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PUFFIn – A New Simplified and Ultra-Fast Dose Simulation Software Tool

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Background and Objective

- A 2017 report by Fermilab, as well as a 2020 IAEA report, conclude that significant impediments remain for *medical device manufacturers* who desire 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, education and tool gaps, not necessarily a lack in technology.
- The Office of Radiological Security (ORS) asked PNNL to assemble an international collaborative team to identify and fill these gaps.
- The collaborative team includes major players in the radiation processing industry, and is named Team Nablo in memory of e-beam and packaging pioneer Sam Nablo.
- This presentation covers a task added in 2021, which was to identify and fill gaps in dose simulation software tools.

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Desired Features for the Software Tool

- As a result of the limitations of current commercial software identified by the survey, the following approach was pursued:
  1) Create a graphical user interface that provides visual representations of accurate dose distribution in items.
  2) Utilize the PENELOPE radiation transport code, which is much more amenable for X-ray and E-beam.
  3) Have a focus of a learning and training tool.
  4) Must be as simple as possible so it can easily be learned and used by individuals who are novices at radiation transport and modeling.
  5) For non-moving/static products only, and of low to medium geometry complexity (in order to achieve simplicity goal).

Desired Features continued -

6) Options for cobalt-60 gamma-ray, X-ray and E-beam fields.

7) Options for multiple beam directions.

8) Provide accuracy and precision of the dose distribution sufficient for a majority of users.

9) Provide the maximum and minimum dose locations and associated Dose Uniformity Ratio (DUR).

10) Minimum labor for training.

11) Simulation/processing times significantly faster than other software.

12) Can utilize a regular laptop or PC.

13) Available to any trained user and at no cost.

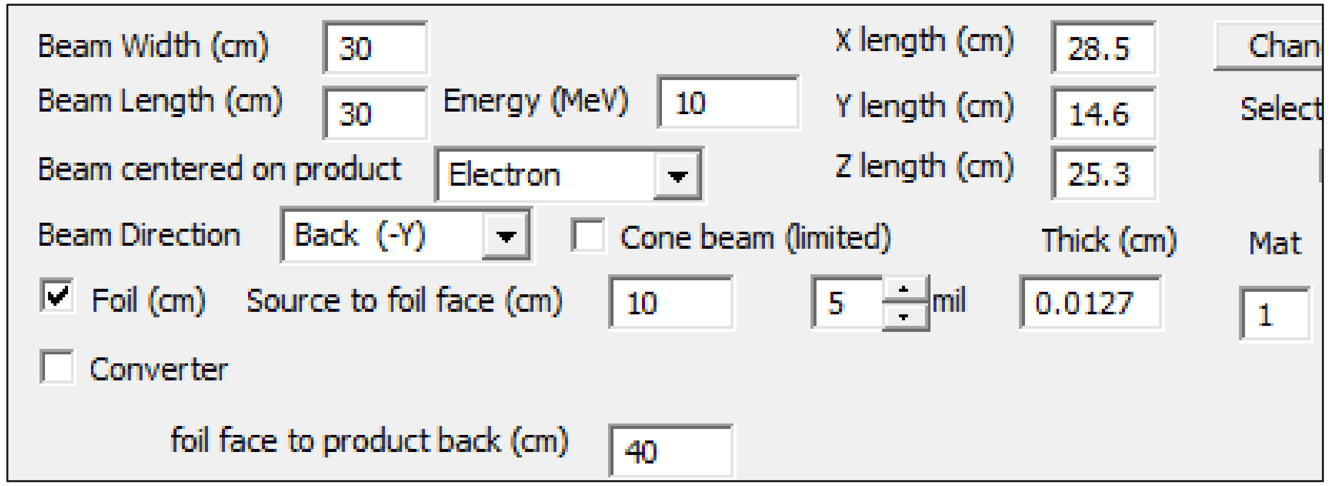
The Resulting PUFFIn software
(Penelope User Friendly Fast Interface)

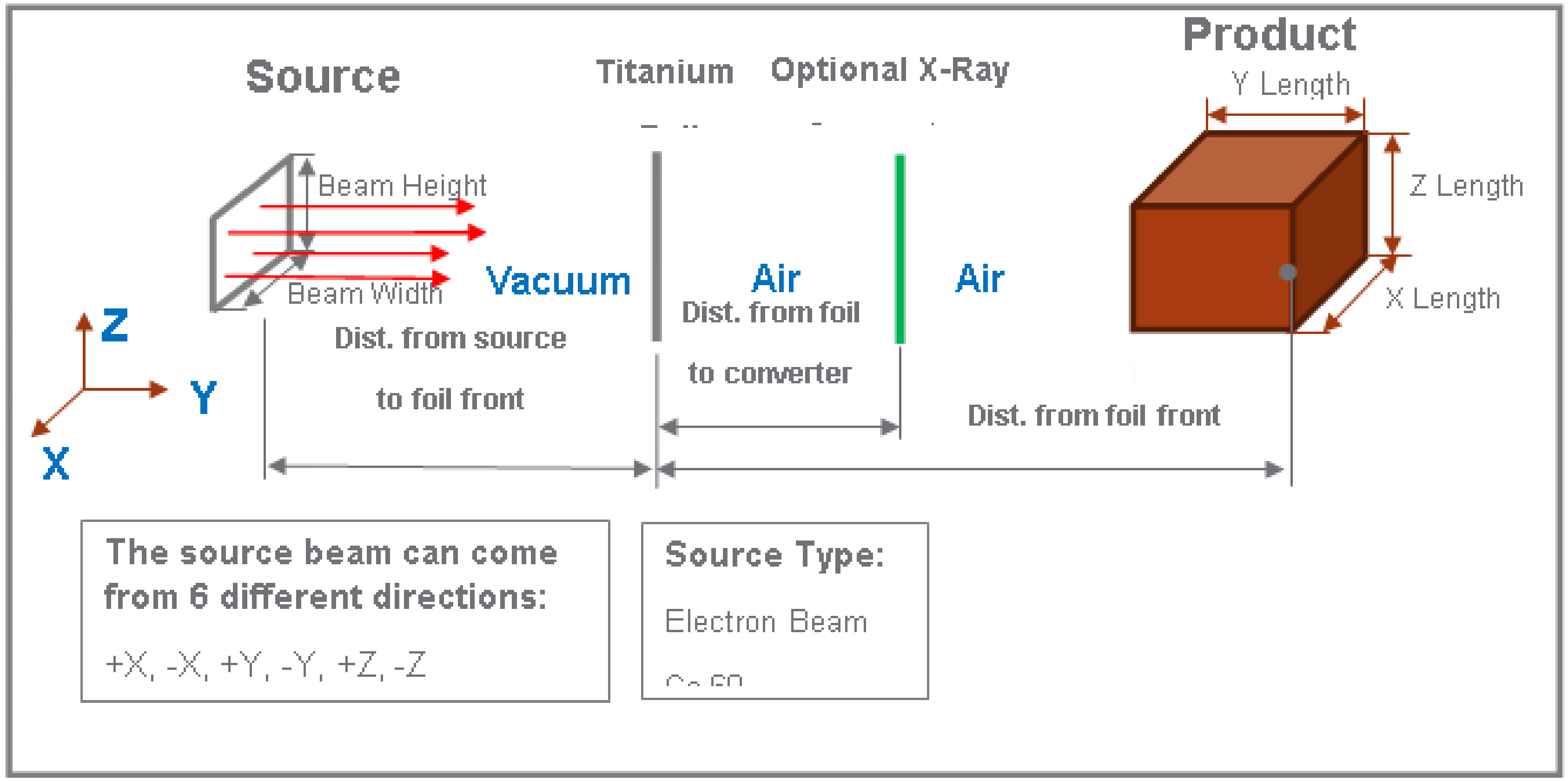
- The user interface uses the PENELOPE Monte Carlo radiation transport code.
- PENELOPE is not integrated into the interface, but called as an external program.
- The interface creates a voxel geometry of the product.
- Multiple options for import file types:
  - Create the geometry within the code
  - Hand-drawn image files (PAINT software?)
  - Any photo
  - Typical 3D CAD files
  - CT scan files (DICOM)
- Up to 20 different materials per item simulated.
- Create own material or select from PUFFIn's large library of common materials.

The Resulting PUFFIn Software continued -

- The source can be changed to show the expected dose from E-beam, X-rays and cobalt-60 gamma-rays for the same product.
- The product can be rotated to show changes in DUR dependent on product orientation.
- Multiple beams can be used.
- Applications include:
  - Teaching/Training
  - New product and/or packaging design
  - Legacy product and/or packaging re-design or re-arrangement for alternative source
  - Determination of influence of source type and energy on dose distribution

Product and beam parameters





User input:

- Outside dimensions of the product (X length, Y length, Z length).
- Distance from the beam to the foil.
- Distance from the foil to the back of the product.
- Foil thickness.
- Energy of the beam (MeV).
- Six different beam directions.
- Source can be e-beam, Co-60 or X-ray.

