The Role of Modeling and Simulation in Industrial Processing

Thomas Kroc

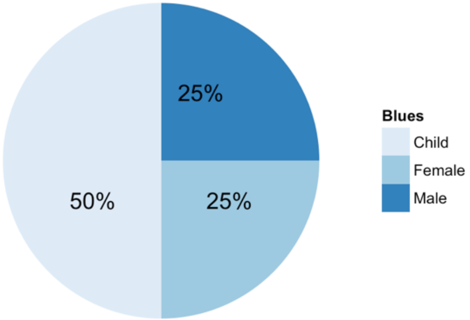
CIRMS 31st Annual Meeting

29 April 2024

Medical Physics – Treatment Planning

More oncology treatment planning systems are incorporating Monte Carlo

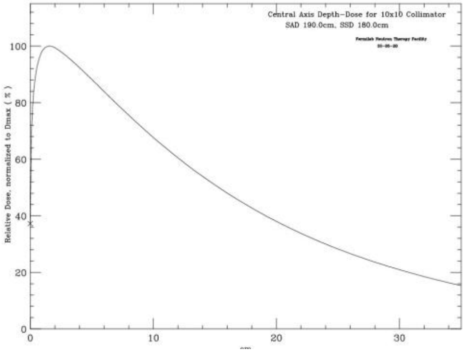
- Protons - Raystation, Raysearch – Monte Carlo, yes
- Protons – Acuros, Varian – Monte Carlo, yes?
- Photons - Eclipse, Varian – Monte Carlo, no
- Photons – Pinnacle, Philips/Elekta – Monte Carlo, no
- Photons – Monaco, Elekta – Monte Carlo, yes

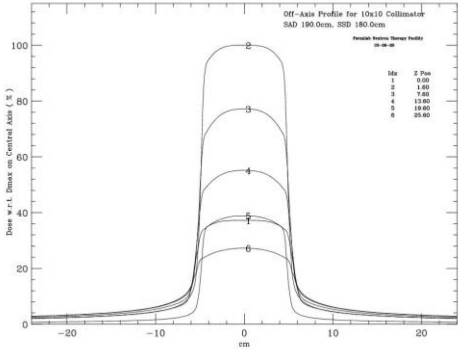


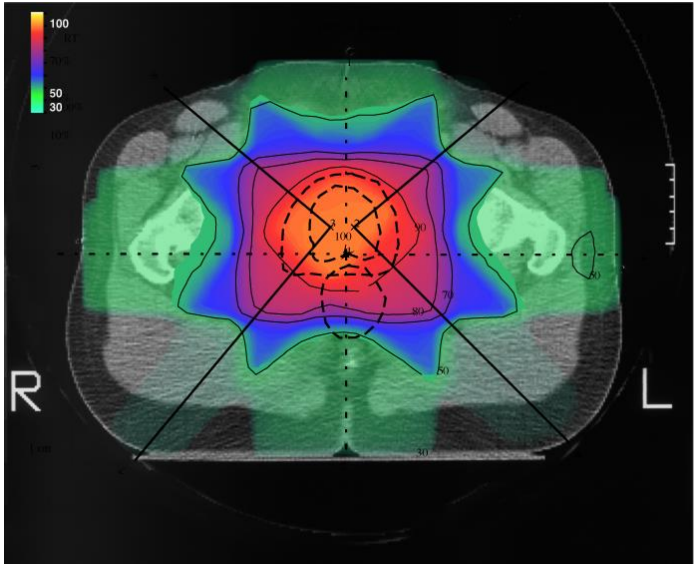
Every slide should have an image. Charts require explanatory titles, axis labels, and legends, and should tell a story to support the desired takeaway.

Medical Physics – Treatment Planning

While we tend to focus on Monte Carlo, it isn't necessarily required



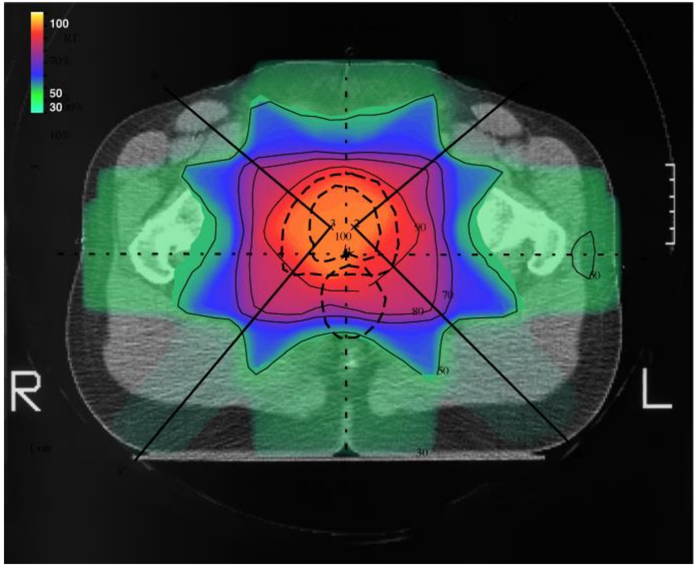




An eight-field prostate plan.
Using percent depth-dose and off-axis ratios.
60x40 grid
Used for Neutron Therapy at Fermilab till 2013

