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User Friendly Fast Interface for Calculating Dose Distribution in Polymer Products

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Fermilab 3rd Medical Device Sterilization Workshop:

Understanding the Possibilities

September 22-24, 2021

PNNL-SA-166322

NNSA/ORS Project and Goals

- A 2017 report by Fermilab, as well as a 2020 IAEA report, conclude that significant impediments remain for *medical device manufacturers* desiring to transition from gamma-ray and ethylene-oxide sterilization modalities to electron-beam or X-ray; and that these impediments are mostly in the form of data and education gaps, not necessarily a lack in technology.
- The Office of Radiological Security (ORS) within the National Nuclear Security Administration (NNSA) has been working with government and private entities that utilize high activity gamma-ray irradiators for various applications, which includes medical product sterilization. One aim is to help advance X-ray and electron beam technologies, and increase their use.
- ORS asked PNNL to build a collaborative team that included major players in the medical sterilization industry.
- The team was charged to focus on data and education gaps, as identified by the Fermilab and IAEA reports.
- This presentation covers a recently added task, which is to identify gaps in dose distribution modeling tools, and brainstorm ways in which to improve these software tools for use by non-experts.

Team Nablo – Active Members

- Pacific Northwest National Laboratory
- Becton-Dickinson
- Stryker
- Sartorius
- Texas A&M University
  - National Center for E-beam Research
  - Mechanical Engineering Department
- Aix Marseille University
- Steri-Tek
- IBA
- Aerial CRT
- AAMI
- Boston Scientific
- Bayer

Team Nablo Collaboration – Progress Since 2018

- To date, the project outputs and outcomes have included:
  - Comprehensive studies on:
    - the influence of radiation DOSE on polymer effects.
    - the influence of radiation DOSE RATE on polymer effects.
    - the influence of RADIATION MODALITY on polymer effects.
  - Presentations at ten conferences
  - Publication of data results in peer-reviewed journals
  - Engagement with relevant AAMI and ASTM subcommittees in order to guide revisions of standards.
  - Currently developing an online library for curating the radiation effects on a broad range of polymers.

Objectives of New Task

- By surveying individuals in the sterilization industry, identify limitations of existing dose distribution software for users desiring to determine the location of the maximum and minimum dose values in existing and conceptual polymer products (individual packages and shipment boxes) sterilized with E-beam and X-ray.
    - Such detailed dose distribution in the boxed product are needed for FDA product qualification
- Improve on existing software by brainstorming ideas to solve these limitations or gaps.
- Execute the solution(s) that have the most promise

Current Approach Being Studied

- The main problem identified in the survey is that, due to its complexity, dose distribution software is out of reach for non-experts, and labor costs for training and getting results are high.
- 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 relatively complex product geometries.
  - Wide range in input files – from hand drawings 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 accurately determined.
  - Use by individuals who are novices at radiation modeling, with a regular personal computer.
  - As compared to existing similar software, much less labor for training and for obtaining dose results.
  - Available to any user and at little to no cost for software and training.
  - Be simple and versatile enough to be used as a training tool for the industry.

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Current Approach continued -

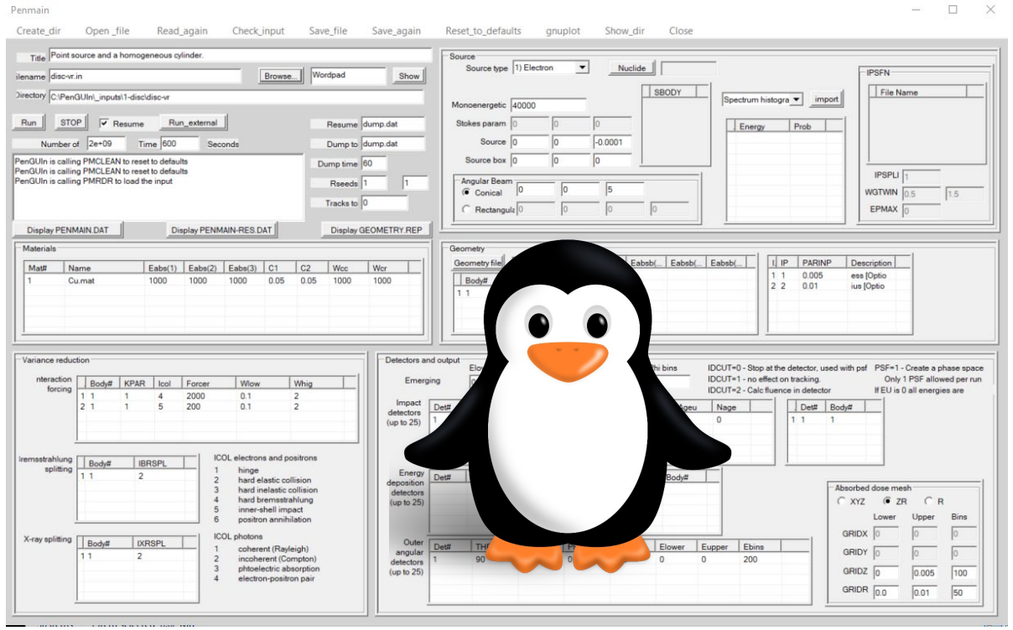
- A user interface that uses the PENELOPE Monte Carlo code.
- PENELOPE will not be integrated into the interface, but called as an external program.
- The interface will create a voxel geometry of the product.
- Initial implementation will be 2D, to be extended to 3D in the next phase.
- The current task and software is being referred to as **PUFFIn** – **P**enelope **U**ser **F**riendly **F**ast **In**terface for electron beam applications.

- The ideal scenario would be a simple enough tool that non-experts can and WILL actually use in the first few steps of dose distribution characterization, then let the modeling experts assist these non-experts with the final dose modeling needed for FDA qualification.

What is PENELOPE?

- **P**enetration and **ENE**rgy **L**oss of **P**ositrons and **E**lectrons.
- Used for the transport of Gammas, Electrons, and Positrons.
- Developed and distributed by the University of Barcelona, Spain.
  - Also available from:
    - Nuclear Energy Agency in France (2018 version)
    - Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory (2014 version).

- Applications include Radiotherapy, Nuclear Medicine, Dosimetry and Detectors.
- PENELOPE can be run through the PENGUIn interface.



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Why PENELOPE?

- **Simple** – The input files are very small 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.
- **Uses Gnuplot**, a world standard graphics package, which is also free and can be distributed with PUFFIn.
- **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 Gigabytes/Regular Computer** – 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.
- **No Cost** – the PENELOPE code has already been incorporated in the GEANT4 code and the source code and executable is free for distribution with the PUFFIn graphical user interface.

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PENELOPE is in GEANT4

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Geant4

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Low Energy Electromagnetic Physics - Penelope

Penelope low-energy electromagnetic models

From version **9.2** of Geant4, the **Penelope** low-energy electromagnetic models for e± and gamma-rays have been **migrated to the new design** (the same as for "Standard EM processes").
From version **Geant4 9.4** a **complete new set of Penelope models** has been made available, which is based on the **version 2008 of Penelope**, rather than version 2001.
All Penelope models are compliant with the multi-thread approach employed in Geant4 from version 10.0.

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PENELOPE is available from the NEA/RSICC

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PENELOPE-2018: A Code System for Monte Carlo Simulation of Electron and Photon Transport

NEA/MBDAV/R(2019)1

Adobe Acrobat PDF Document - on 10/8/20 at 3:25 PM

Codes and programs | English | Proceedings

Workshop Proceedings, Barcelona, Spain 28 January-1 February 2019

The computer code system PENELOPE (version 2018) performs Monte Carlo simulation of coupled electron-photon transport in arbitrary materials for a wide energy range, from a few hundred eV to about 1 GeV. Photon transport is simulated by means of the standard, detailed simulation
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consisting of homogeneous bodies limited by quadric surfaces, i.e., planes, spheres, cylin
provide the user with the necessary information to understand the details of the Monte Ca

RSICC

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Package Details

Computer Code Name: PENELOPE2014

Computer Code Number: C00782

Code System for Monte Carlo Simulation of Electron and Photon Transport.

Keywords:
high energy
positron
gamma-ray
monte carlo
bremsstrahlung

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PENELOPE Documentation

PENELOPE, a code system for Monte Carlo simulation of electron and photon transport

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Diagonal 645, E-08028 Barcelona, Spain.

Abstract

The computer code system PENELOPE (version 2018) performs Monte Carlo simulation of coupled electron-photon transport in arbitrary materials for a wide energy range, from a few hundred eV to about 1 GeV. Photon transport is simulated by means of the standard, detailed simulation scheme. Electron and positron histories are generated on the basis of a mixed procedure, which combines detailed simulation of hard events with condensed simulation of soft interactions. A geometry package called PENGEOM permits the generation of random electron-photon showers in material systems consisting of homogeneous bodies limited by quadric surfaces, *i.e.*, planes, spheres, cylinders, etc. This report is intended not only to serve as a manual of the PENELOPE code system, but also to provide the user with the necessary information to understand the details of the Monte Carlo algorithm.

KEYWORDS: Radiation transport. Electron-photon showers. Monte Carlo simulation. Sampling algorithms. Constructive quadric geometry.