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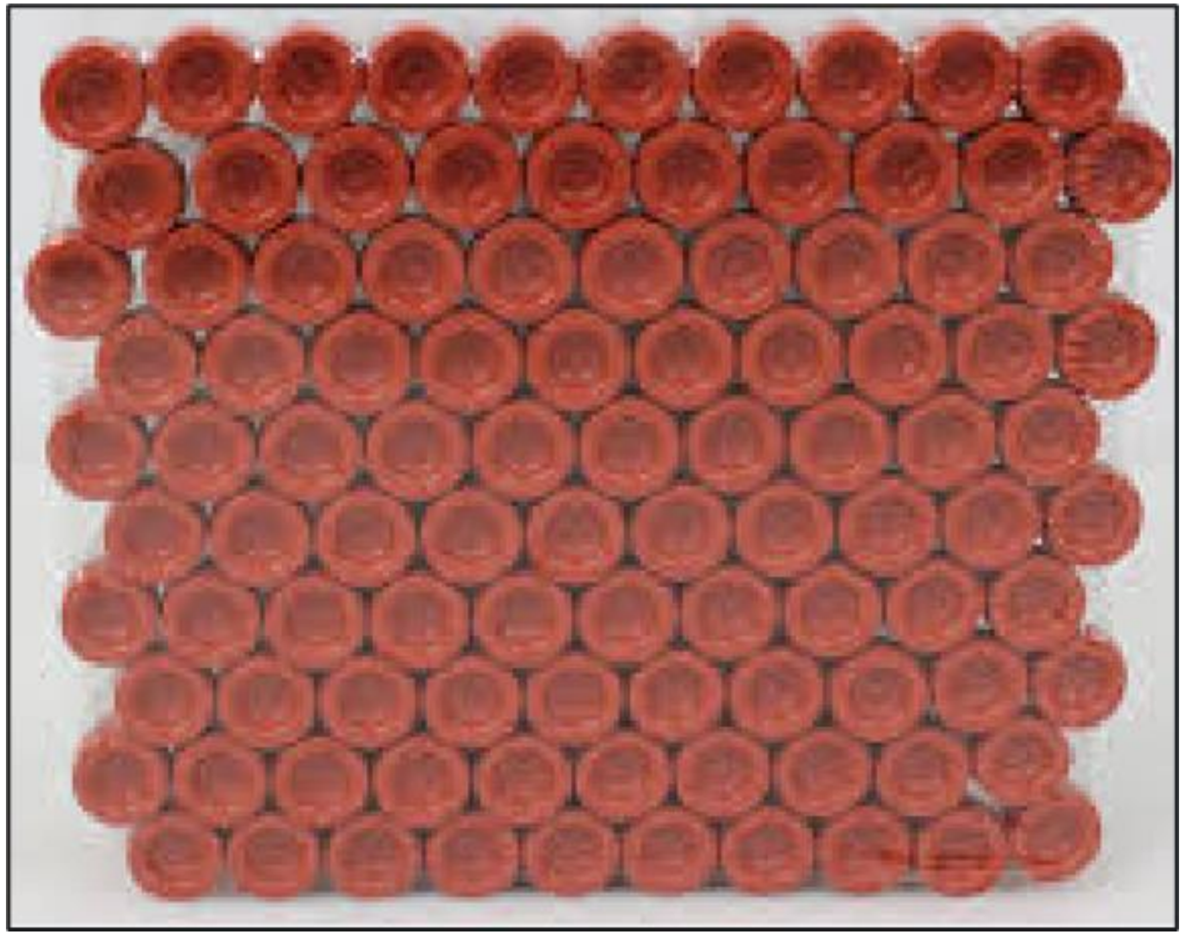
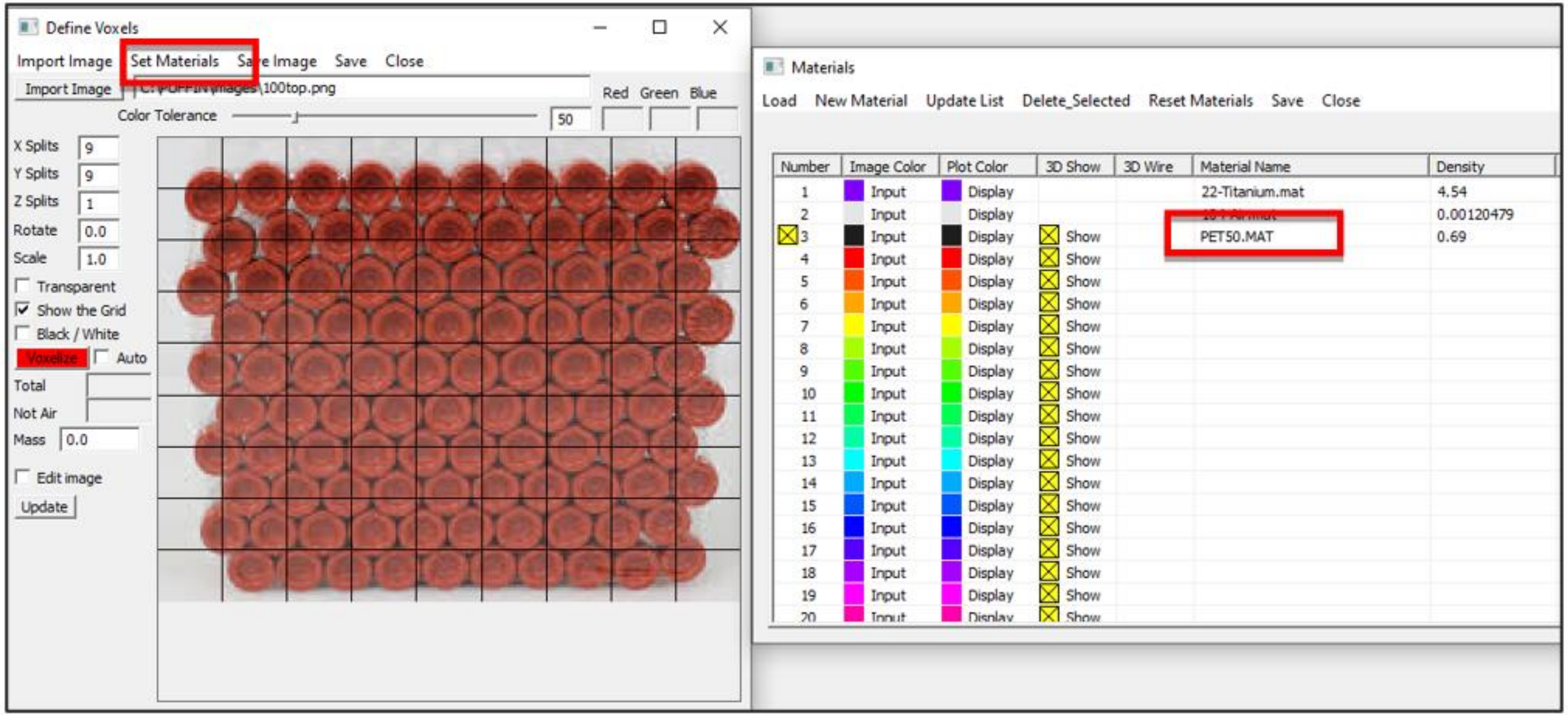
Using Photo of Item – Blood Collection Tubes

Single material and consistent geometry and average density throughout



Voxelizing Photo and Selecting Materials

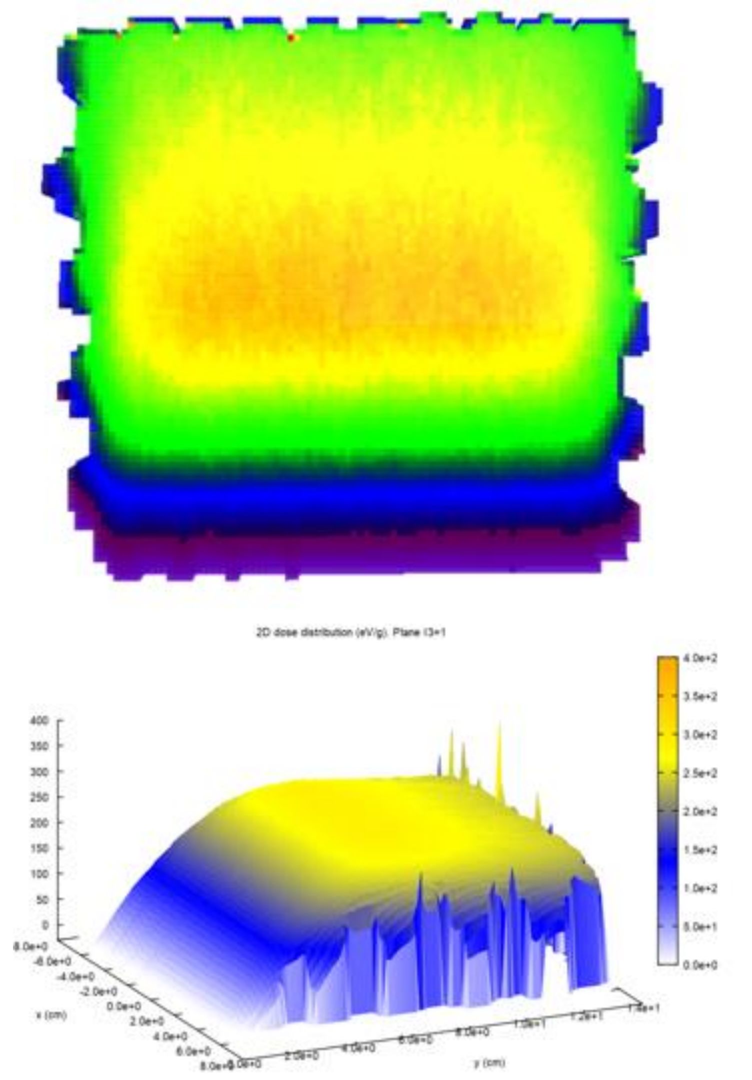
Pixels = 2D   Voxels = 3D



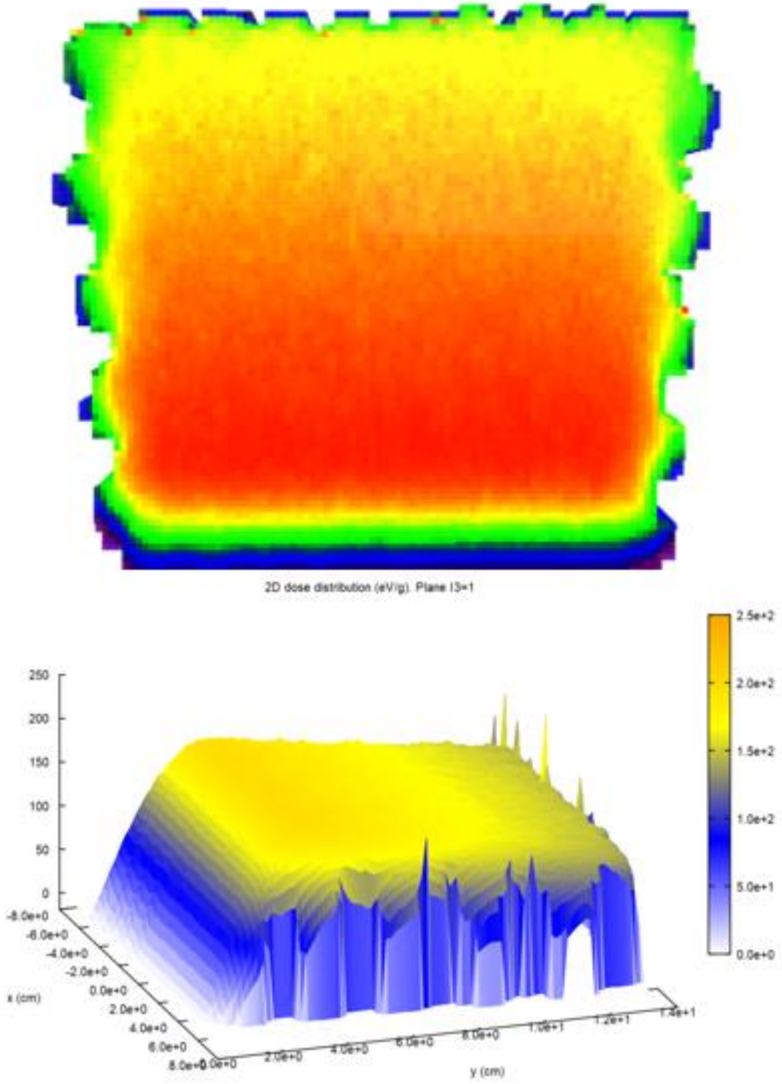
Because the tubes are hollow, a 50% density PET material is used.