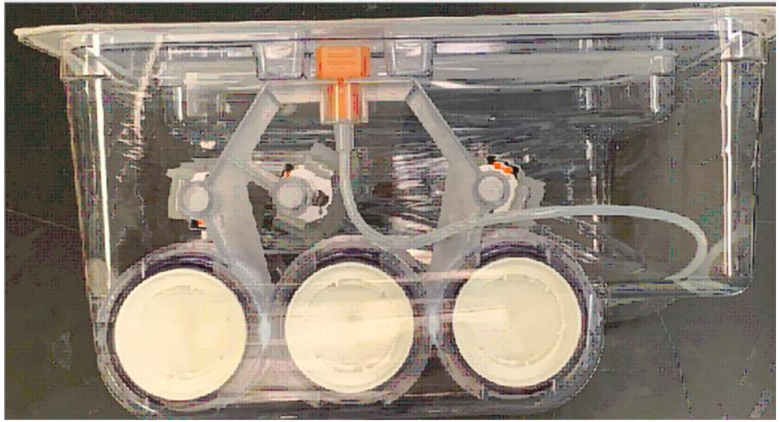
What is different between people and medical devices

- External Beam Radiation Therapy
  - Assume the object is homogenous, or nearly so
  - Electronic equilibrium

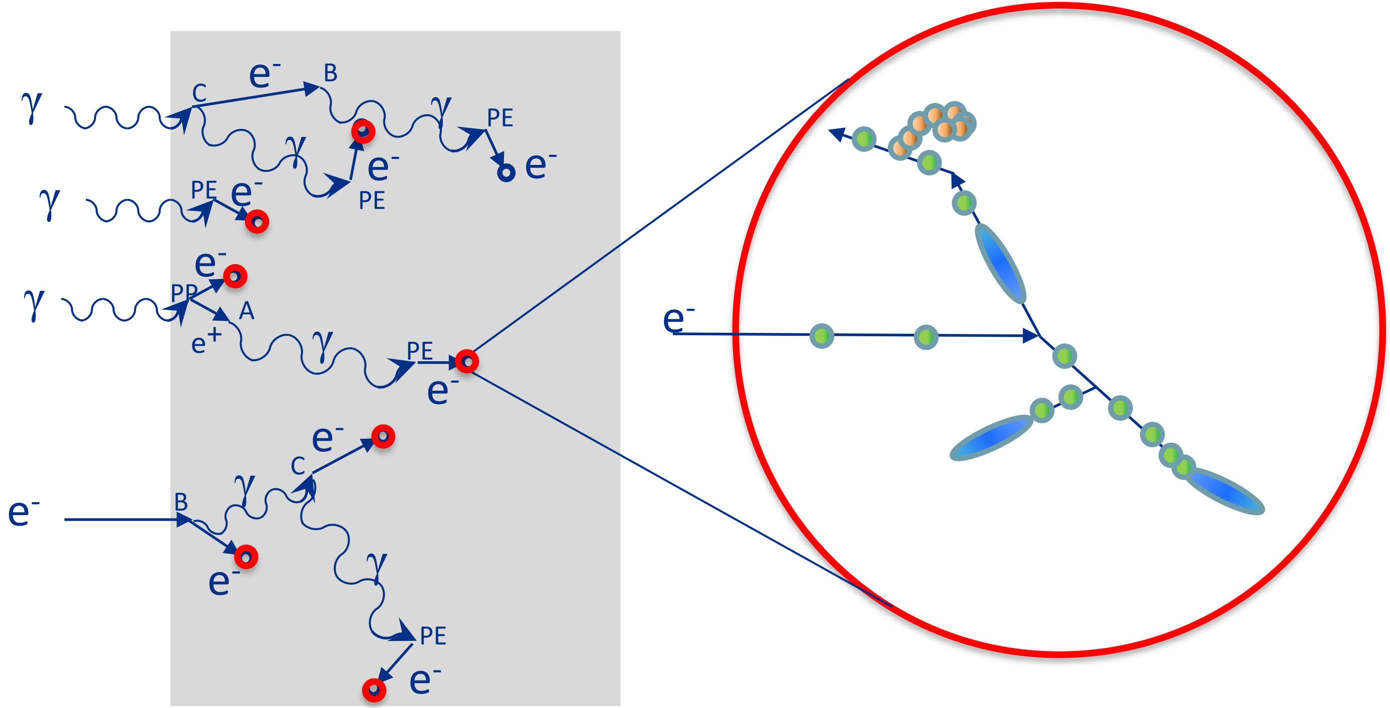


Assumed ρ = 1.017 g/cm^3

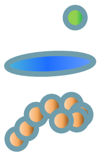
- Medical Devices
  - Many voids, many densities
  - Voids may lead to repeated build-up areas
  - Reestablish electronic equilibrium