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PENELOPE Benchmarks

Experimental benchmarks of the Monte Carlo code PENELOPE

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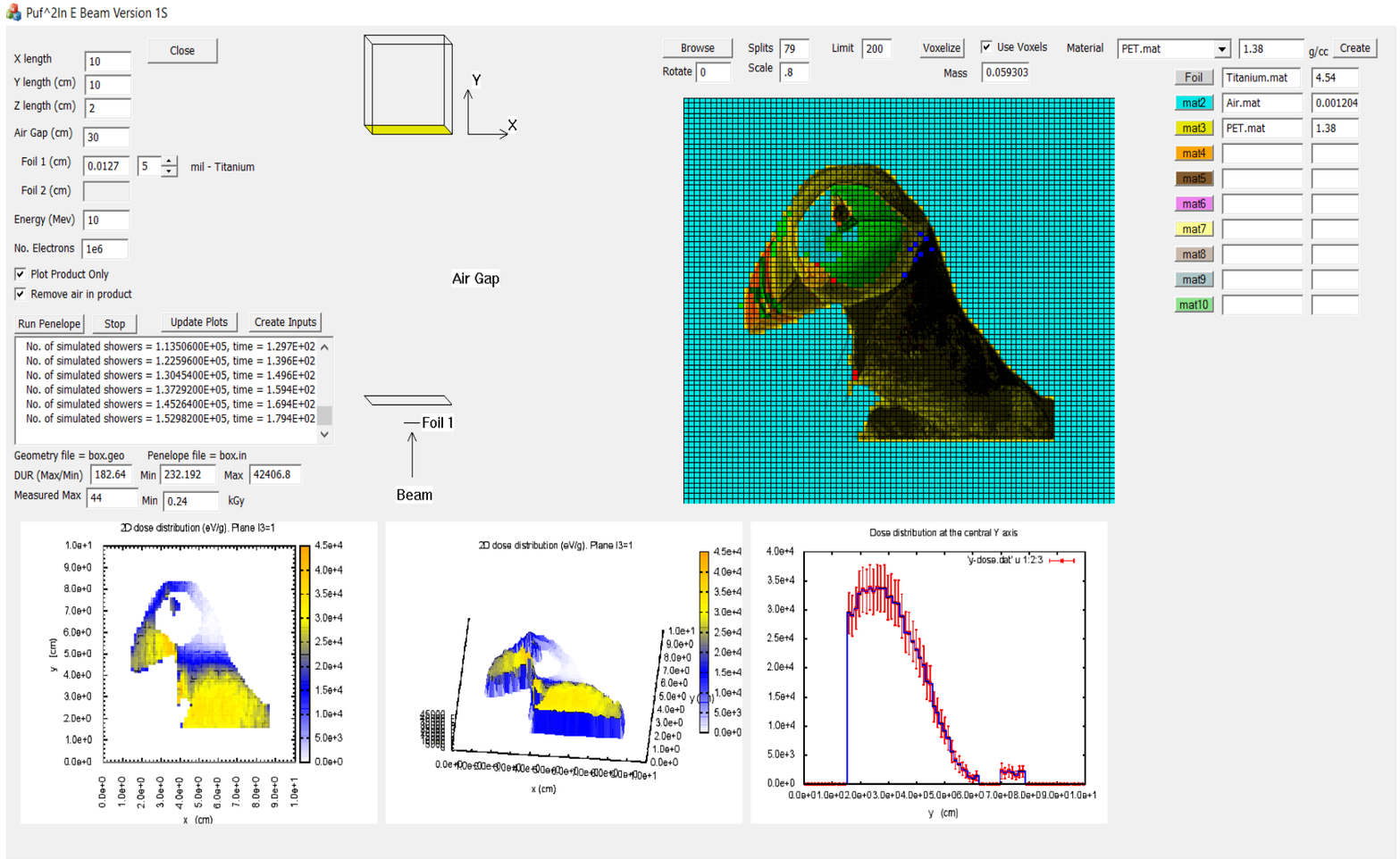
Received 1 August 2002; received in revised form 17 December 2002

Abstract

The physical algorithms implemented in the latest release of the general-purpose Monte Carlo code PENELOPE for the simulation of coupled electron–photon transport are briefly described. We discuss the mixed (class II) scheme used to transport intermediate- and high-energy electrons and positrons and, in particular, the approximations adopted to account for the energy dependence of the interaction cross-sections. The reliability of the simulation code, i.e. of the adopted interaction models and tracking algorithms, is analyzed by means of a comprehensive comparison of simulation results with experimental data available from the literature. The present analysis demonstrates that PENELOPE yields a consistent description of electron transport processes in the energy range from a few keV up to about 1 GeV.

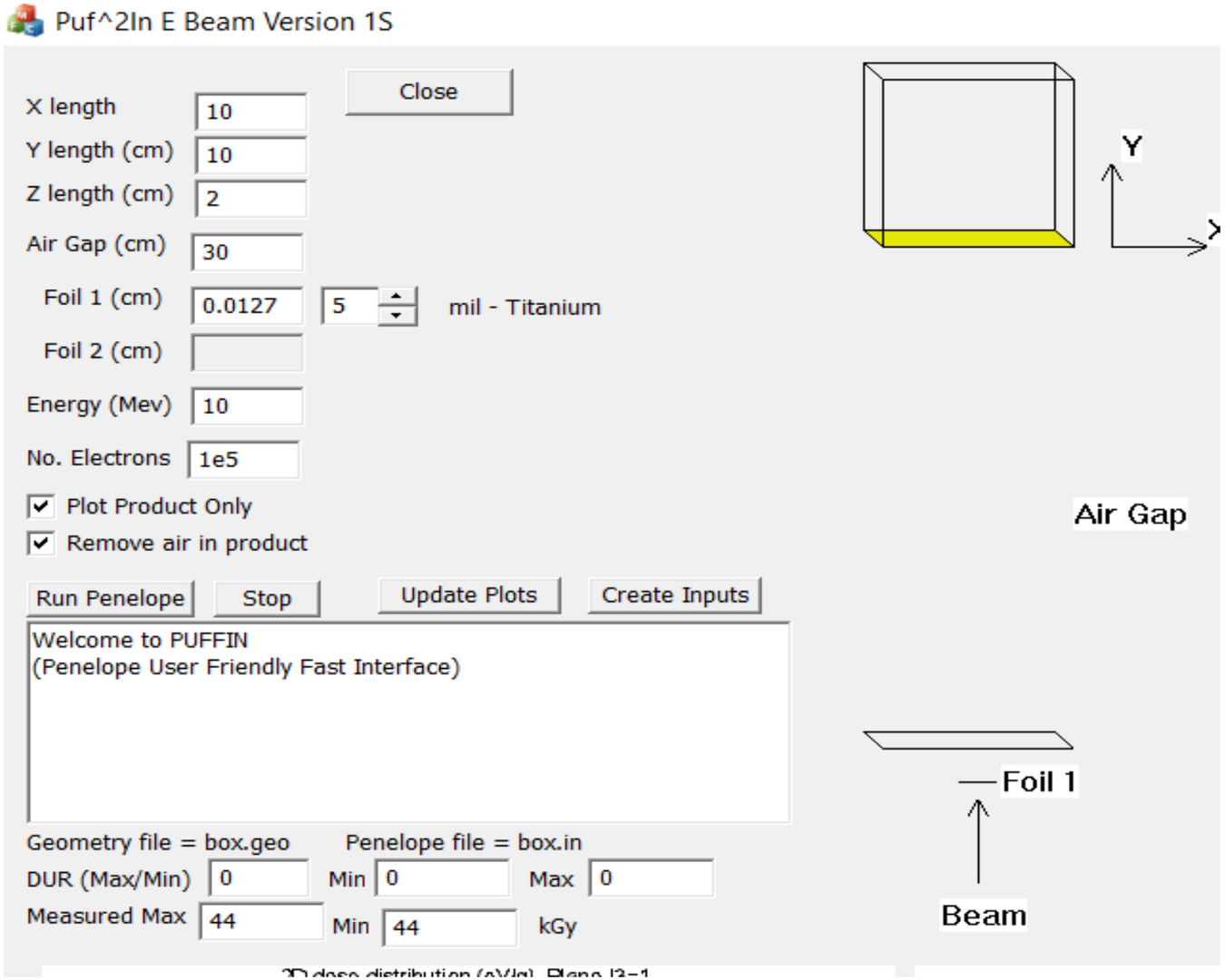
PACS: 78.70.–g
Keywords: Radiation transport; Monte Carlo simulation; Electron–gamma showers

PUFFIn – Overview



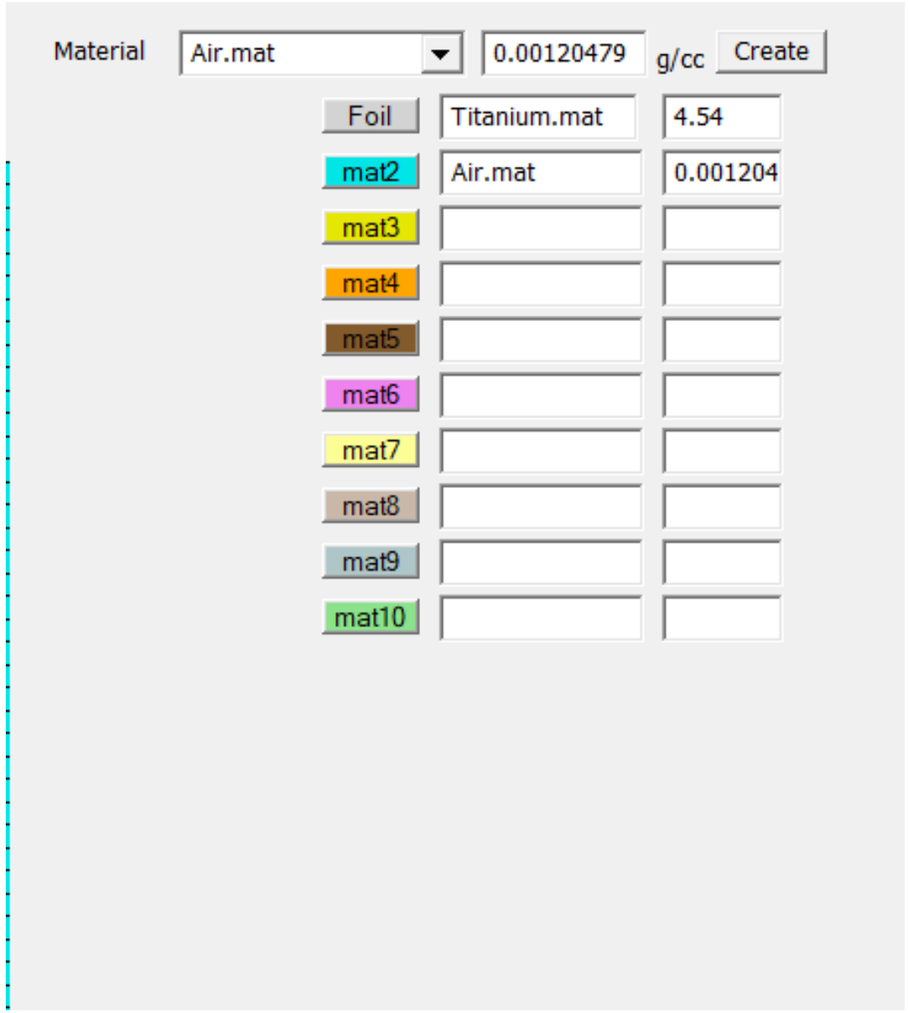
- **User input:**
- All input and output is displayed in a single window.
- The geometry description is intuitive and easy to define.
- It is easy to run PENELOPE from the interface.
- Plots generated by PENELOPE are shown in the interface.