Generating Dose Distribution for Various E-beam Energies

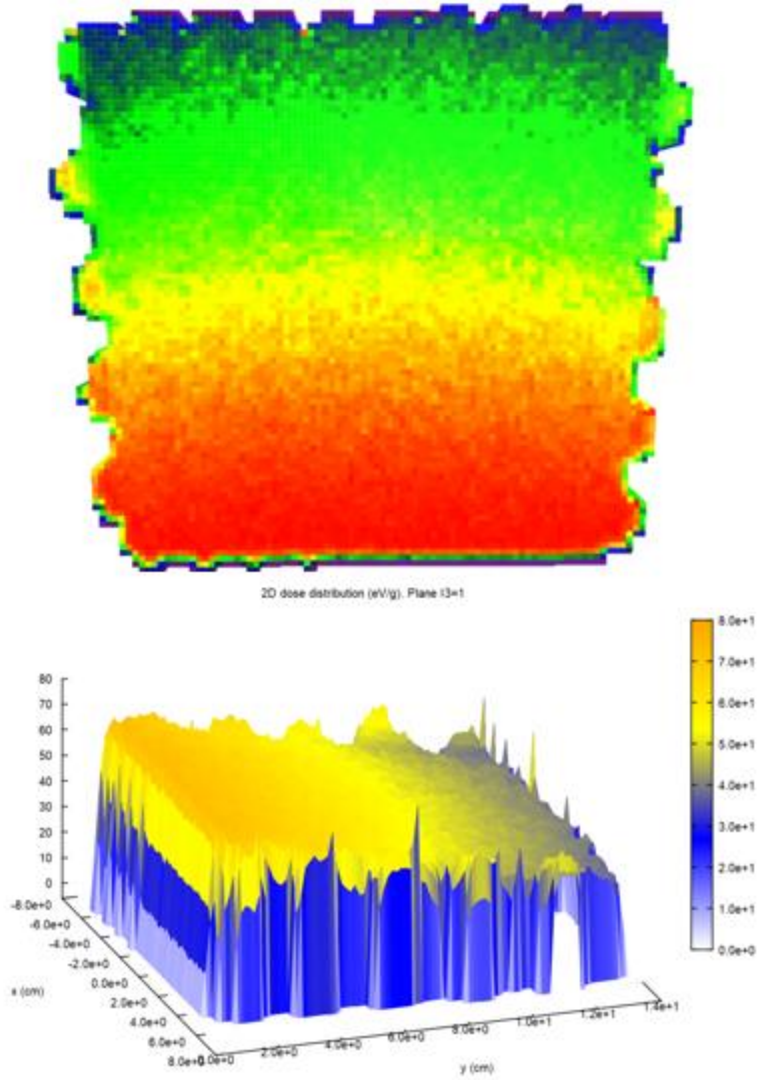
10 MeV



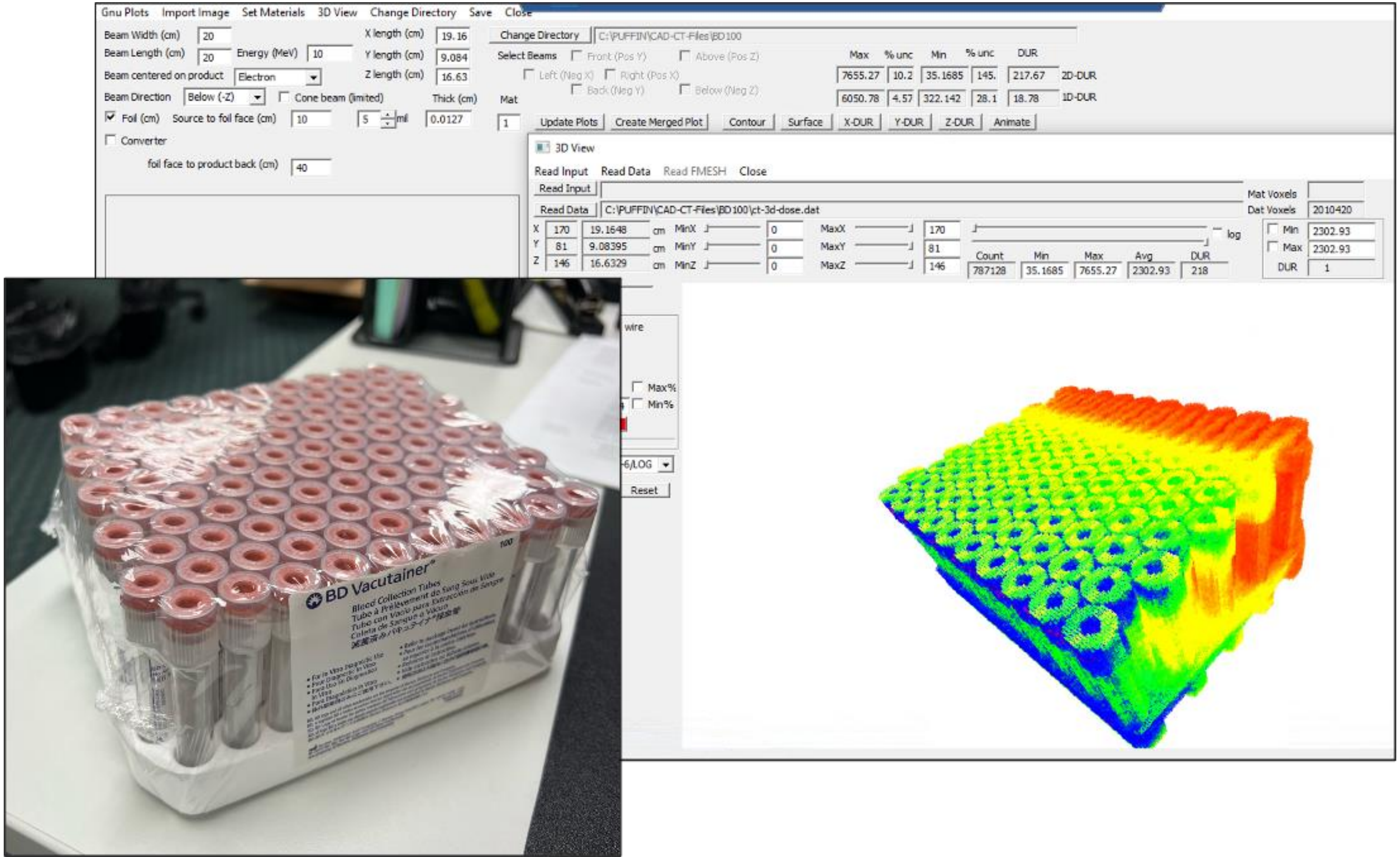
5 Mev



1 MeV



3D Dose Distribution from a CAD File



Steps to Convert CAD Files for PUFFIn

Step1:
Build products using CAD Software

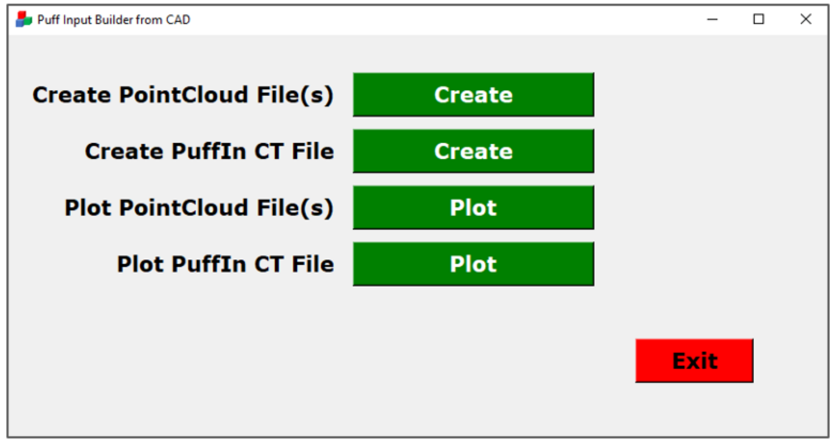
SOLIDWORKS

AutoCAD

Other CAD Software

Step2:
Exported a single STL file for each material.

Step3:
Open the CAD2PUFFIN GUI



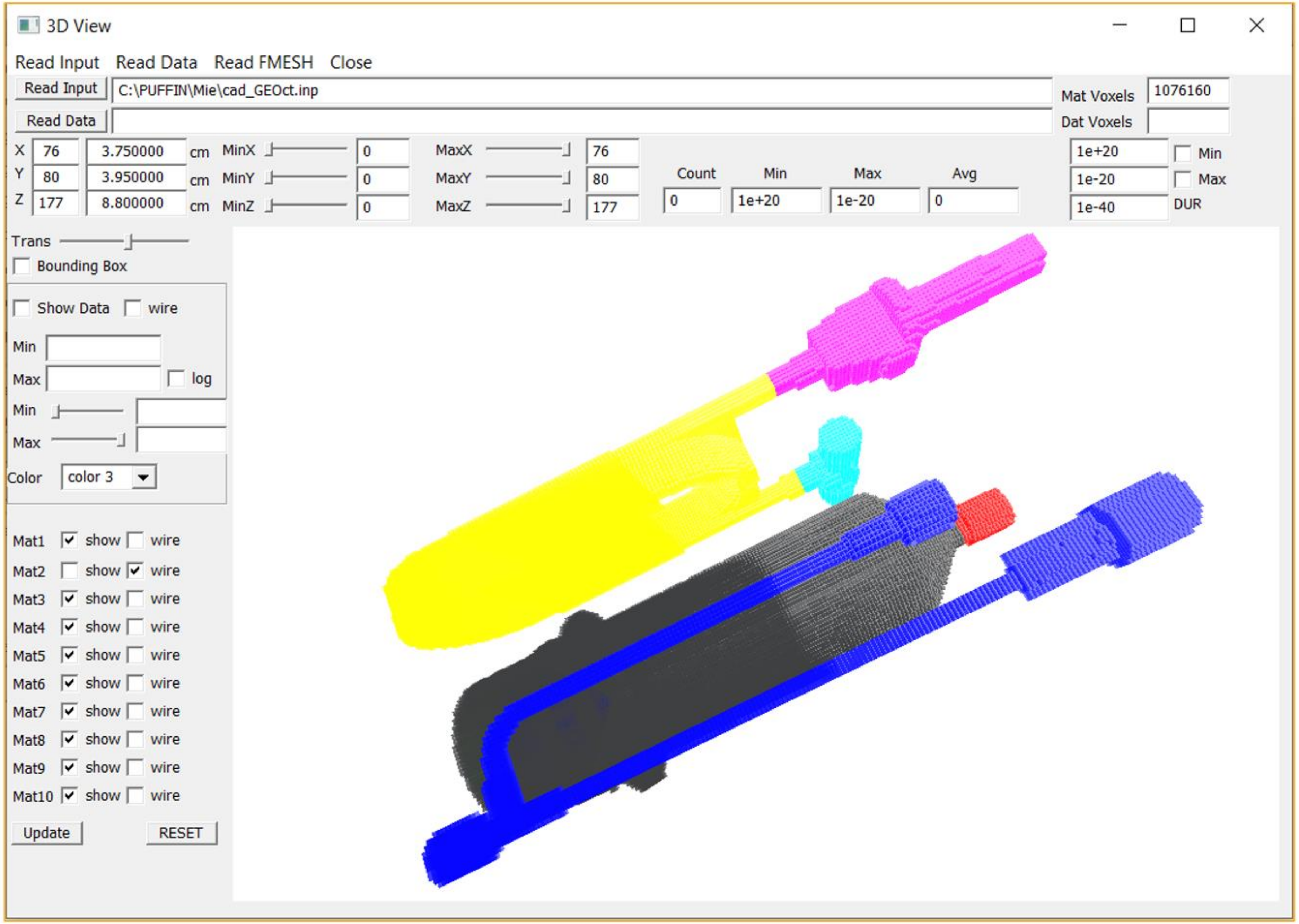
Step4:
Execute CAD2PUFFIn

Step5:
PUFFIn CT file is built

PuffIn CT File

PuffIn

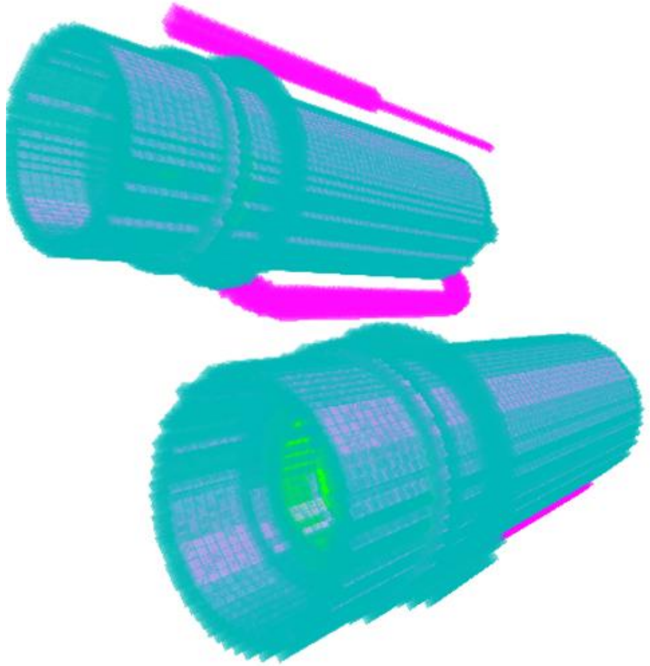
3D Dose Profile of Medical Device – 10 MeV E-beam