Photon Interactions with Atoms



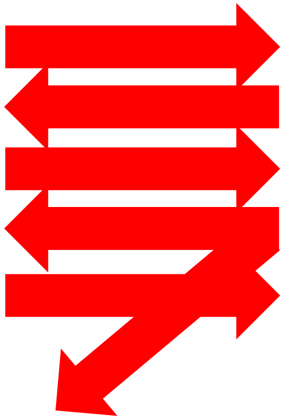
A - Positron Annihilation, B - Bremsstrahlung,
C - Compton Scattering,
PE - Photoelectric Effect, PP - Pair Production



Spur: 0-100 eV, ~65%
Blob: 100 – 500 eV, ~15%
Short track: 500 – 5000 eV, ~20%

The Photon-Electron Cascade

- Photons Produce Electrons
  - Compton Scattering
  - Photo-electric Effect
  - Pair Production
  - Photon Auger

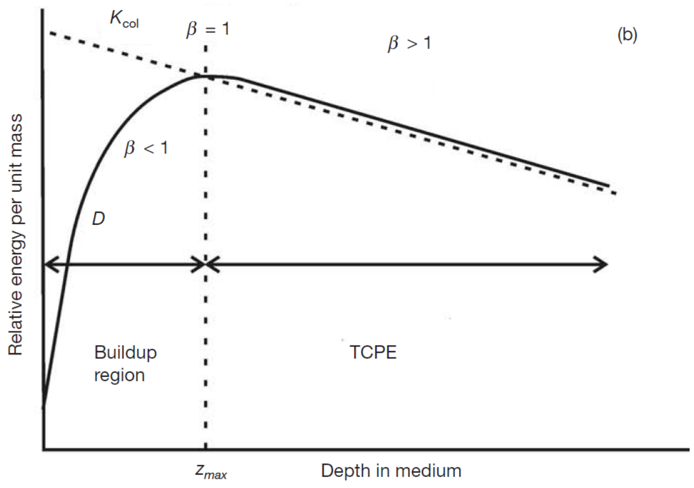


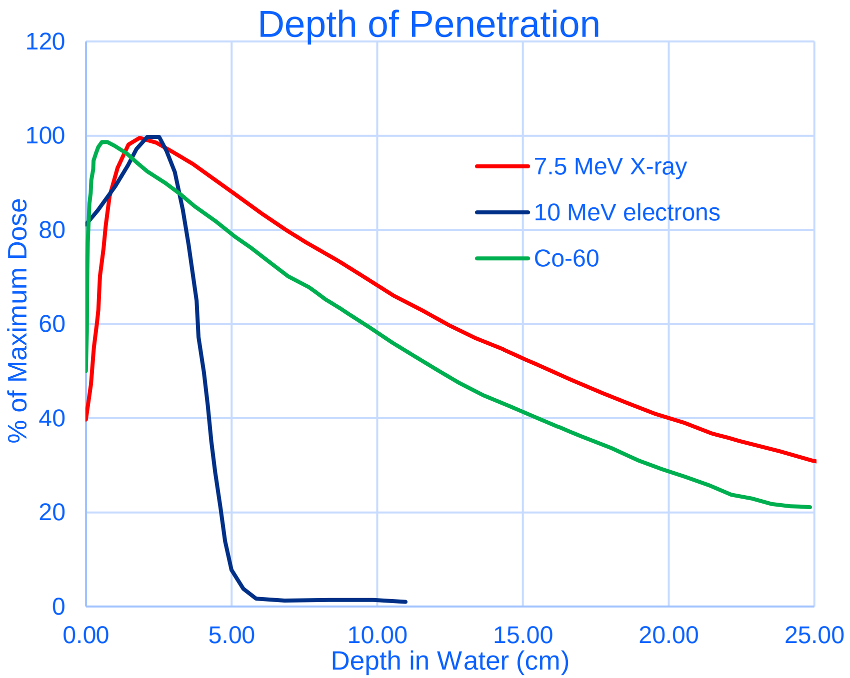
- Electrons Produce Photons
  - Bremsstrahlung
  - Positron Annihilation
  - Electron X-rays
  - Fluorescence

- Electrons Produce Electrons
  - Electron Auger
  - Delta Rays (Knock-on)