PUFFIn – 2D



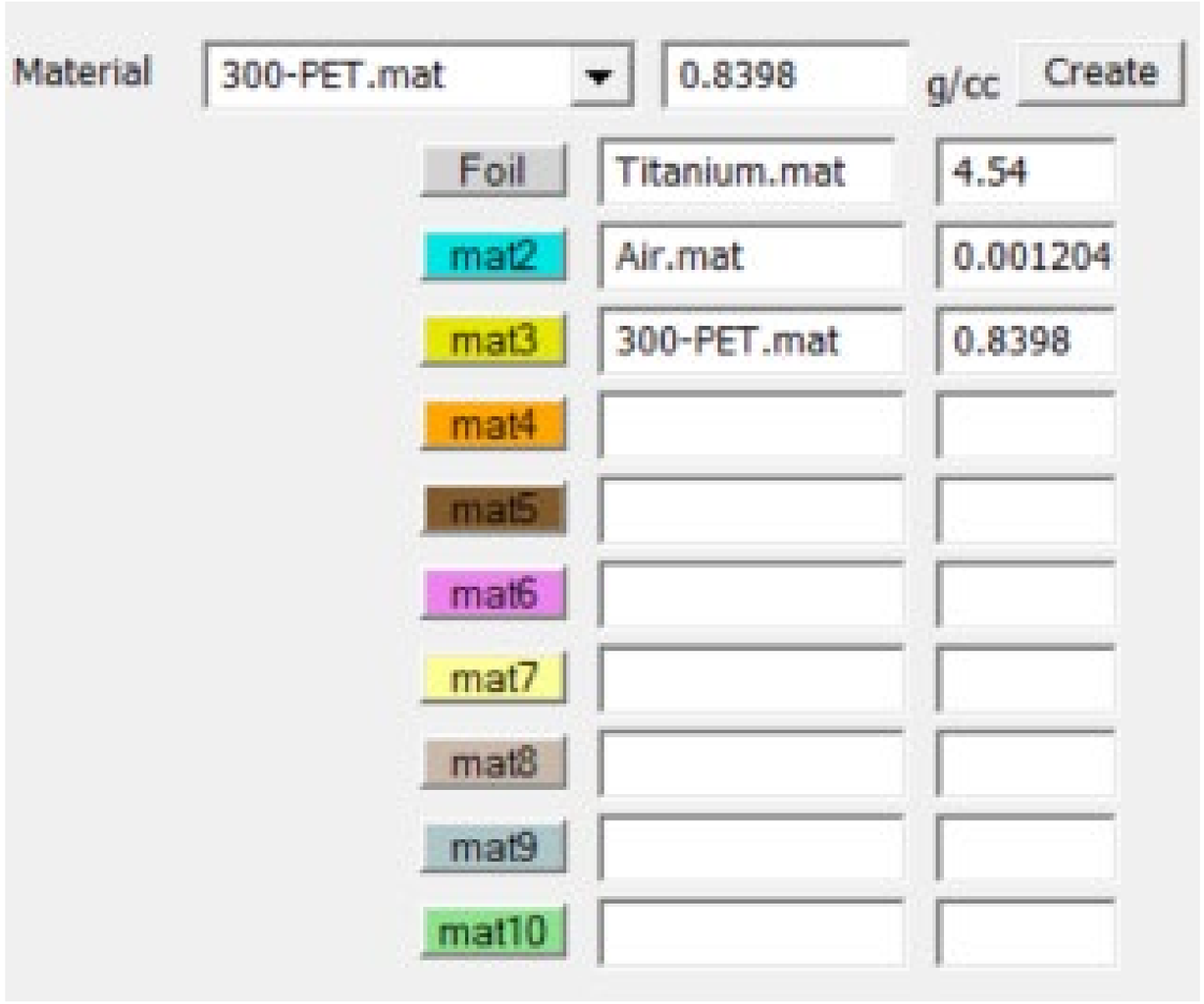
- **User input:**
- Outside dimensions of the product (X length, Y length, Z length)
- Distance from the beam to the product (Air Gap).
- Foil thickness (mil) – Only 1 foil is currently supported.
- Energy of the beam (MeV).
- Scatter plate or equivalent
- Number of electron showers to run.

PUFFIn – 2D – Materials

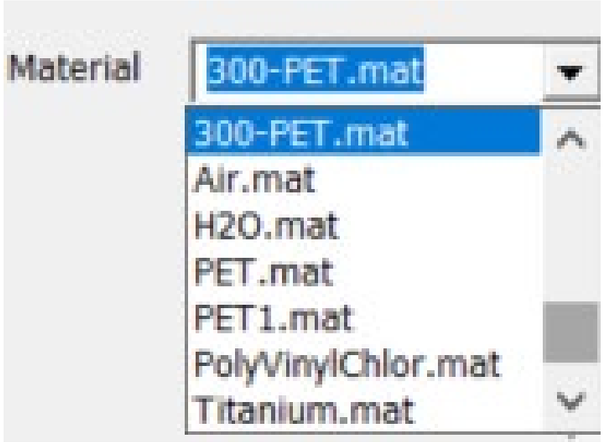


- **User input:**
- Standard PENELOPE materials are used.
- Available materials are determined by the material files found in the default directory.
- New materials can be created using PENELOPE.
- The default foil material is Titanium.
- Air material is used for the region between the beam and product.
- Additional materials can be set by the user - up to 10 materials.

PUFFIn – 2D – Materials

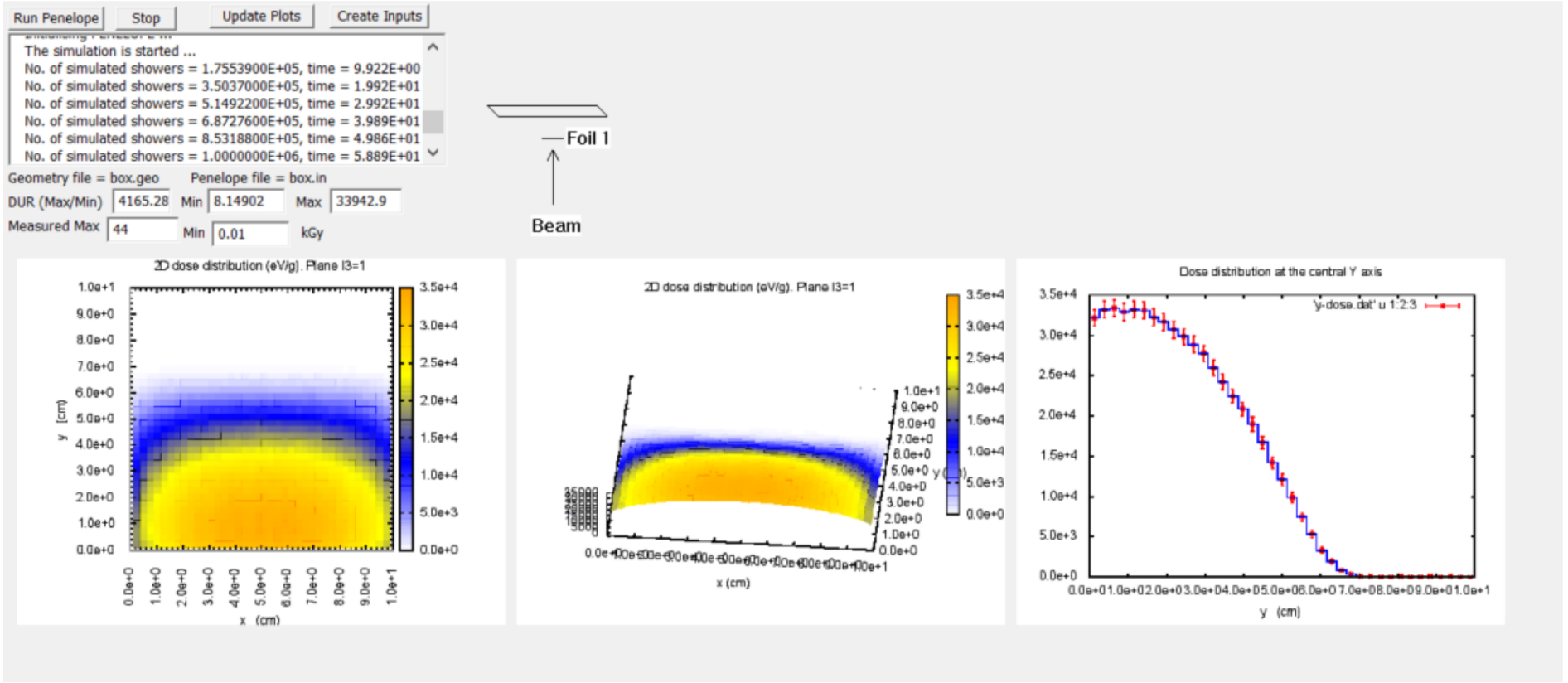


- **User input:**
- The foil material and the air material are set be default.
- The user must set at least one product material.



PUFFIn – 2D – Run PENELOPE

- Selecting “Run Penelope”, creates a PENELOPE input file and PENELOPE geometry file.
- PENELOPE is run as a sub process.
- PENELOPE plots are displayed.
- The DUR is calculated.