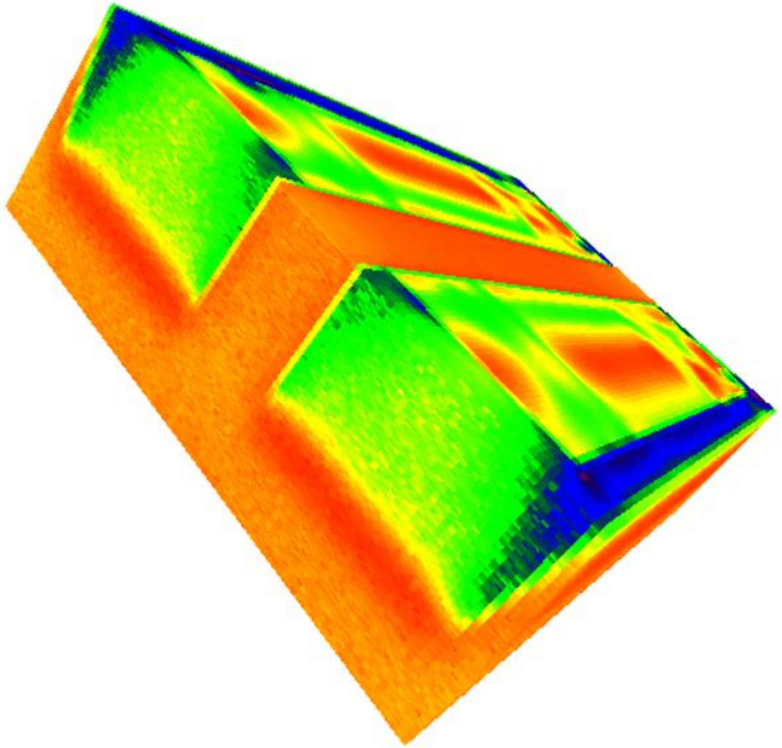
- Voxelize the CAD file
- Import the file
- Run PENELOPE
- Show regions of min and max dose to help with the placement of dosimeters

3D Dose Profile of Medical Device – 10 MeV E-beam

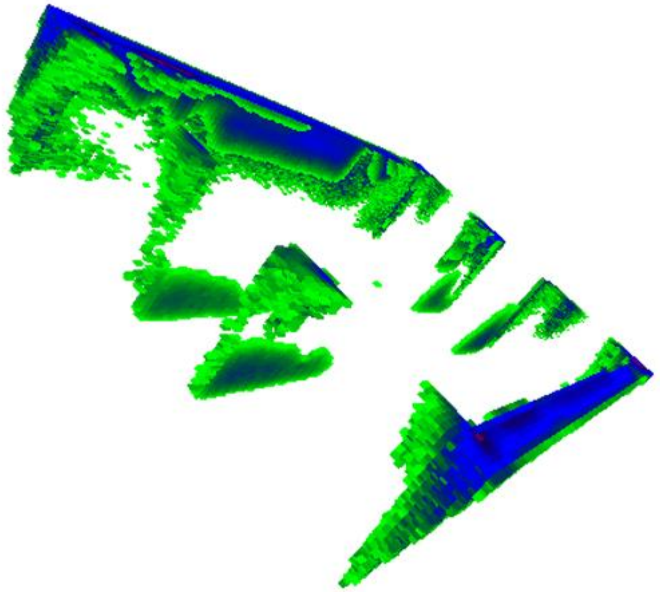
Geometry



Electron Dose



Min Dose



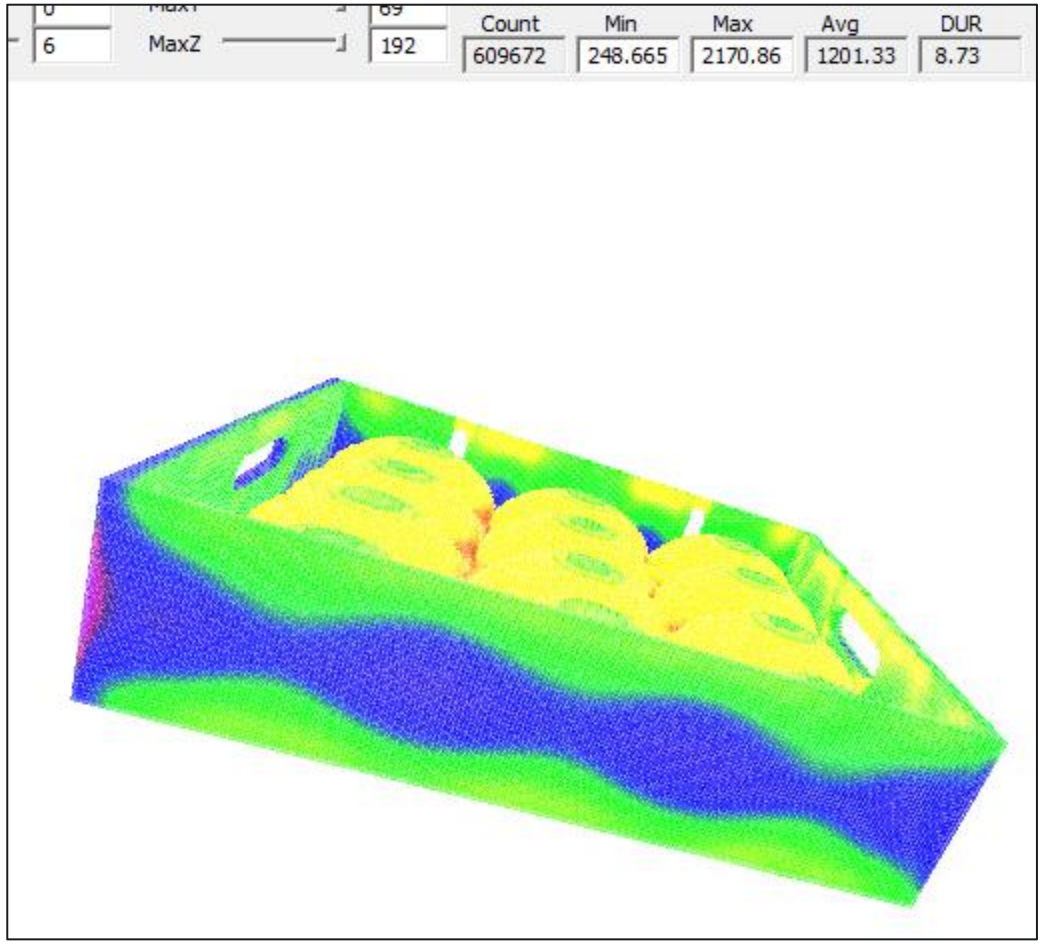
Max Dose

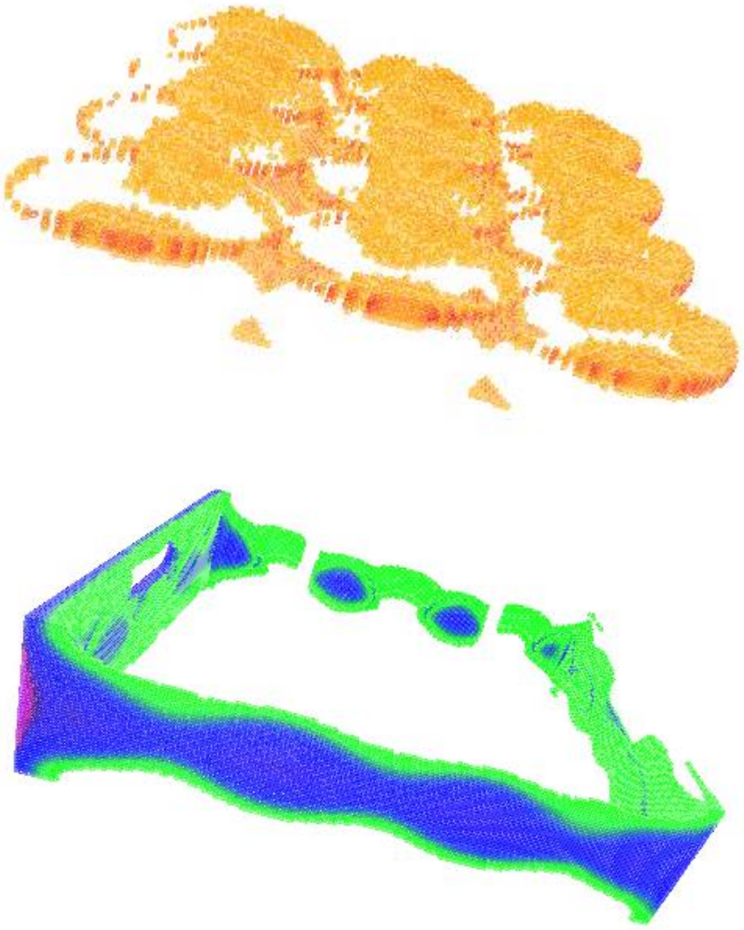
Beam from Bottom direction

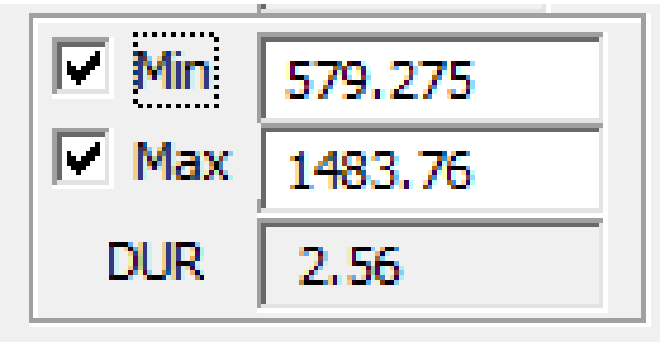
Box of Mangos – Visualize Min and Max Dose Locations