Electronic Equilibrium

It takes time for dose to build up





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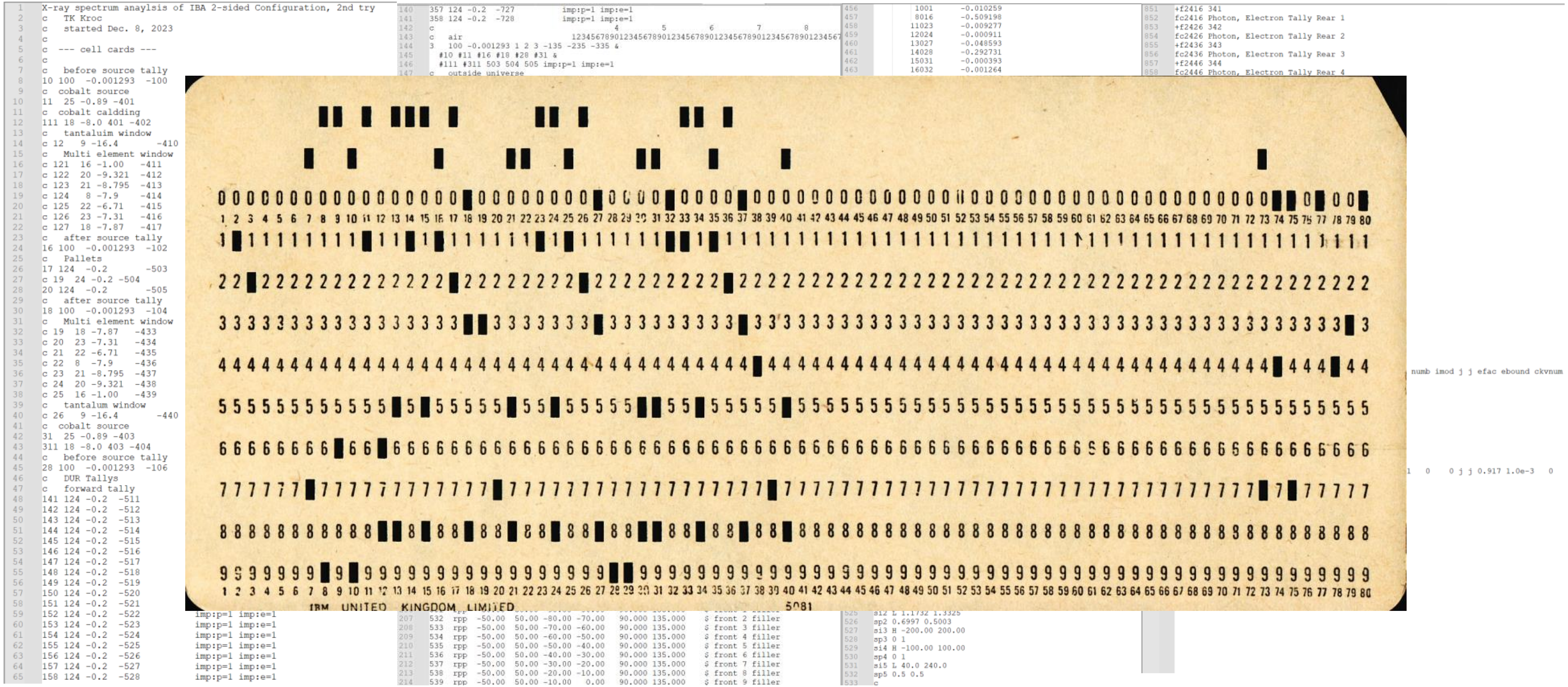
CPU Intensive

What is Available for Industrial Application (Medical Devices) ?

- PUFFIN
  - PENELOPE
    - Developed by PNNL
- RayXpert
  - Geant4
    - TRAD
- DoseInsight
  - Geant4
    - TripleRing
- MCNP6
  - LANL
- Geant4
  - CERN
- PENELOPE
  - University of Barcelona

MCNP



X-ray spectrum anaylsis of IBA 2-sided Configuration, 2nd try
c TK Kroc
c started Dec. 8, 2023
c
c --- cell cards ---
c
c before source tally
10 100 -0.001293 -100
c cobalt source
11 25 -0.89 -401
c cobalt caldding
111 18 -8.0 401 -402
c tantaluim window
c 12 9 -16.4 -410
c Multi element window
c 121 16 -1.00 -411
c 122 20 -9.321 -412
c 123 21 -8.795 -413
c 124 8 -7.9 -414
c 125 22 -6.71 -415
c 126 23 -7.31 -416
c 127 18 -7.87 -417
c after source tally
16 100 -0.001293 -102
c Pallets
17 124 -0.2 -503
c 19 24 -0.2 -504
20 124 -0.2 -505
c after source tally
18 100 -0.001293 -104
c Multi element window
c 19 18 -7.87 -433
c 20 23 -7.31 -434
c 21 22 -6.71 -435
c 22 8 -7.9 -436
c 23 21 -8.795 -437
c 24 20 -9.321 -438
c 25 16 -1.00 -439
c tantalum window
c 26 9 -16.4 -440
c cobalt source
31 25 -0.89 -403
311 18 -8.0 403 -404
c before source tally
28 100 -0.001293 -106
c DUR Tallys
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141 124 -0.2 -511
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155 124 -0.2 -525 imp:p=1 imp:e=1
156 124 -0.2 -526 imp:p=1 imp:e=1
157 124 -0.2 -527 imp:p=1 imp:e=1
158 124 -0.2 -528 imp:p=1 imp:e=1
357 124 -0.2 -727 imp:p=1 imp:e=1
358 124 -0.2 -728 imp:p=1 imp:e=1
c air
3 100 -0.001293 1 2 3 -135 -235 -335 &
#10 #11 #16 #18 #28 #31 &
#111 #311 503 504 505 imp:p=1 imp:e=1
c outside universe
1001 -0.010259
8016 -0.509198
11023 -0.009277
12024 -0.000911
13027 -0.048593
14028 -0.292731
15031 -0.000393
16032 -0.001264
+f2416 341
fc2416 Photon, Electron Tally Rear 1
+f2426 342
fc2426 Photon, Electron Tally Rear 2
+f2436 343
fc2436 Photon, Electron Tally Rear 3
+f2446 344
fc2446 Photon, Electron Tally Rear 4
numb imod j j efac ebound ckvnum
532 rpp -50.00 50.00 -80.00 -70.00 90.000 135.000 $ front 2 filler
533 rpp -50.00 50.00 -70.00 -60.00 90.000 135.000 $ front 3 filler
534 rpp -50.00 50.00 -60.00 -50.00 90.000 135.000 $ front 4 filler
535 rpp -50.00 50.00 -50.00 -40.00 90.000 135.000 $ front 5 filler
536 rpp -50.00 50.00 -40.00 -30.00 90.000 135.000 $ front 6 filler
537 rpp -50.00 50.00 -30.00 -20.00 90.000 135.000 $ front 7 filler
538 rpp -50.00 50.00 -20.00 -10.00 90.000 135.000 $ front 8 filler
539 rpp -50.00 50.00 -10.00 0.00 90.000 135.000 $ front 9 filler
sp2 0.6997 0.5003
si3 H -200.00 200.00
sp3 0 1
si4 H -100.00 100.00
sp4 0 1
si5 L 40.0 240.0
sp5 0.5 0.5
IBM UNITED KINGDOM LIMITED
5081