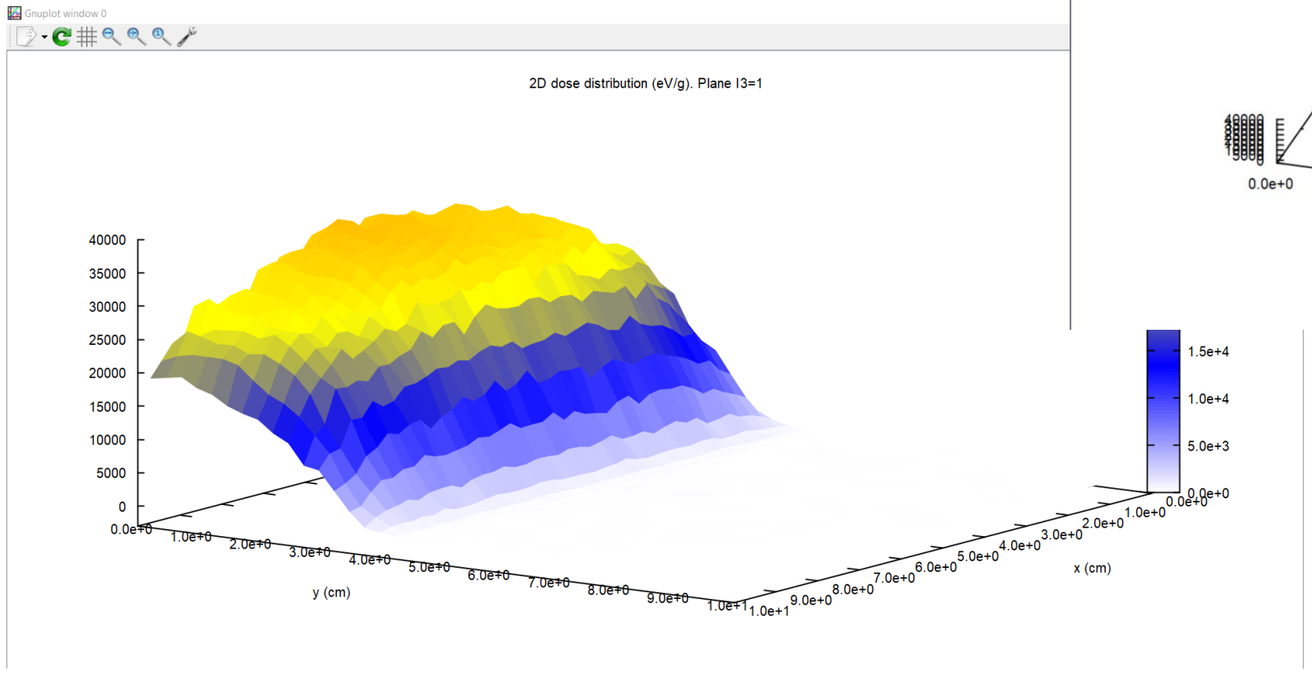
PUFFIn – 2D – Run PENELOPE

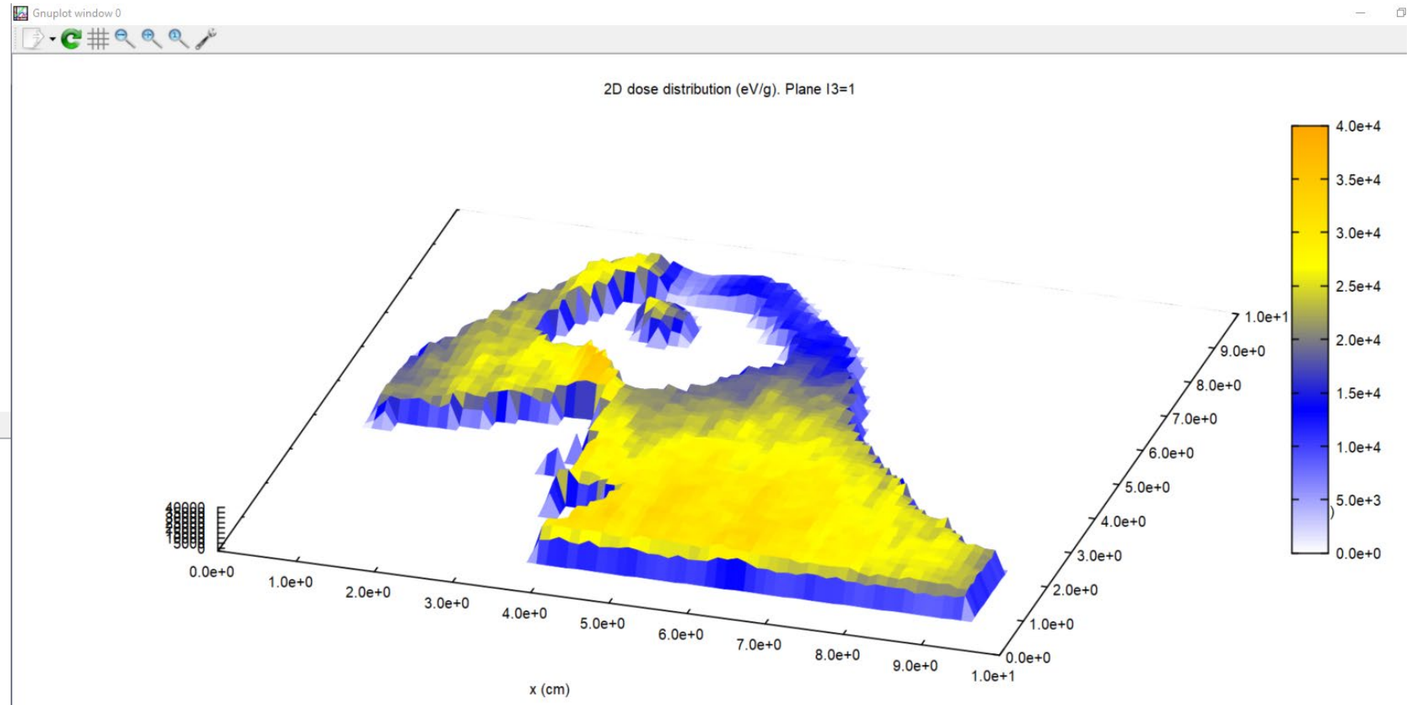
```
TITLE  PUF^2In Generated Input for a box lattice
      Created on: Wednesday August 18, 2021 11:36
       >>>>>>>> Source definition.
SKPAR  1        [Primary particles: 1=electron, 2=photon, 3=positron]
SENERG 1e+07           [Initial energy (monoenergetic sources only)]
SPOSIT 5.000000 -100 1.000000             [Coordinates of the source]
SRECTA 89.427 90.573 87.138 92.862  [Rectangular beam; angles in deg]
       >>>>>>>> Material data and simulation parameters.
MFNAME Titanium.mat                                [Material file, up to 20 chars]
MSIMPA 1E5 1E4 1E5 0.05 0.05 5E3 5E3        [EABS(1:3),C1,C2,WCC,WCR]
MFNAME Air.mat                             [Material file, up to 20 chars]
MSIMPA 1E5 1E4 1E5 0.05 0.05 5E3 5E3        [EABS(1:3),C1,C2,WCC,WCR]
MFNAME 300-PET.mat                            [Material file, up to 20 chars]
MSIMPA 1E5 1E4 1E5 0.05 0.05 5E3 5E3        [EABS(1:3),C1,C2,WCC,WCR]
       >>>>>>>> Geometry and local simulation parameters.
GEOMFN box.geo                         [Geometry file, up to 20 chars]
        >>>>>>>> Absorbed dose distribution.
GRIDX   0 10.0000   39         [X coords of the box vertices, no.of bins]
GRIDY  0.0000   10.0000   39 [Y coords of the box vertices, no.of bins]
GRIDZ   0 2.0000 1          [Z coords of the box vertices, no.of bins]
       >>>>>>>> Job properties.
DUMPTO dump.dat                    [Generate this dump file, 20 chars]
DUMPP    10                                  [Dumping period, in sec]
LTRACK 1000                  [Generate shower files for visualisation]
NSIMSH 1e+06                     [Desired number of simulated showers]
TIME   2E9                        [Allotted simulation time, in sec]
END
```

- Input and geometry files are automatically created.
- A knowledgeable user can see all the parameters used in the calculation.
- Allows for independent review of the calculation.
- All input and output files are available, along with data files and plots.
- These files can be run in PENELOPE, outside of the graphical user interface.

PUFFIn – 2D – Plots using Gnuplot

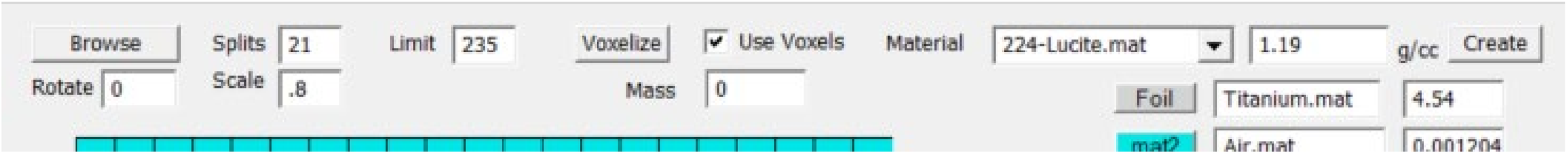
- The Gnuplots are re-directed to the interface, but can be viewed directly with gnuplot outside of PUFFIn.