DUR – 8.73

10% DUR – 2.56





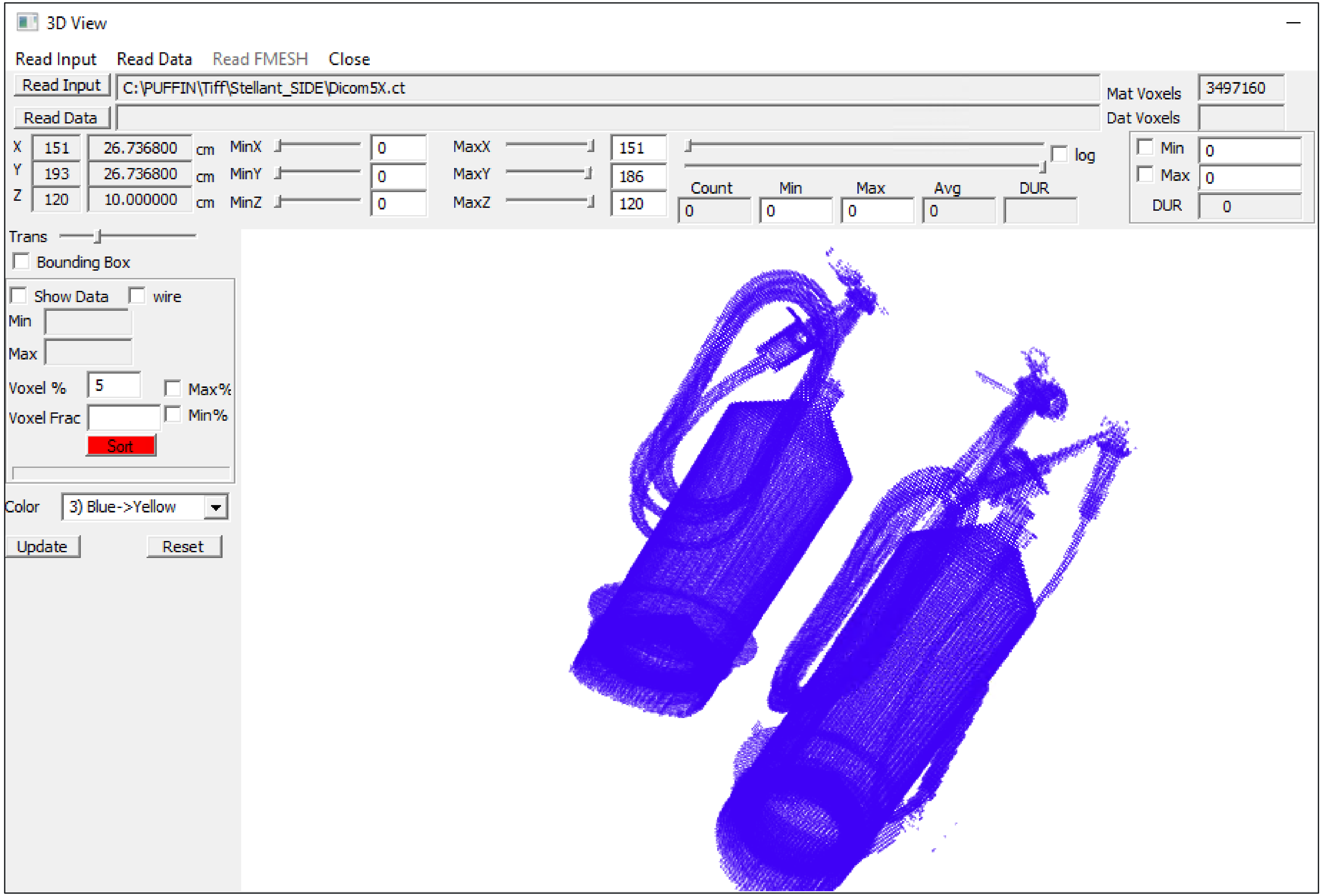


10 MeV E-beam

X-ray Tomography Scan of Medical Device

User options:

- Scan using X-ray Tomography
- Generate data
- Convert to PUFFIn
- Display results



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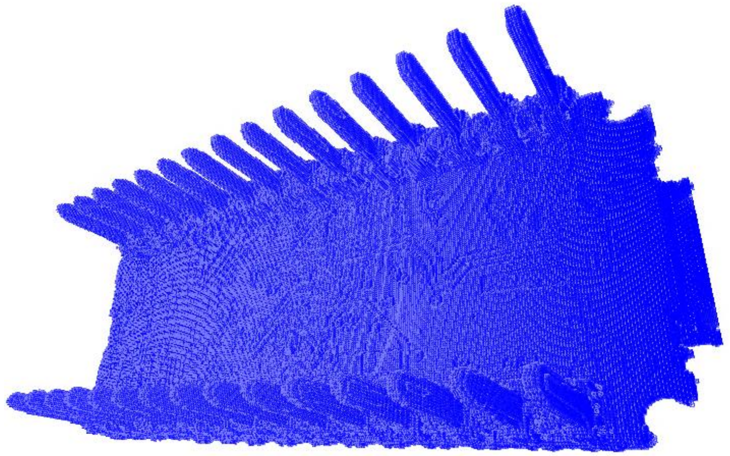
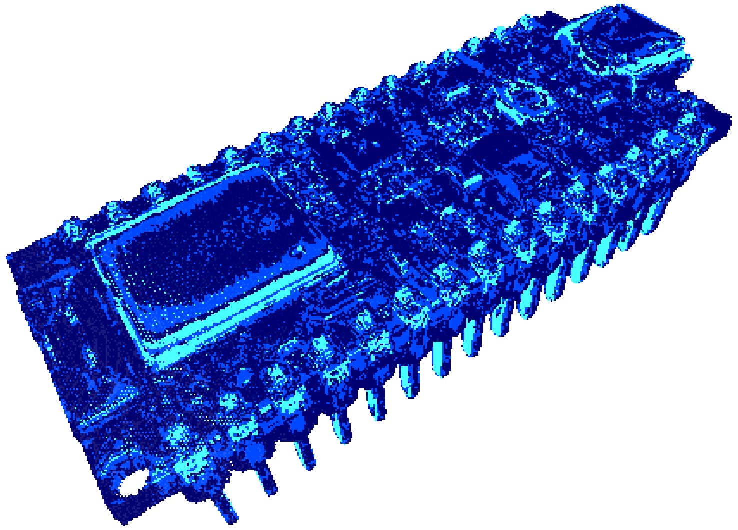
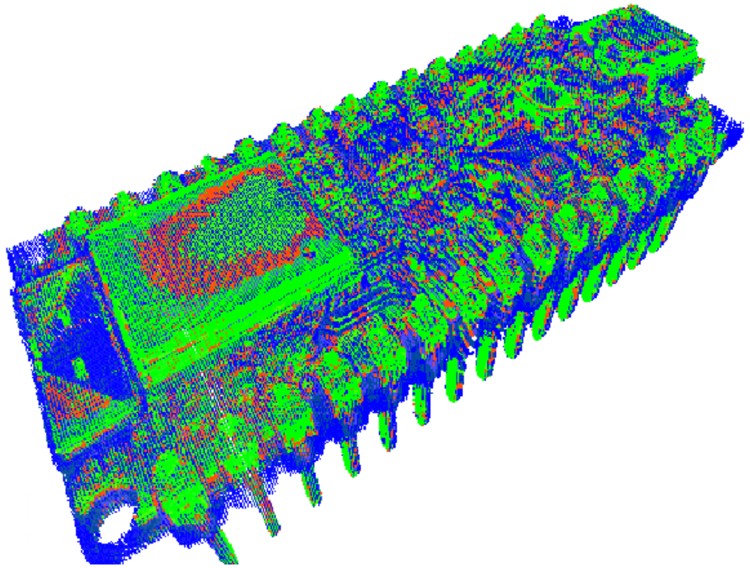
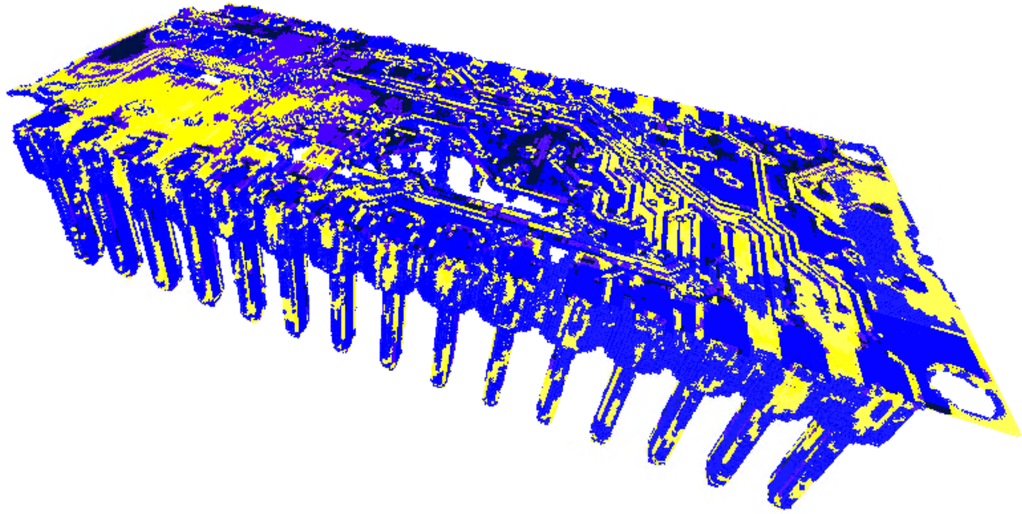
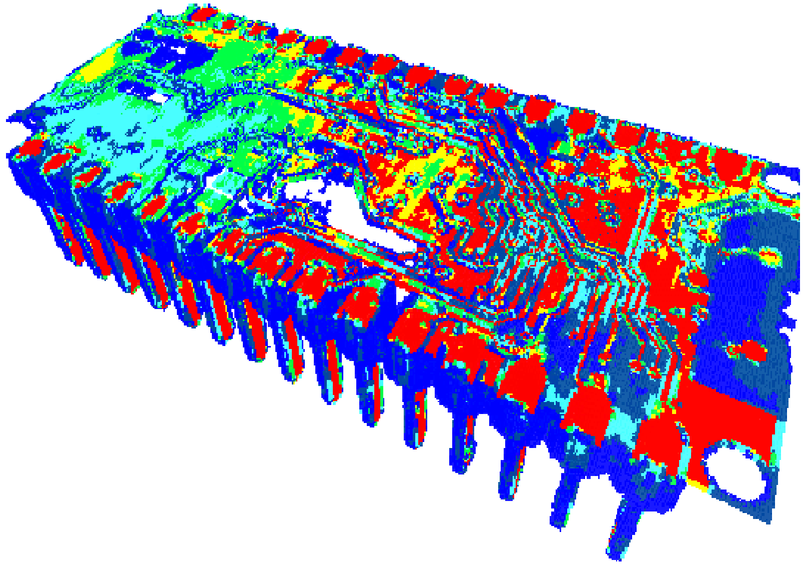
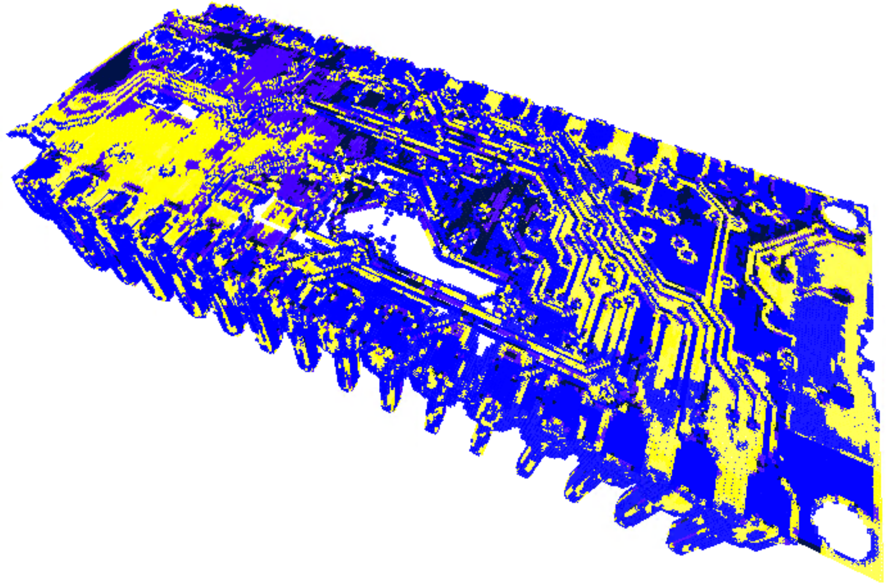
DICOM file from X-ray Tomography Scan of an electronics component – Uploaded into PUFFIn