The Resulting PUFFIn software
(Penelope User Friendly Fast Interface)

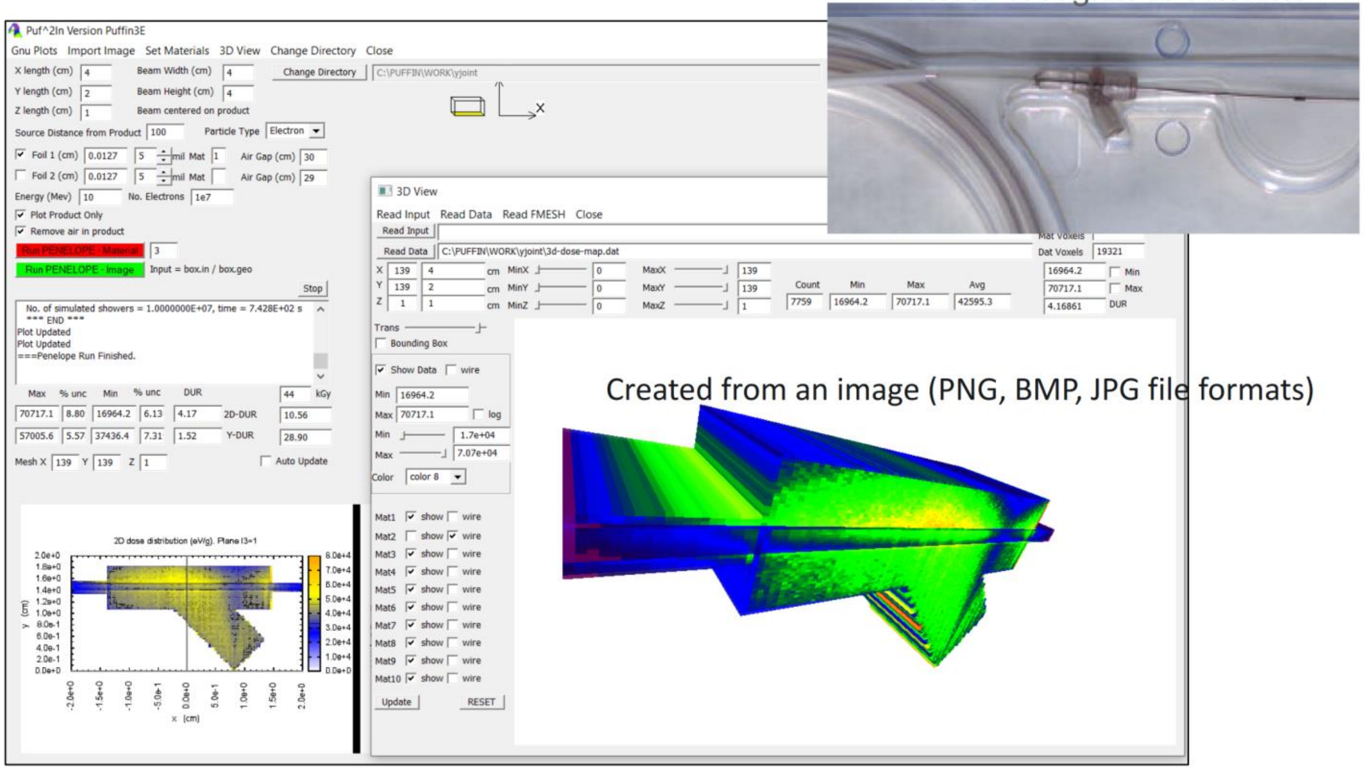
- The user interface uses the PENELOPE Monte Carlo radiation transport code.
- PENELOPE is not integrated into the interface, but called as an external program.
- The interface creates a voxel geometry of the product.
- Geometry is created within the code or imported from images or 3D data sets.