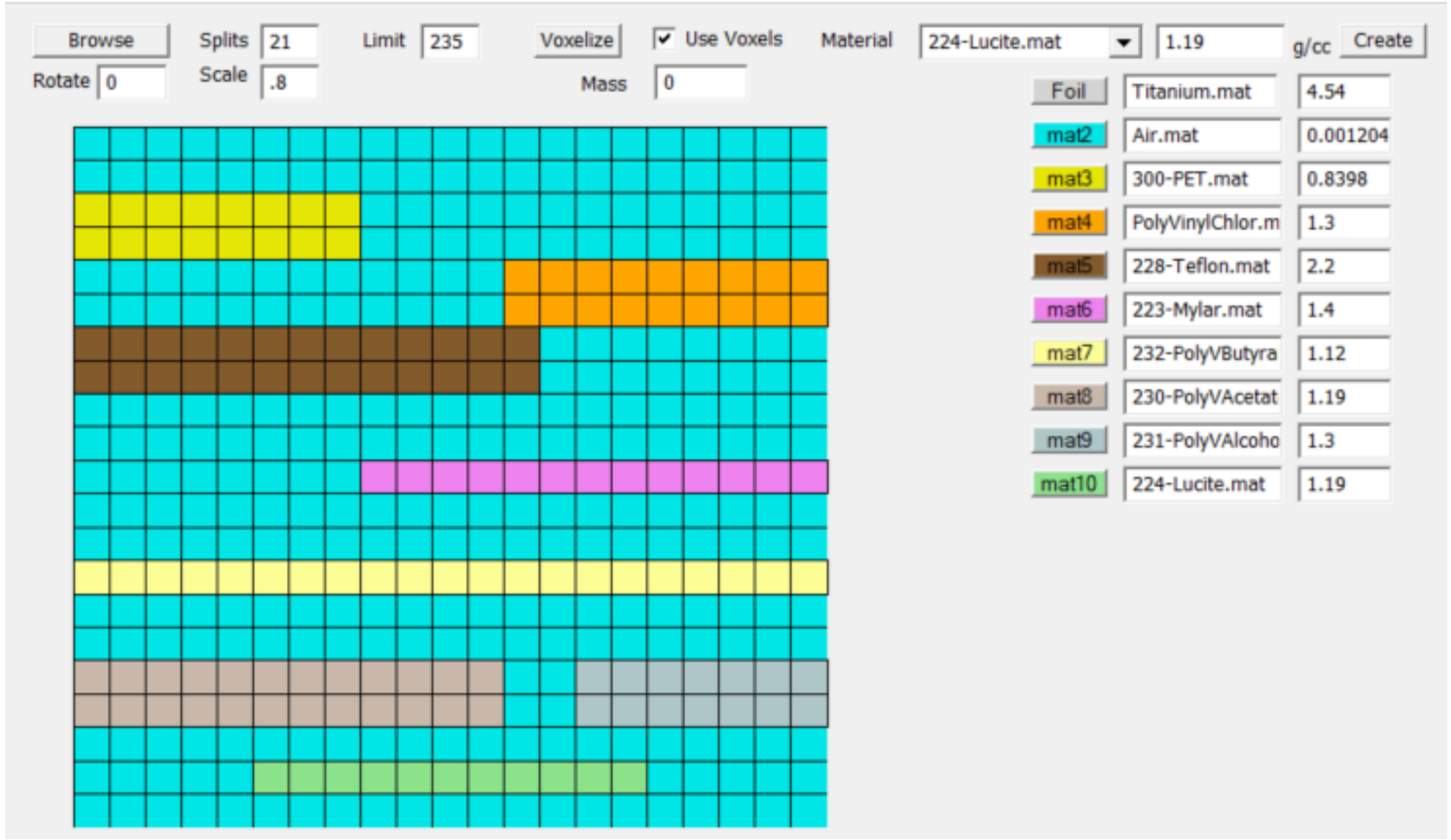


PUFFIn – 2D – Voxelization

- The user enters the number of voxels to create (splits).
- The user enters the RGB level (1-255) to determine what is air and what is product for the initial voxelization.
- Once voxelization has completed, the user can further modify the material in the voxels by clicking and or dragging the mouse to select the voxels.
- The total mass (grams) from the sum of the voxels is calculated as an independent check.

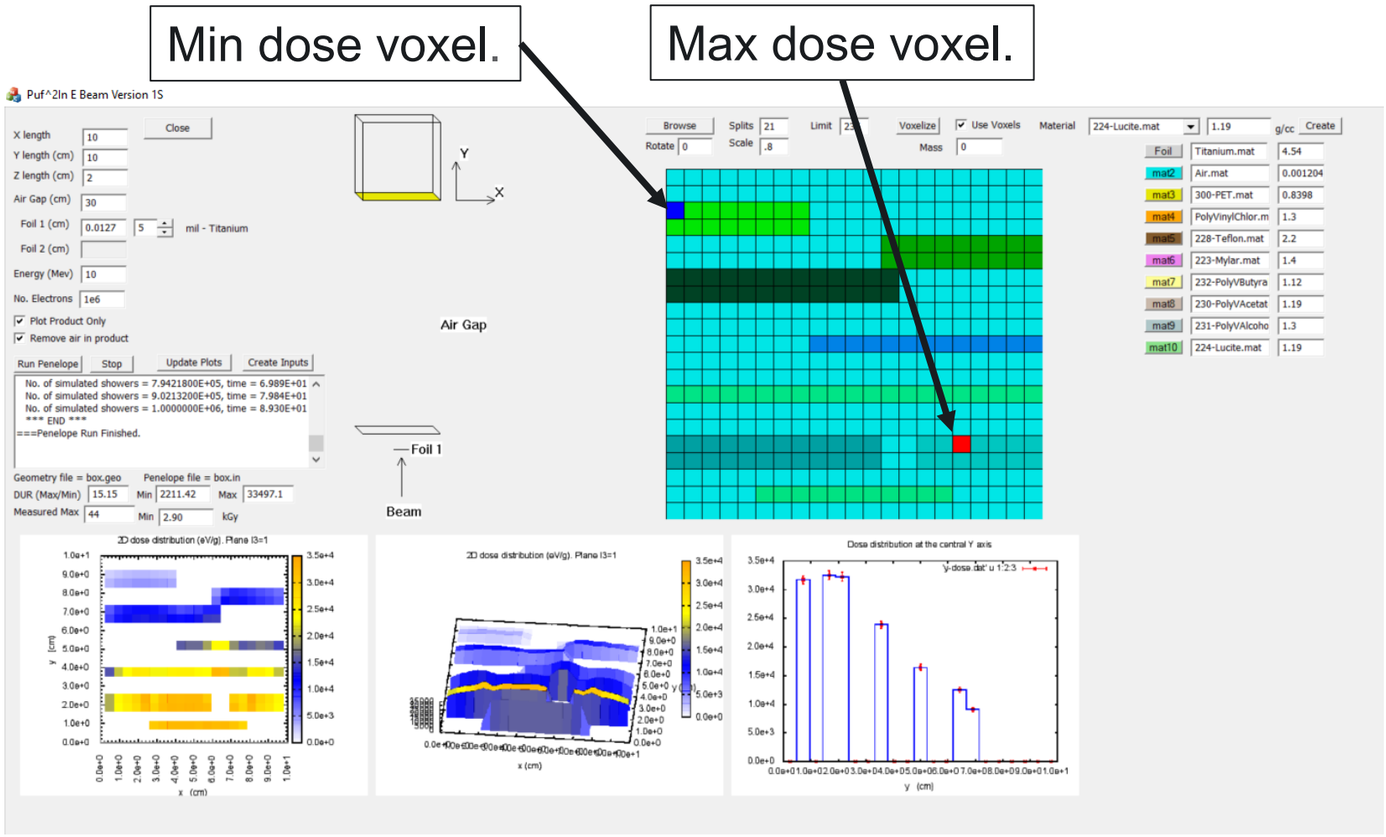


PUFFIn – 2D – Simple Voxel Geometry



- Load a blank image.
- Set the level of voxelization (21 splits).
- Select voxelize to define air in all voxels.
- Set the material definitions.
- Drag or click with the mouse to set the material within a voxel or group of voxels.
- Run PENELOPE.