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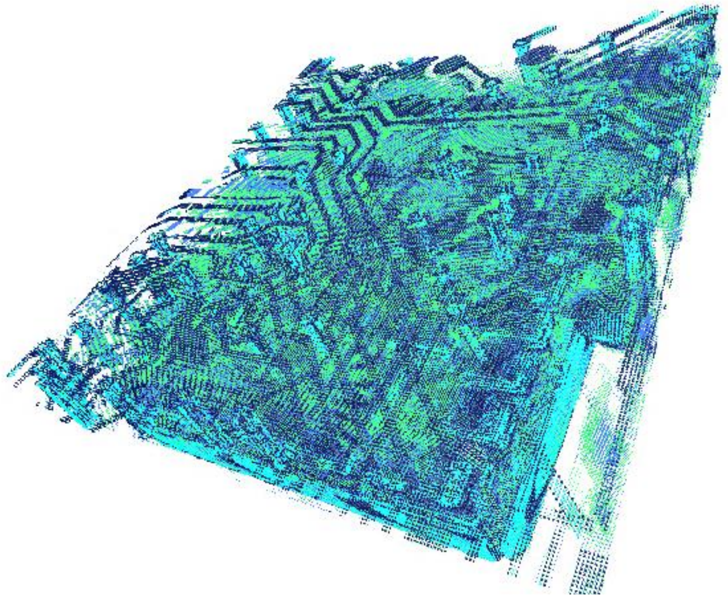
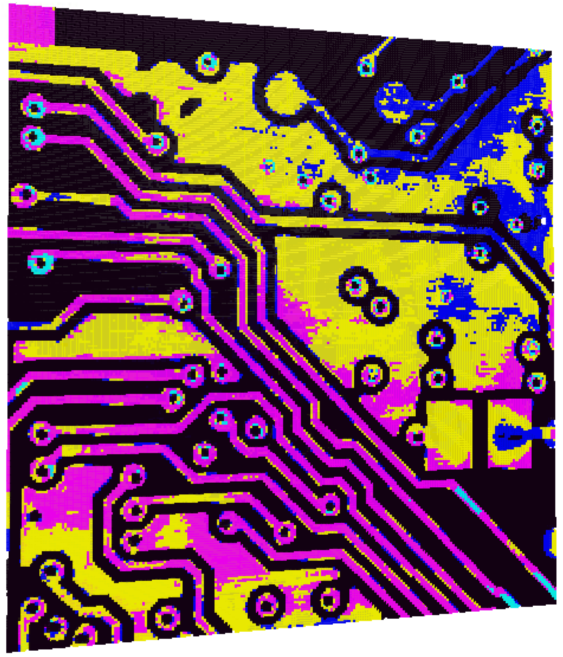
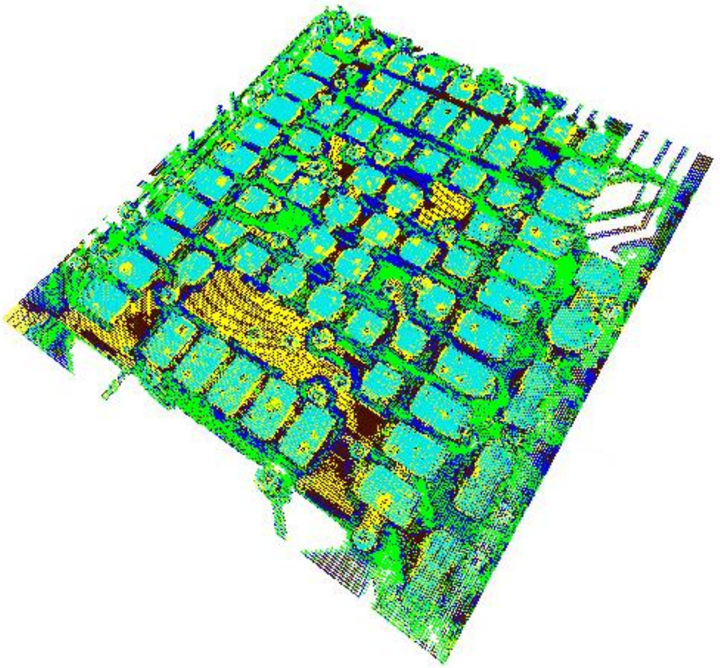
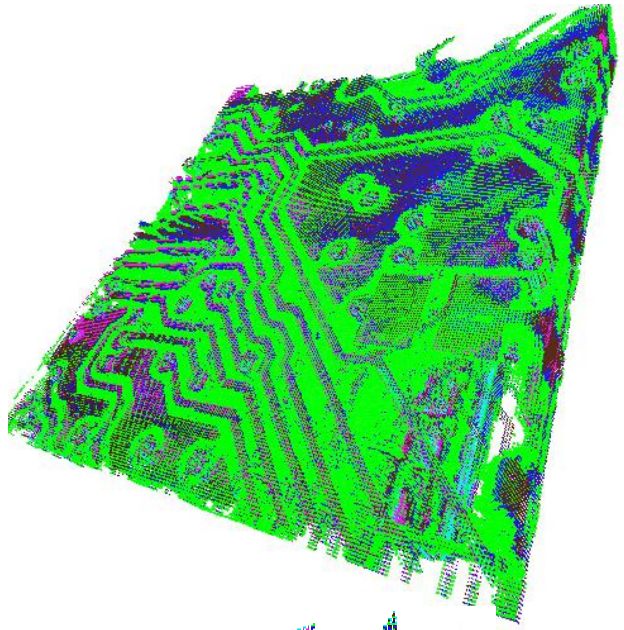
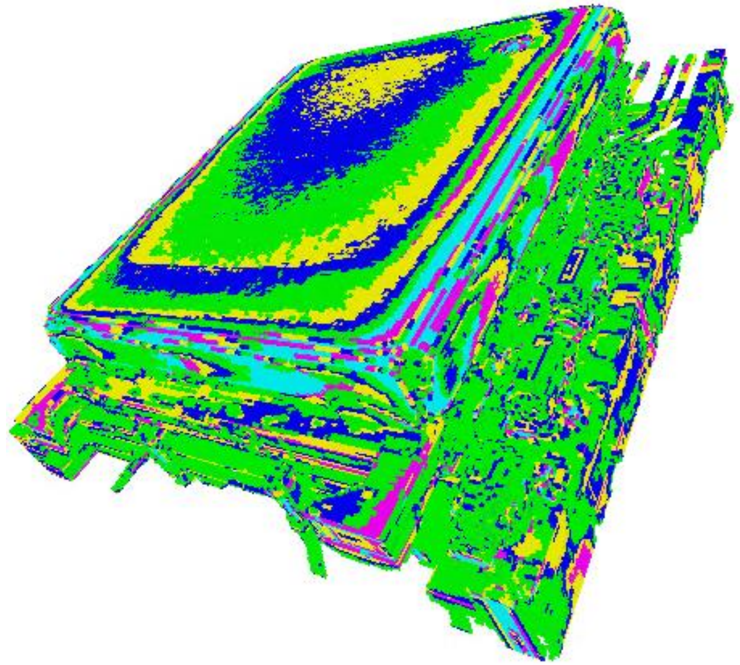
DICOM file from X-ray Tomography Scan of an electronics component – Uploaded into PUFFIn