The Resulting PUFFIn Software continued -

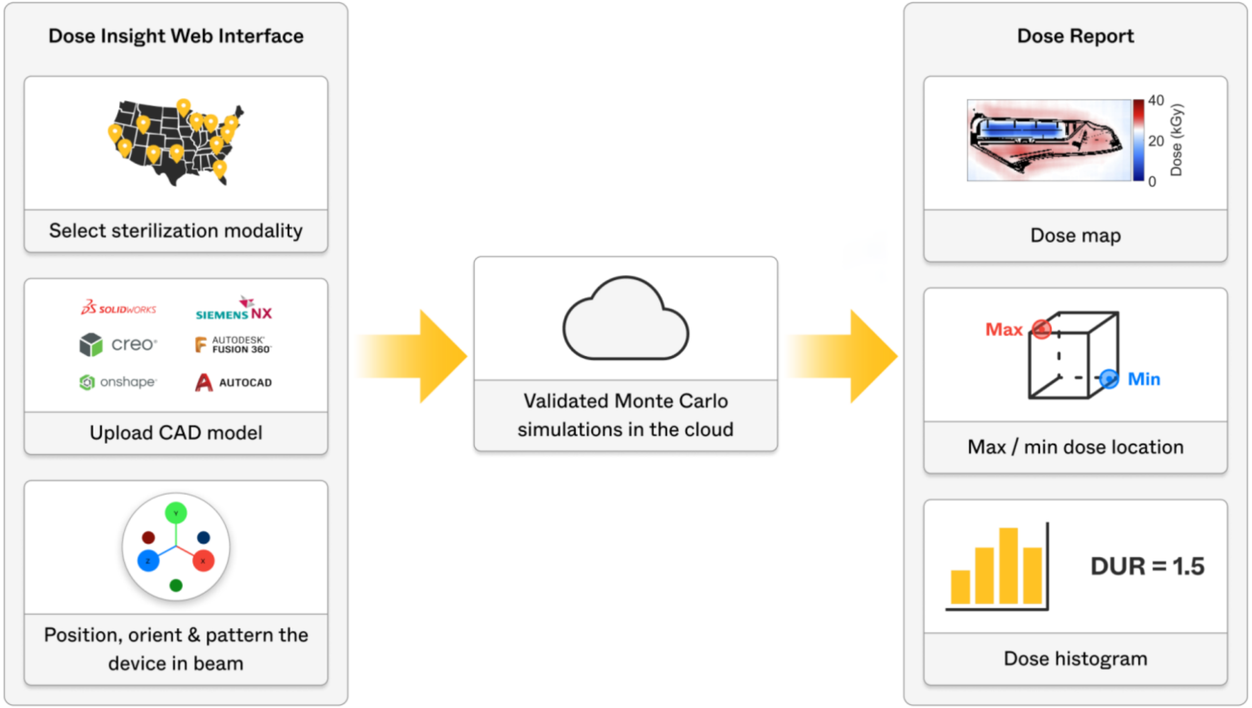
- PUFFIn can be used to model geometries to show the expected dose response for different materials.
- The source can be changed to show the expected dose from E-beam, X-rays and cobalt-60 gamma-rays for the same product.
- The product can be rotated to show changes in DUR dependent on product orientation.
- Multiple beams can be used.
- CAD geometries can be converted and imported.
- X-Ray Tomography files can be converted and imported.
- Applications include:
  - Teaching/Training
  - New product and/or packaging design
  - Legacy product and/or packaging re-arrangement or re-design for alternative source
  - Influence of source type and energy on dose distribution

Puffins 2D Version – Dose Distribution for Simple Geometries, and Training Tool

Photo of region of concern



Dose Insight



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Dose Insight

- Triple Ring Technologies, a co-development firm was awarded an SBIR Phase I grant by the Food and Drug Administration entitled An e-beam sterilization dose map simulation tool.

- simulation tools that predict the outcome of radiation sterilization without the need to have a fully engineered or manufactured product in hand. Sterilization of medical devices is often an afterthought. Yet, once a device is fully engineered and manufactured, the costs of failing to meet regulatory sterilization requirements can be astronomical. Even when well-planned, sterilization configurations are modified by trial and error through an expensive and time-consuming process.

- "The tool leverages the massively parallel architecture of Graphical Processing Units (GPUs) to make simulations fast and user-friendly. From only the Computer Aided Design (CAD) model of the device, the software tool will calculate the full three-dimensional dose distribution delivered during radiation sterilization processing. The simulation tool scores the dose distribution on a GPU, as well as implements the physics of radiation sterilization"

- This project is supported by the Food and Drug Administration (FDA) of the U.S. Department of Health and Human Services (HHS) as part of a financial assistance award [FAIN] with 100 percent funded by FDA.