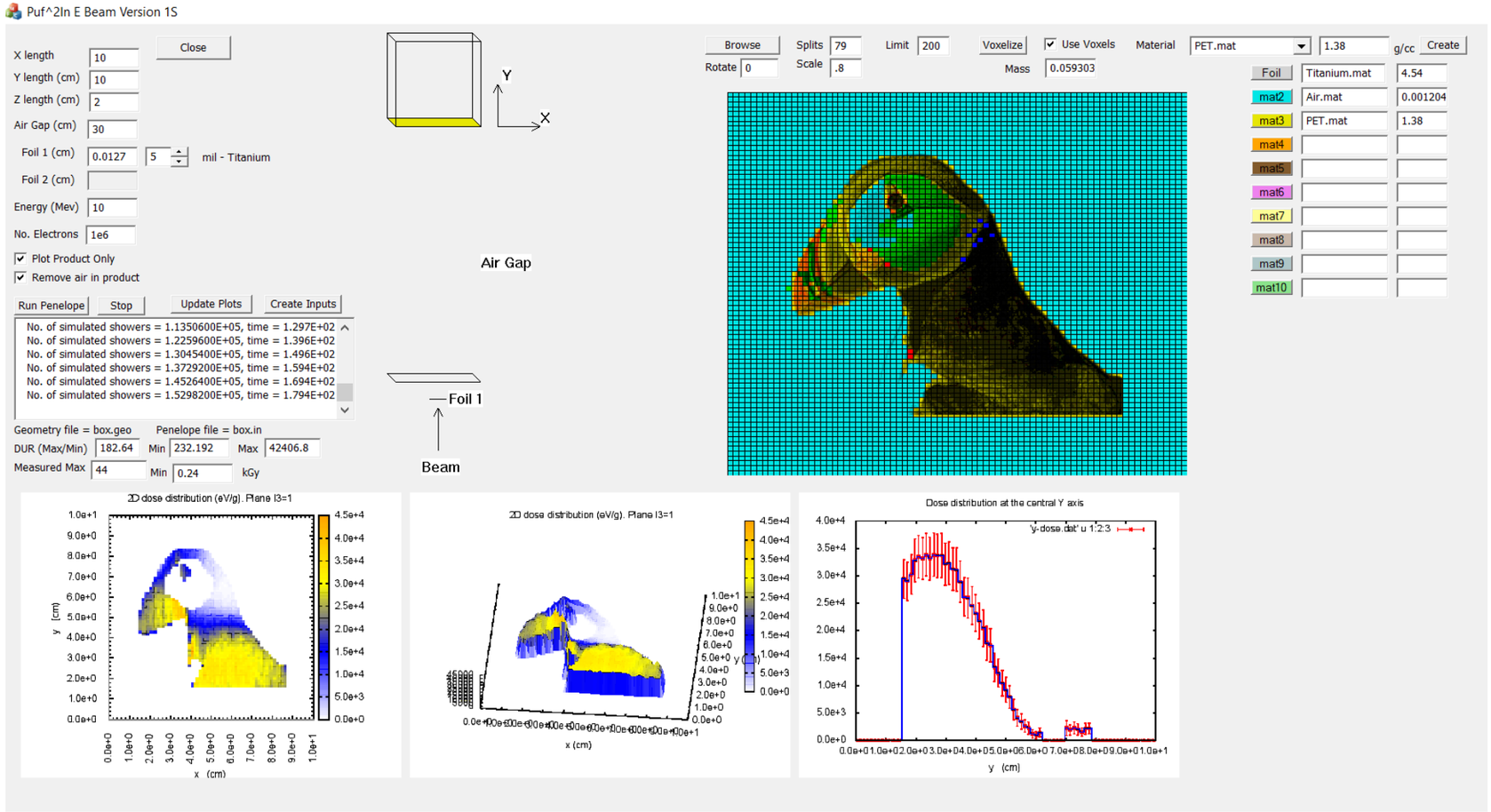
PUFFIn – 2D - Multiple Materials



- PENELOPE is run and the DUR is calculated with a blue square showing the minimum location, a red square showing the maximum location.
- The ratio of min to max is calculated (DUR).
- The min value is normalized to the beam intensity (kGy).

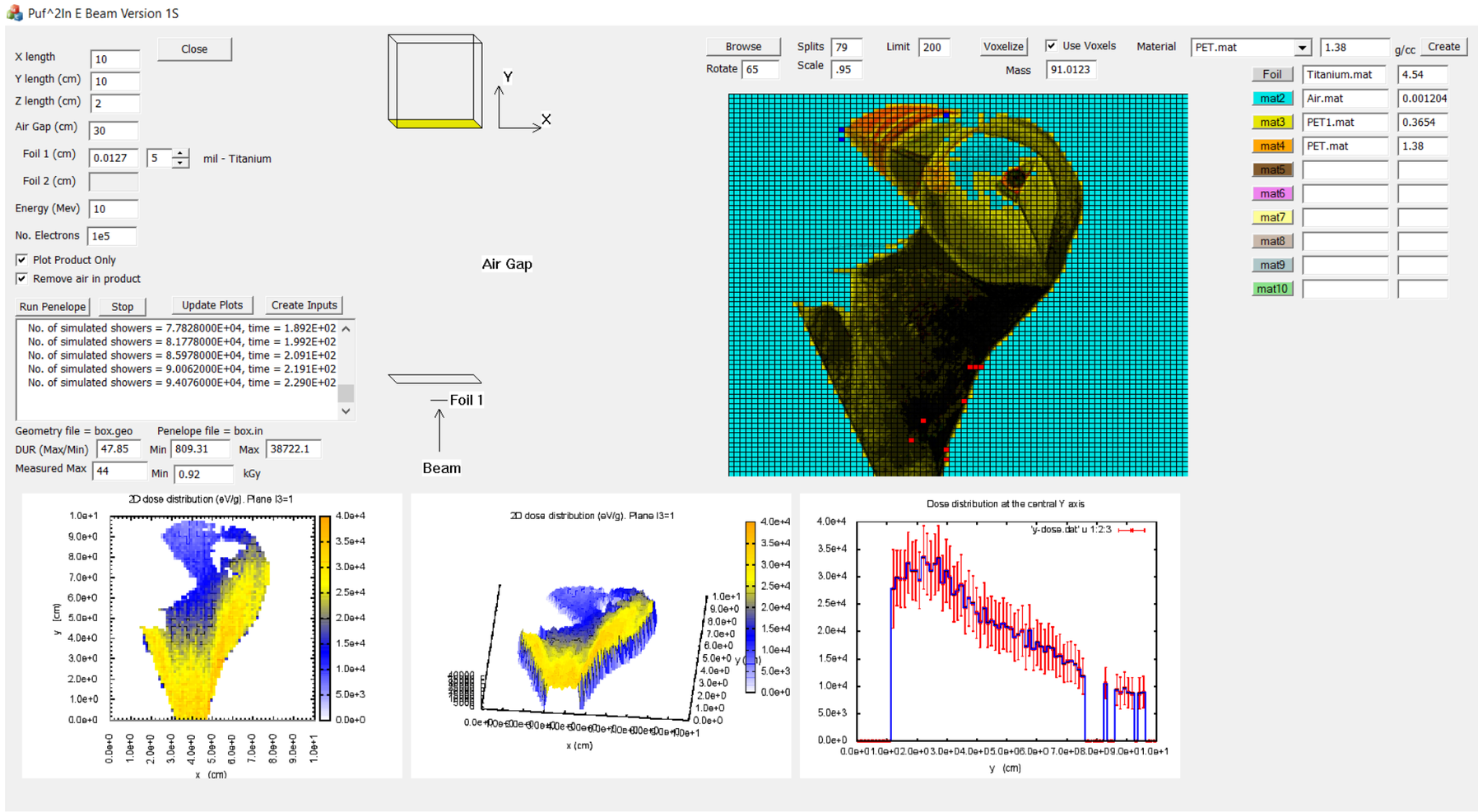
PUFFIn – 2D – Photo geometry

- Photos can be uploaded and voxelized.
- PNG, JPG, and BMP files are supported.
- Once uploaded, the image can be voxelized.
- Additional changes can be made with the mouse.
- PENELOPE is then run on the voxelized geometry.



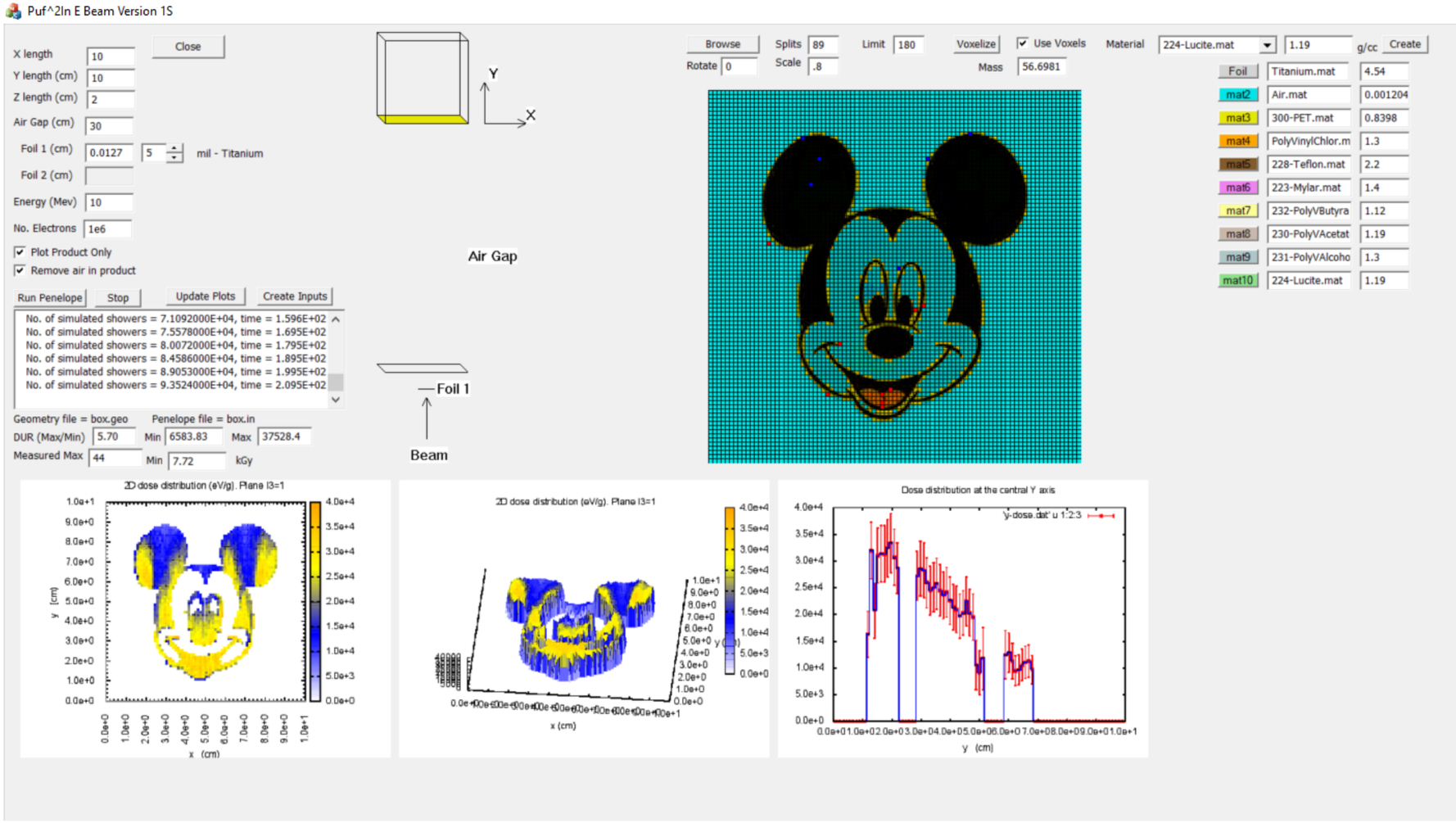
PUFFIn – 2D – Photo geometry

- Images can be rotated or resized.