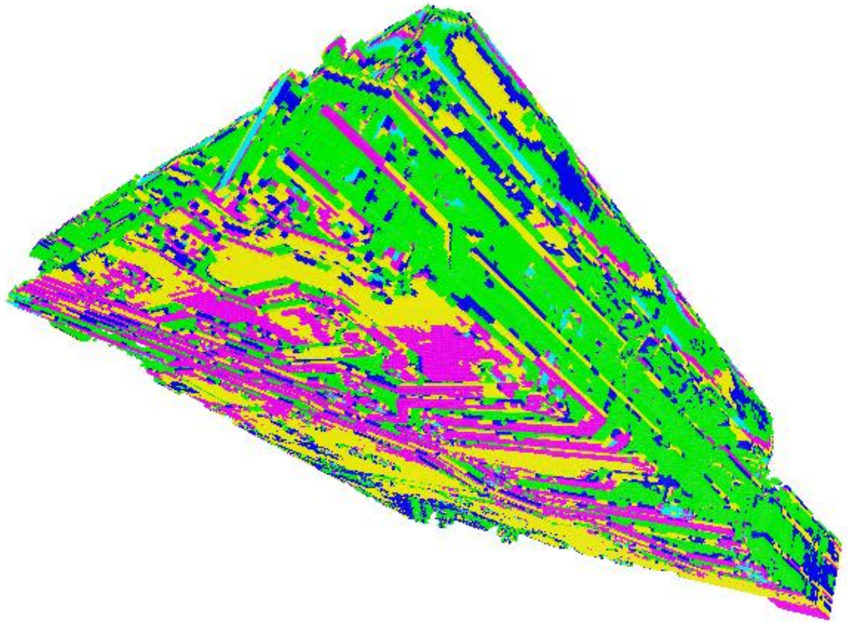


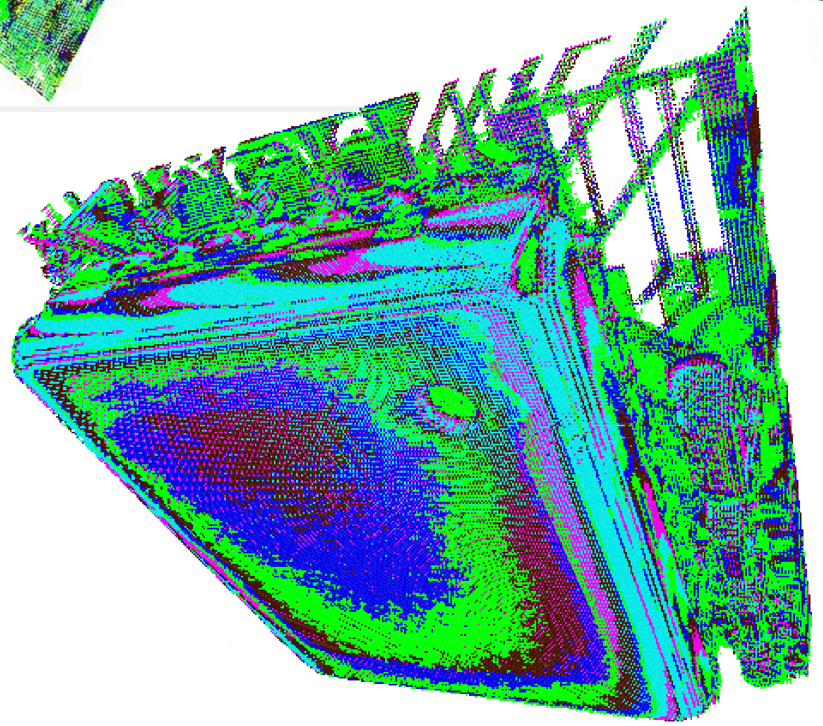




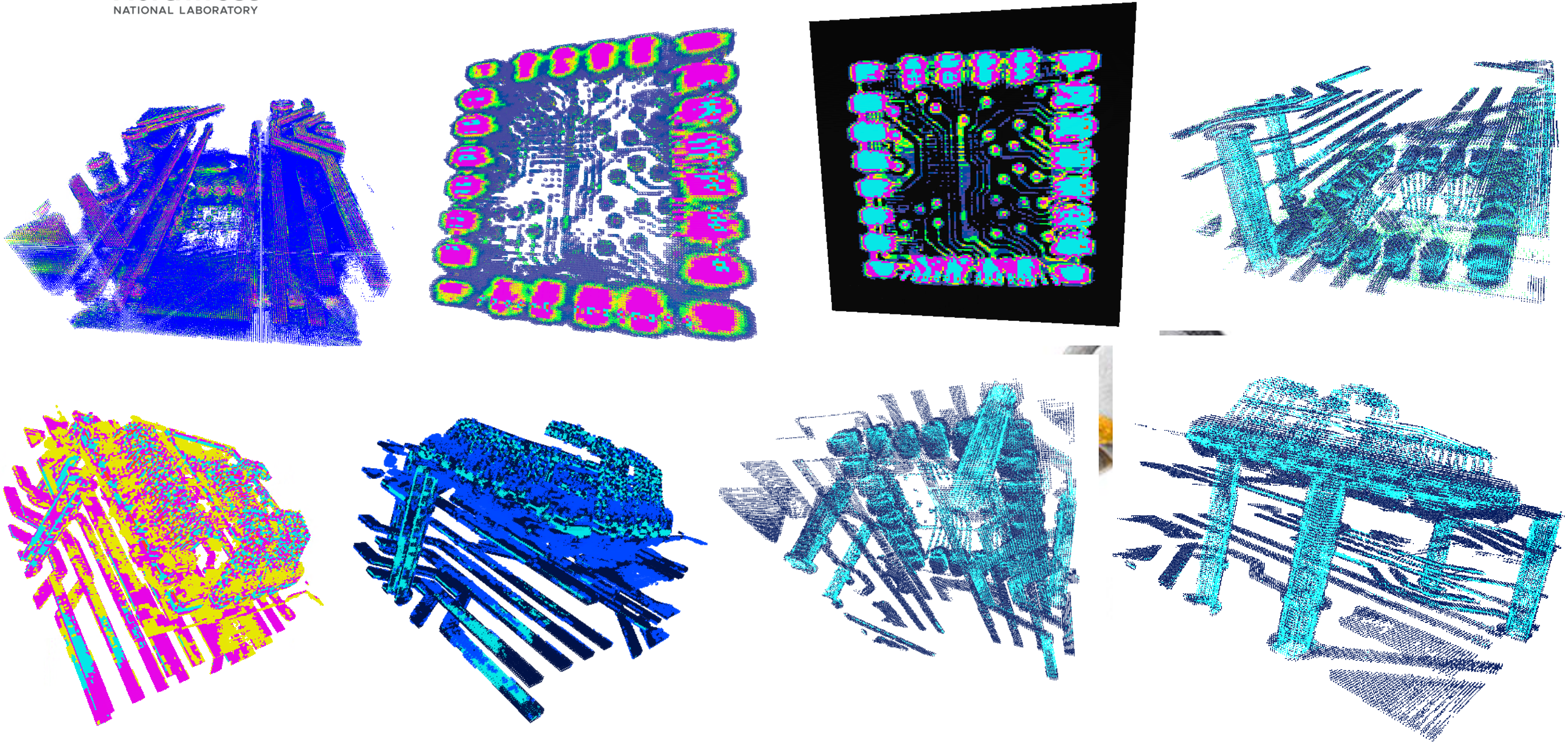




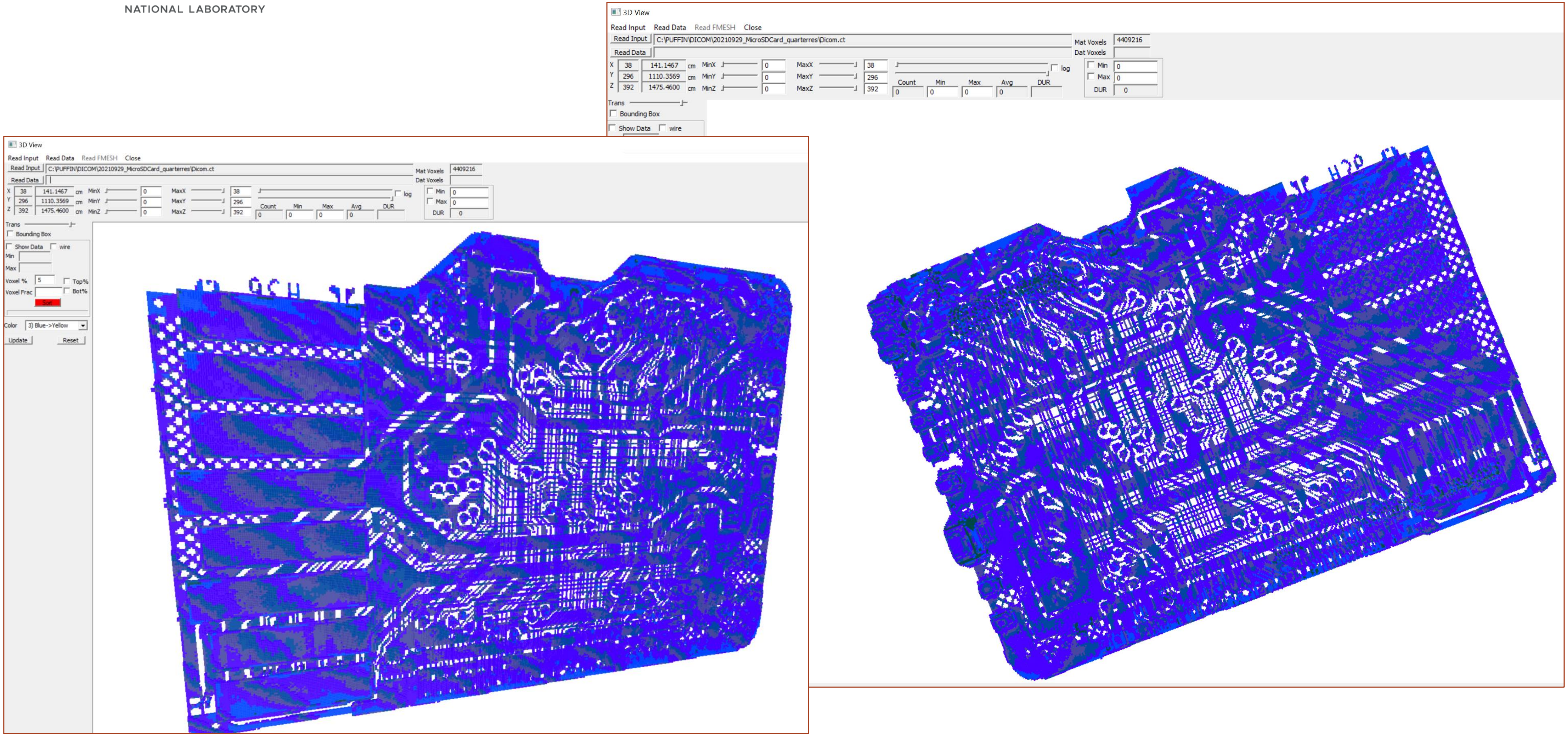




DICOM file from X-ray Tomography Scan of an electronics component – Uploaded into PUFFIn

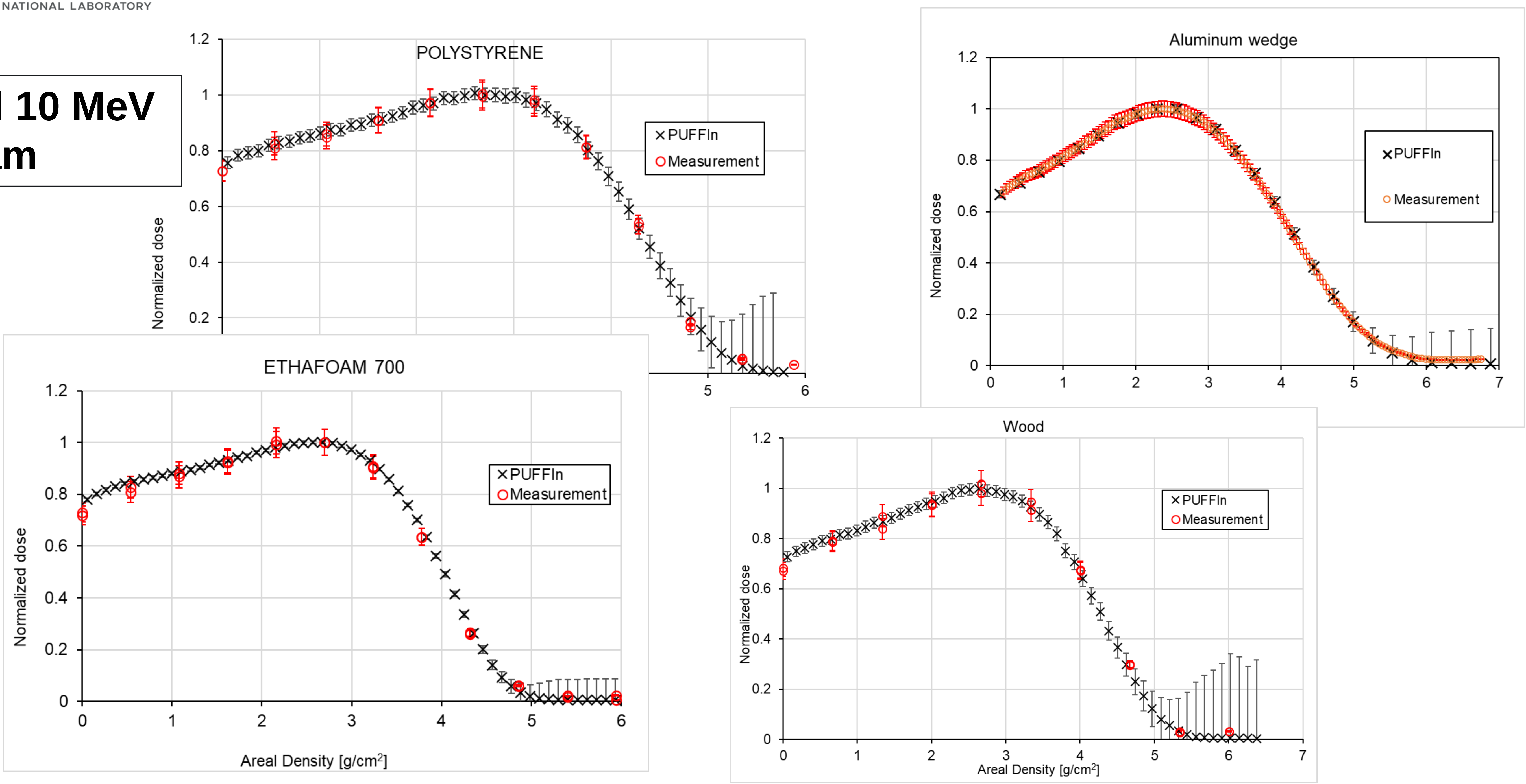


DICOM file from X-ray Tomography Scan of an SD Card – Uploaded into PUFFIn – 4.4 Million Voxels