- Project: “An e-beam sterilization dose map simulation tool” Monte Carlo simulations are a powerful tool to predict the outcome of radiation sterilization. A major advantage is that these simulations can be performed early in the medical device design process when only CAD models of the device exist. Further packaging configurations and sensitivity to variations in placement of the device can be explored virtually whereby enabling a rigorous and reliable design for sterilization process. Monte Carlo simulations for radiation transport are a well-established tool with various open-source packages available for use. One of the most prominent tools is the Geant4 library, which was originally developed by CERN and is now supported by an international collaboration of scientists and software developers. The downside of such tools is that they are slow in terms of computation times. In this Phase I SBIR grant Triple Ring Technologies has developed a custom simulation tool that significantly speeds up the simulation times by using modern Graphics Processing Unit (GPU) cards. Currently photon physics has been implemented. To also enable simulations of the e-beam sterilization process full electron physics is proposed to be implemented in a subsequent Phase II grant. We compared the performance of our new simulation engine to Geant4 and to experiments. We find that our GPU engine and Geant4 agree within 2% for most cases and we find that in the low energy range which is less relevant for sterilization agreement is slightly less (on the order of 5%). Further, we find that comparison to experiments gives agreement within 5.6% with the GPU and within 5% with Geant4. In summary, we find excellent agreement between the two simulation engines with the advantage of a 1000x speed up of our new tool compared to single-threaded Geant4.

Dose Insight – Design for Sterilization

Presented at Medical Device Sterilization:
Past, Present, and Future
September 20-21, 2023
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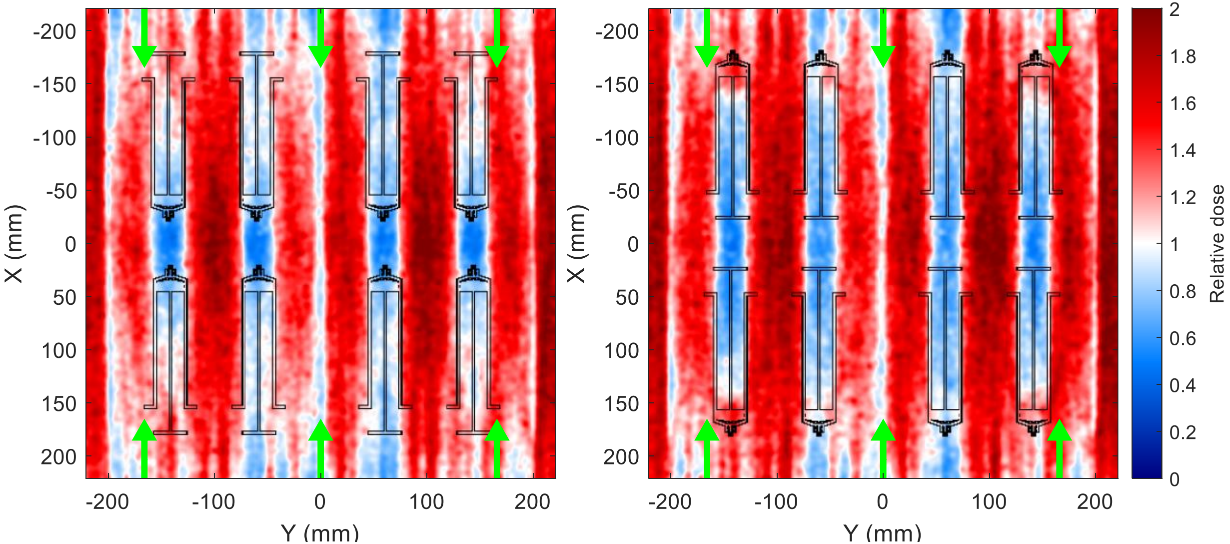
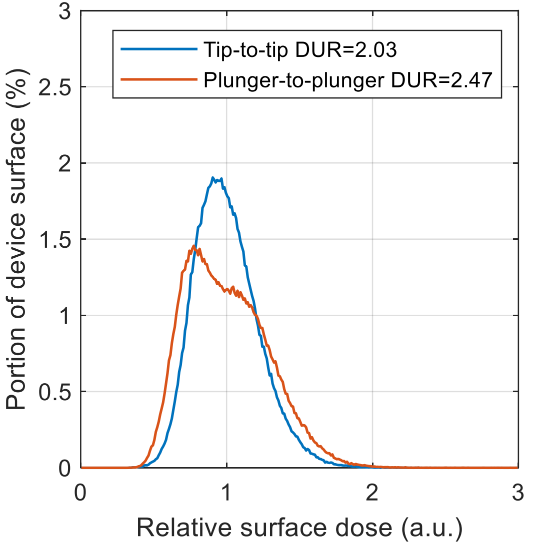
Beam direction is 0 degree