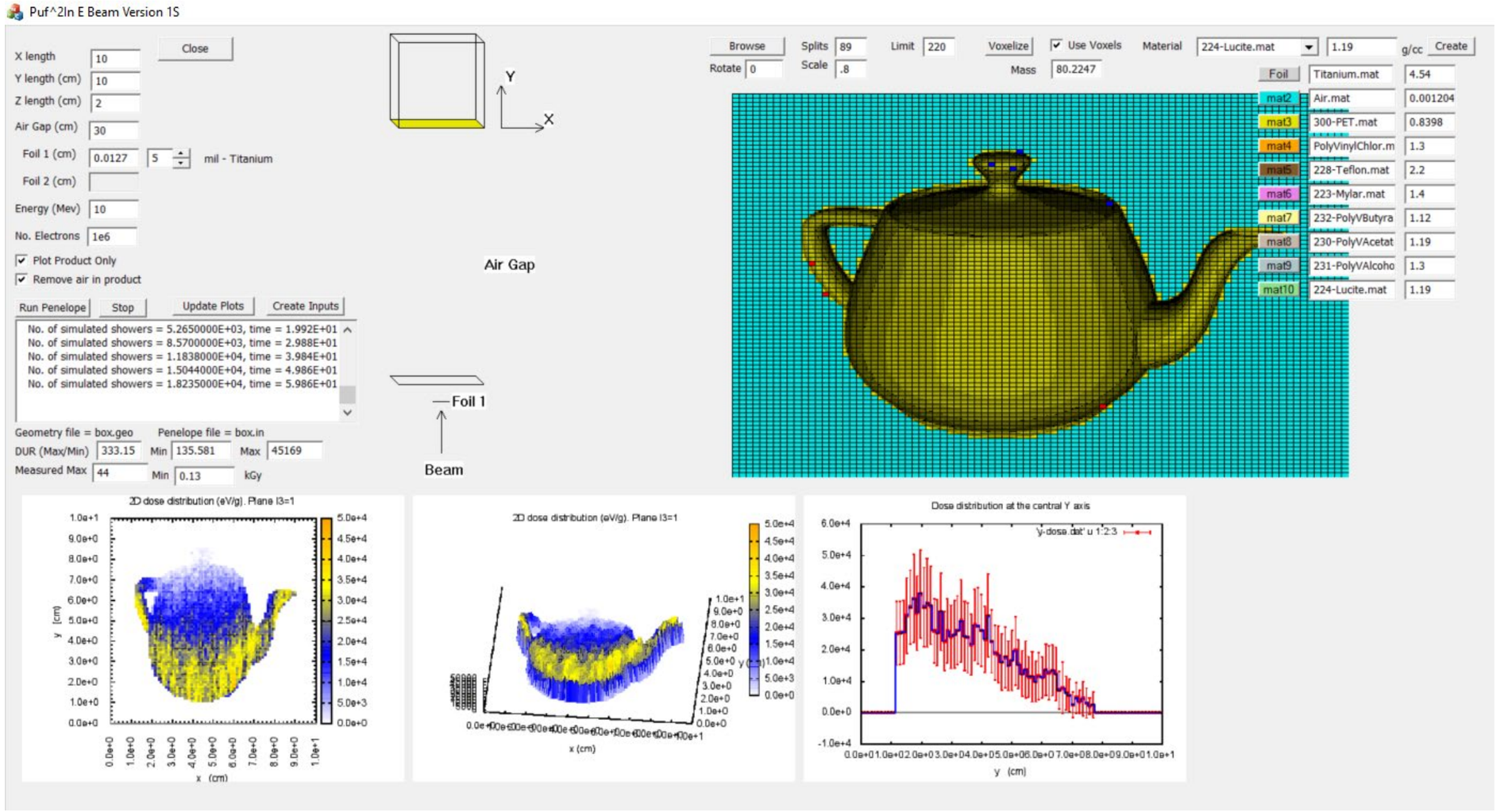
PUFFIn – 2D – Photo geometry

- Any image can be voxelized.



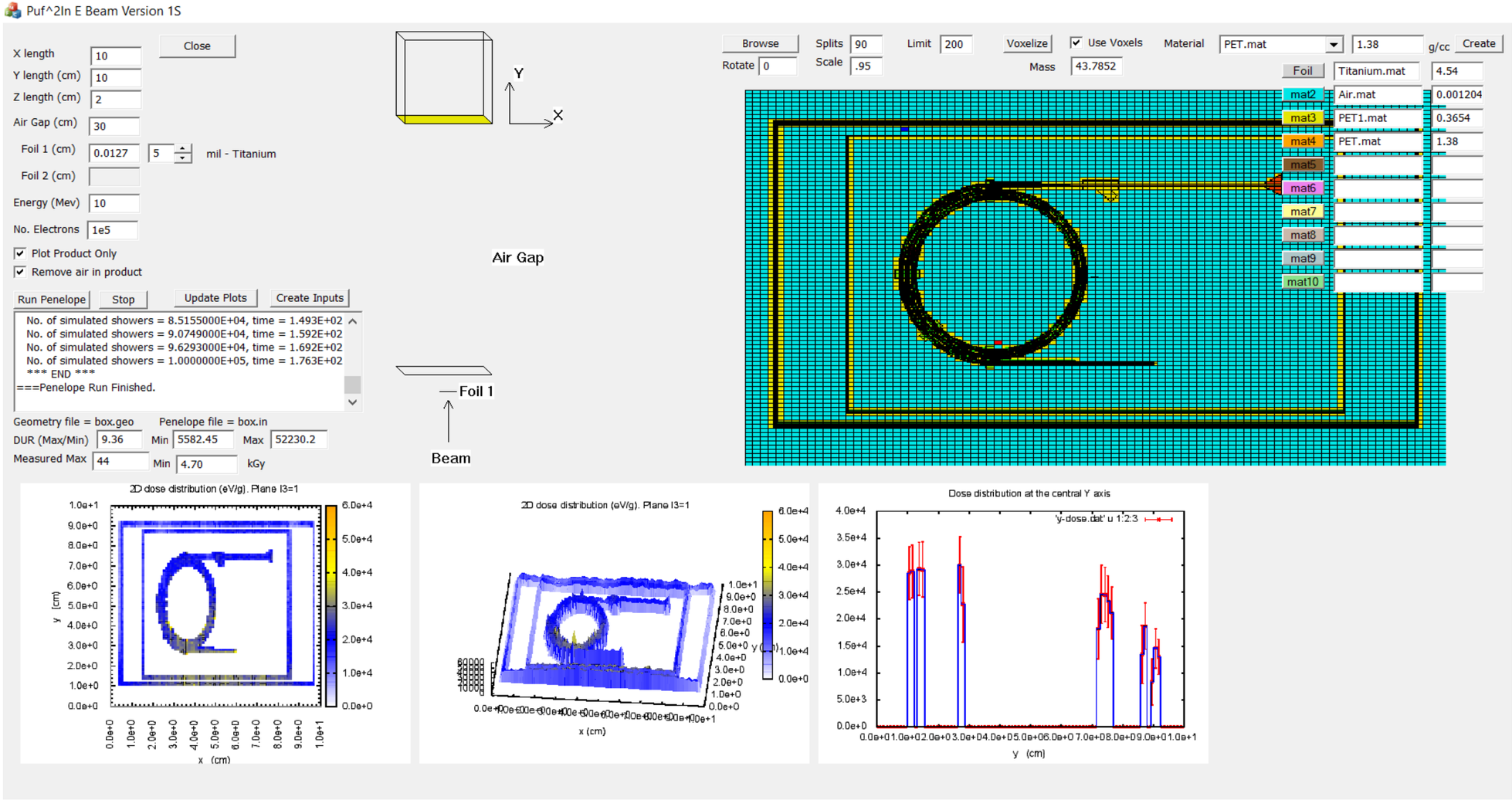
PUFFIn – 2D – CAD Teapot

- Plots from CAD can be voxelized.

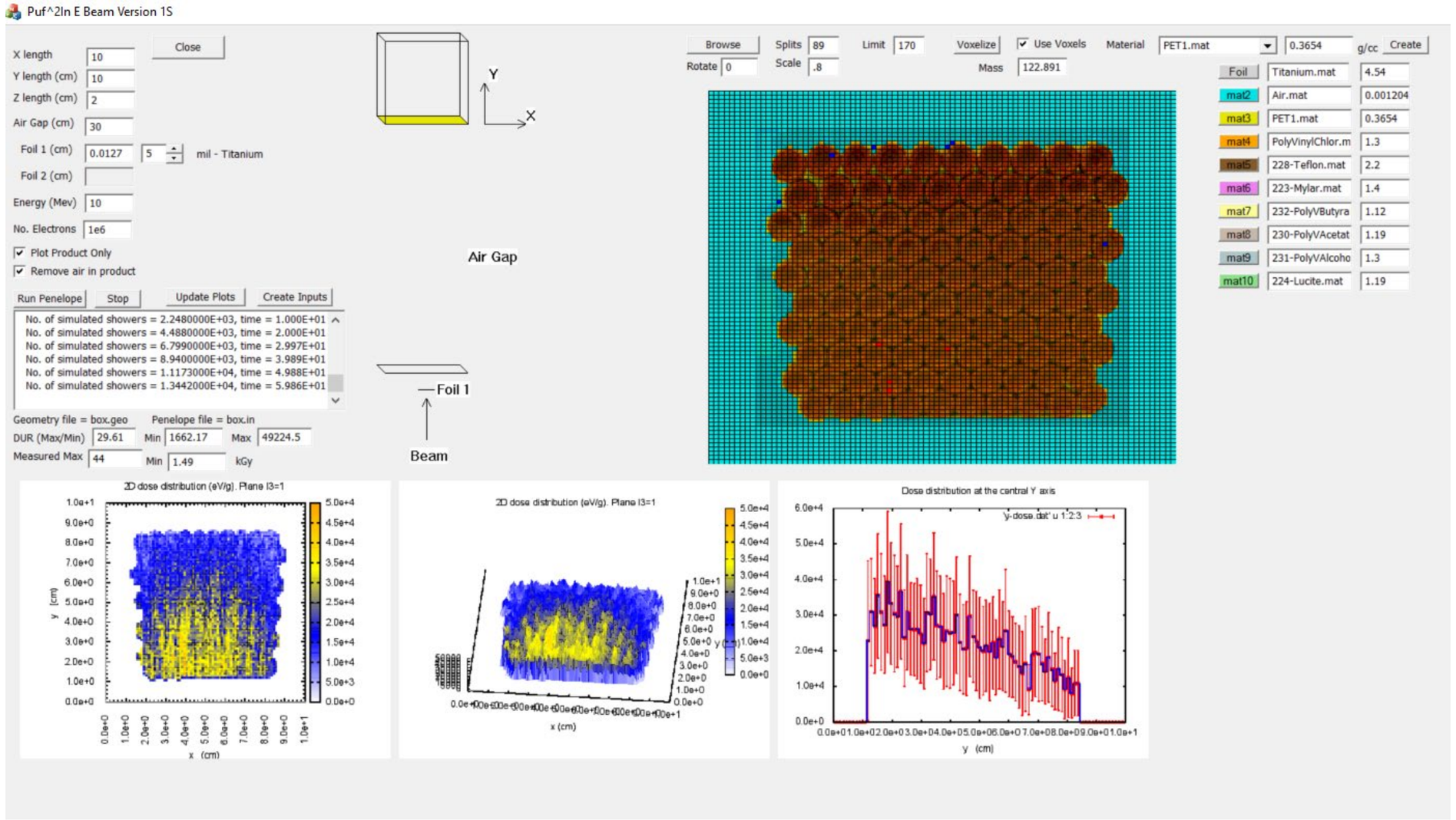


PUFFIn – 2D – Geometry Plot.