Puffin DUR versus Measured DUR for Various Materials

Aerial 10 MeV E-beam



Conclusions for PUFFIn

- Can determine the accurate dose distribution within various materials and geometries, for cobalt-60 gamma-rays and various energies of E-beam and X-rays.
- Allows users to create a conceptual item/product design or upload a 2D image or 3D CAD or DICOM file.
- Allows users to quickly and easily locate the minimum and maximum dose locations (thus locations for dosimetry), and resulting ratio (DUR).
- For most applications the processing time is ~10X faster than similar software.
- Novices can use tool effectively after a 3-4 day training workshop.
- For most applications (up to ~1-2 million voxels) a regular laptop can be used.

Conclusions for PUFFIn – continued

- Overall, allows user to optimize product and/or packaging design for dose distribution.
- Only for NON-MOVING/STATIC items, and best for low to medium complexity items. Other software exists for the more complex MOVING/NON-STATIC items for which surrounding structures are modeled, and for which very high dose resolution is required.
- **Is an ideal LEARNING/EDUCATIONAL TOOL to quickly and easily obtain estimates for dose distribution in conceptual or real items, and how source type and energy and item geometry influences this dose distribution.**

Future Plans

- Planned future versions of PUFFIn:
  - Allow large geometries (pallets of product for X-ray?)
  - Add features desired for electronics component applications
  - Other ideas?

- Planned future 3-4 day training workshops:
  - October 2024 –Texas A&M University Electron Beam facility
  - Spring 2025 – Aerial CRT, Strasbourg, France

- If you would like to host a public workshop or invite the PUFFIn team to your site for a private workshop, please contact

  Mark Murphy at mark.murphy@pnnl.gov

Acknowledgements

- Todd Powell (Bayer Corporation) for providing medical products for CAD and CT scan/DICOM development
- Suresh Pillai (Texas A&M University) for performing PUFFIn validation measurements using E-beam
- Florent Kuntz and Abbas Nasreddine (Aerial CRT) for performing comprehensive PUFFIn validation measurements using E-beam
- Tamas Varga (PNNL) for performing the X-ray tomography scans.

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Thank you

Questions?

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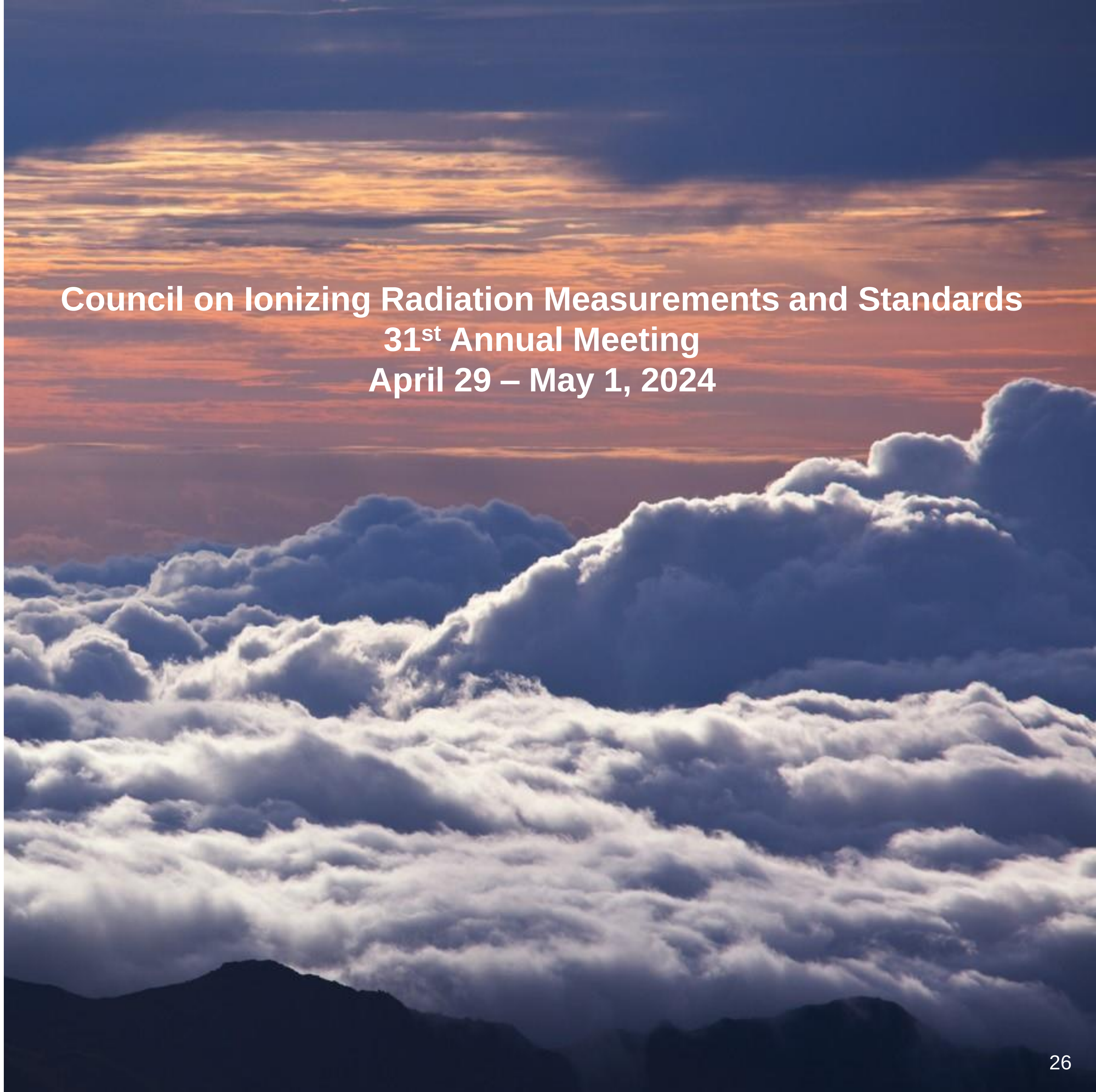


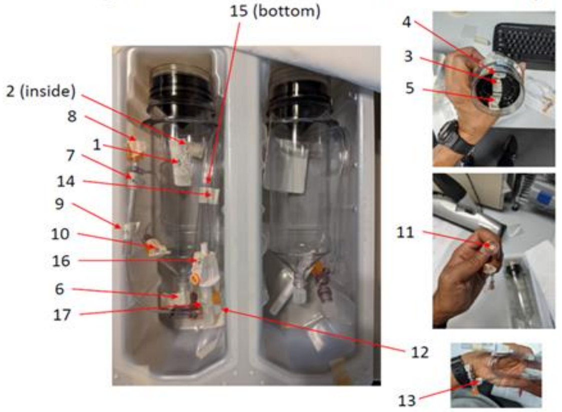
Puffin DUR versus Measured DUR for Medical Device

Bayer – Stellant Product

Measured DUR left/right = 2.16 | 2.59

PUFFIn DUR using 2D version = 2.13

Bayer Stellant - Individual package



Single sided, 1 pass

Sample	mean Irr1 (kGy)	std dev (kGy)	mean Irr2 (kGy)	std dev (kGy)
C1	15.567		14.663	0.09154
1	15.6323	0.00651	15.4863	0.04809
2	18.788	0.00265	18.458	0.01871
3	13.6527	0.01301	14.5053	0.01924
4	15.587	0.01929	18.41	0.0894
5	13.863	0.00954	13.9947	0.01776
6	15.7017	0.04554	13.2887	0.05702
7	17.005	0.01179	14.0127	0.01724
8	15.5373	0.01305	15.8347	0.01742
9	15.68	0.00889	15.575	0.01507
10	16.934	0.00872	17.1087	0.01953
11	17.0497	0.0165	15.591	0.02729
12	15.664	0.01539	15.9737	0.02663
13	17.471	0.01513	16.4537	0.02344
14	15.6623	0.02376	15.7567	0.04356
15	10.599	0.01054	12.72	0.02588
16	15.5627	0.02577	15.3797	0.12799
17	15.4953	0.03166	15.366	0.03342
Max	18.788		18.458	
Min	10.599		12.720	
DUR	1.77262		1.451101	

Right

	A	B	C	D	E
1	12.369	18.155	22.039	28.757	30.088
2	14.832	18.166	22.375	22.163	28.351
3	12.347	20.406	21.617	31.249	31.989
4	15.058	18.9	21.706	28.646	29.102
5	13.6	15.359	30.384	26.433	26.565
6	13.363	18.101	26.204	21.767	26.69
7	15.78	17.14	22.76	25.894	27.771
8	13.894	18.272	27.26	24.149	28.006
9	17.667	21.998	19.227	33.06	27.439
10	16.559	22.153	21.244	33.181	28.013

Left

	A	B	C	D	E
1	15.764	15.676	20.271	24.755	28.657
2	14.352	20.98	20.845	21.668	29.618
3	17.017	16.969	20.021	29.124	28.757
4	14.134	16.418	19.251	30.469	29.695
5		18.26	19.994	24.114	20.559
6	20.533	14.437	16.067	26.668	19.973
7	16.336	18.259	20.338	30.619	28.456
8	17.799	19.548	18.671	32.08	28.126
9	12.45	21.992	25.031	24.033	27.884
10	15.147	22.016	26.049	30.64	28.181

- Max. limit (mechanical testing): ~76.75 kGy
- Right
  - DUR: 2.59
  - On top of product DUR: 2.39
  - Min. limit: 29.62 kGy
- Left
  - DUR: 2.16
  - On top of product DUR: 2.58
  - Min. limit: 35.60 kGy