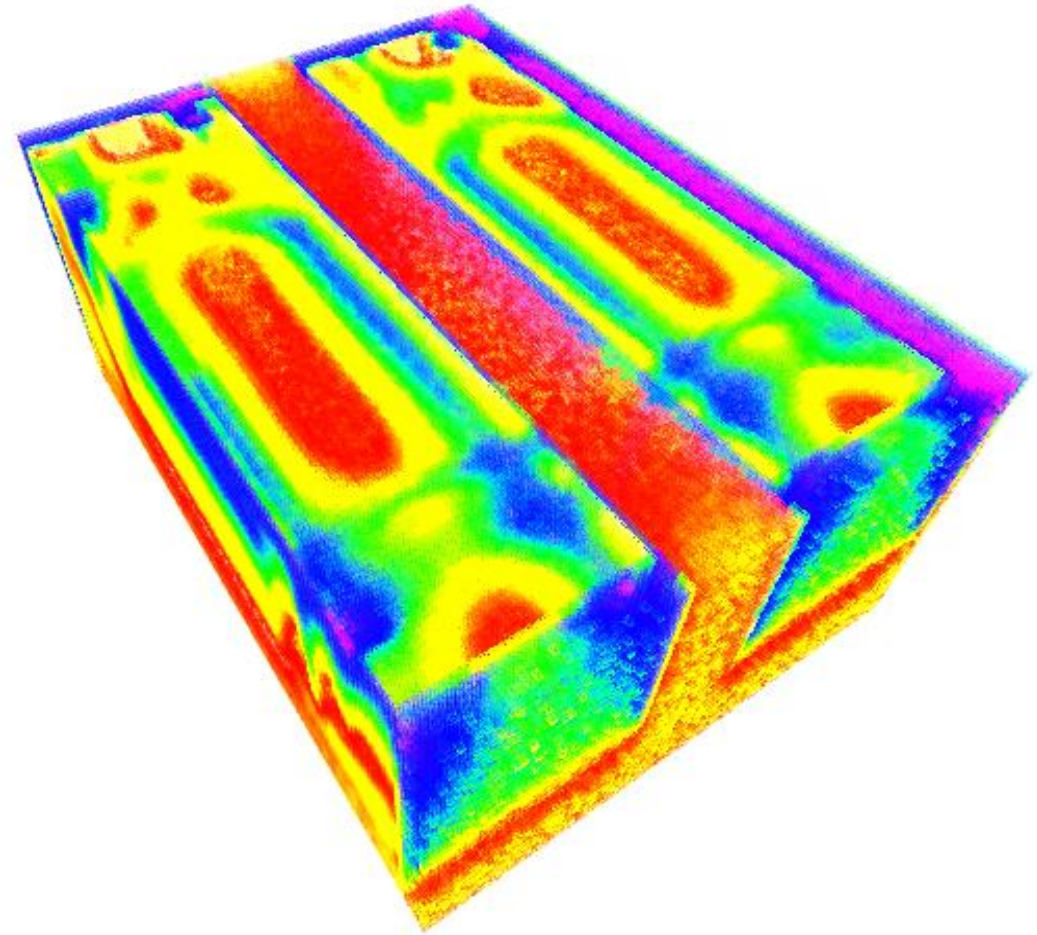


PUFFIn 3D – Bayer Stellant Dose

1 MeV Photons



10 MeV Electrons



PUFFIn – Summary

- ▶ A graphical user interface is being developed that will allow for 2D and 3D calculations of dose distribution in a product/material.
- ▶ The PENELOPE code is used to do the calculations.
- ▶ Users do not need extensive knowledge of PENELOPE, since the geometry and input is created by PUFFIn.
- ▶ Geometry information/input can be in the form of 2D images or more complex 3D data sets.
- ▶ The target users are those needing detailed dose distribution information for polymer-based products with simple to moderately complex geometries.
- ▶ The software package will be available to any user at no cost.
- ▶ Can be used as a training tool.



Thank you

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