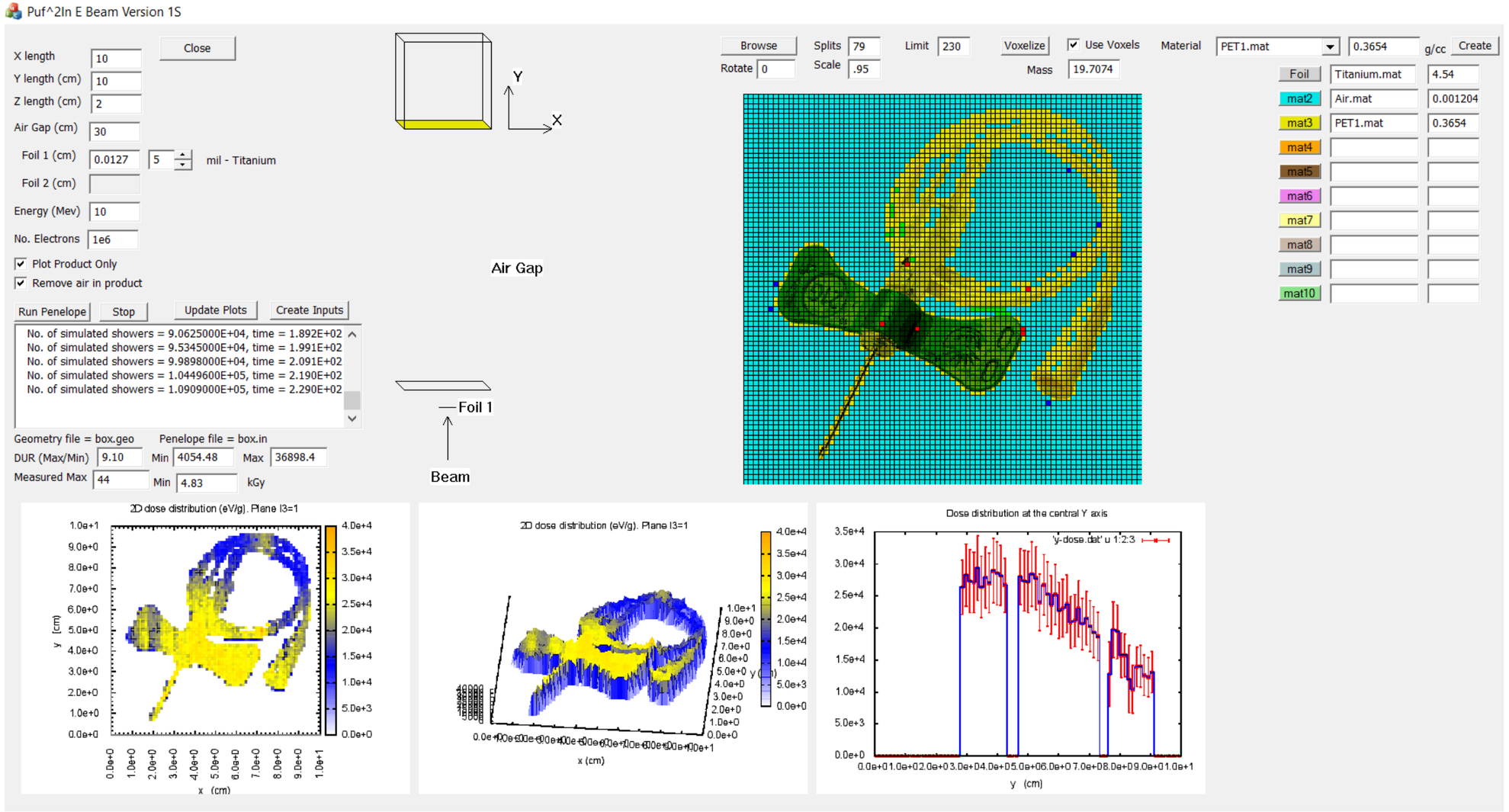
- Plots from other codes can be voxelized.



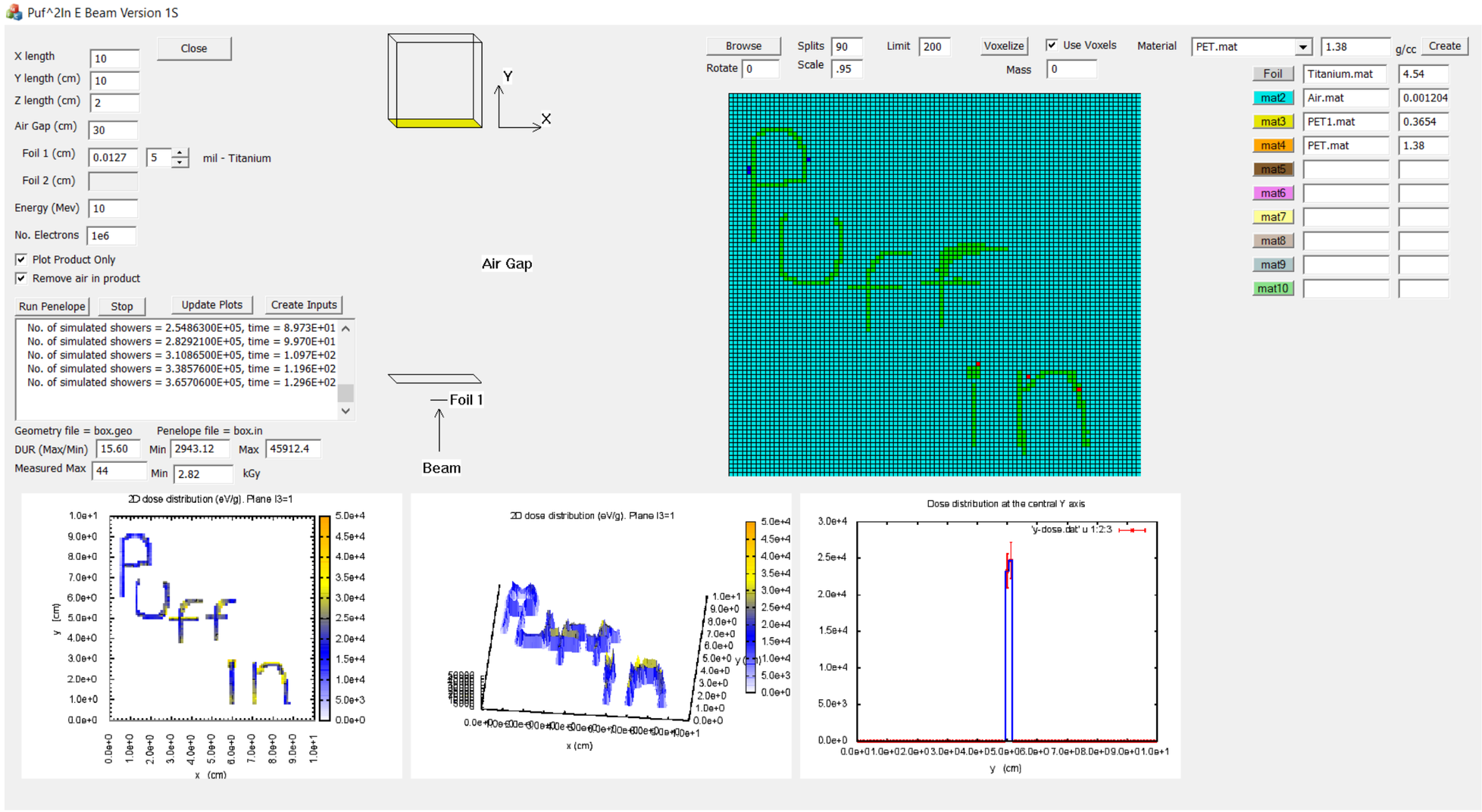
PUFFIn – 2D – Box of BD Tubes



PUFFIn – 2D – BD Push Button



PUFFIn – 2D – Free Hand Drawing



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Future Work

- Once the 2D software is developed sufficiently, compare to product dose mapping measurements, and revise as needed.
- Have several select individuals in the industry pilot test the software, and use their experience/feedback to revise as needed.
- If the testing of the 2D version indicates that this approach/tool could have the accuracy, precision, speed and user friendliness needed to allow non-experts to use with minimal training, and that the labor and time to obtain results is minimal, then continue with development of 3D version.
- Explore the best way to extend to 3D.
  - Multiple photos or images
  - 3D photos used for 3D printing.
  - X-ray images.
  - CAT scan images.
  - CAD geometry.

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Fermilab 3rd Medical Device Sterilization Workshop:

Understanding the Possibilities

September 22-24, 2021

Thank you

Questions?

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