Tip-to-tip   Plunger-to-plunger

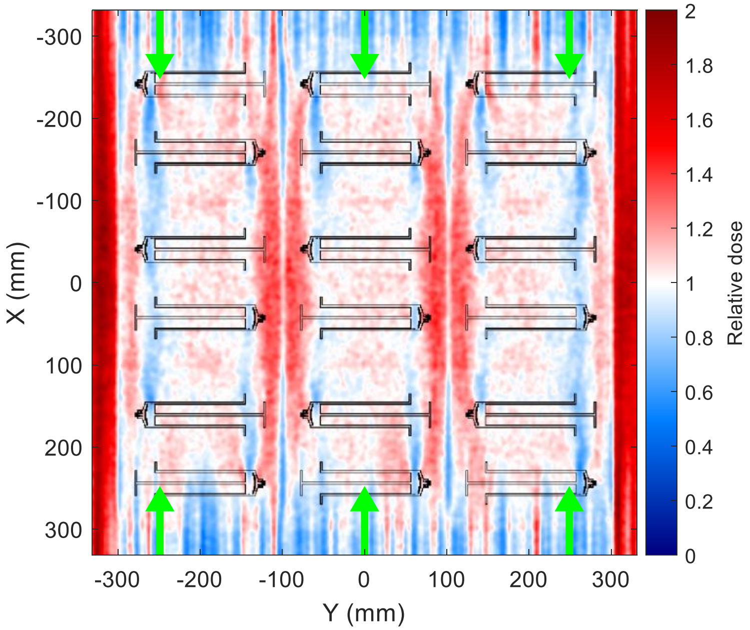


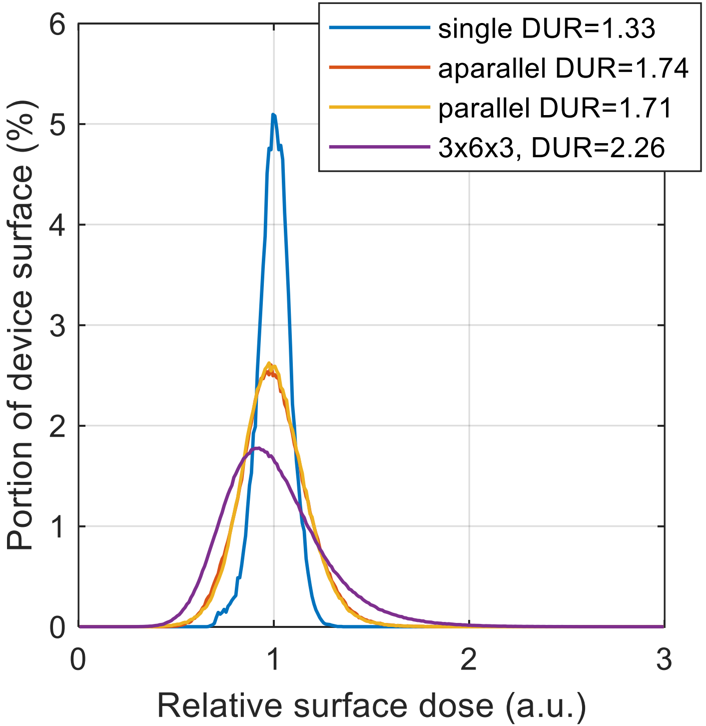


Tip-to-tip configuration has significantly lower DUR

Dose Insight – Design for Sterilization

Final packaging configuration: 3x6x3 syringes





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RayXpert

3D MODELING AND CAD IMPORT

The interface allows to quickly realize realistic 3D modeling , on the one hand by combining **simple solid shapes**, and on the other hand by **importing 3D CAD models** made from standard **CAD software (CATIA, SolidWorks, Pro -E, AutoCad**, etc…).

- Import of CAD geometry
- User interface, modeling toolboxes
- Shapes reconstruction
- Equipment manager
- Integrated libraries of materials and isotopes

DOSE CALCULATION BY MONTE CARLO

Particles in the a 3D structure are monitored using the **Monte-Carlo method**. The management of physical processes for particle-matter interactions was programmed based on the physics processing of ***GEANT4,*** but entirely redeveloped by TRAD Tests & Radiations **since the 2000s**.

This function gives access to the dose rate calculation in a 3D scene with composed sources of **isotopes emitting photons** (gamma and X-ray), **electrons** (line and Beta spectrum), **positrons** (line and Beta + spectrum) and **Neutrons** (optional) and / or sources of **radiation emitted by devices**.

Convergence indicators have been implemented in RayXpert®. Each calculated quantity (energy, total dose, H * 10 dose, etc.) is associated by a series of indicators to best estimate the level of convergence of the results by giving information on the **evolution of the result and of the sigma** during the simulation.

RayXpert

3D MAPPING

3D mapping is a feature that automatically creates a virtual mesh of detectors in the geometry and thus provides some **3D visualization of dose rates, flows and deposited energies**; for photons, electrons, positrons and neutrons (optional module).
This function also makes it possible to **merge several mapping** relating to the same model and to display the different radiological zones according to a **legal Zoning** which is directly integrated into RayXpert.
A conditional display is available in order to, for example, filter with one click on a type of particle or on all the results having a sigma lower than X%.

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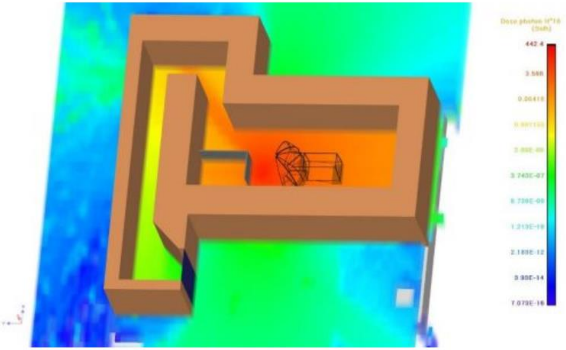

3D mapping of the dose rate around and inside a Co60 bunker

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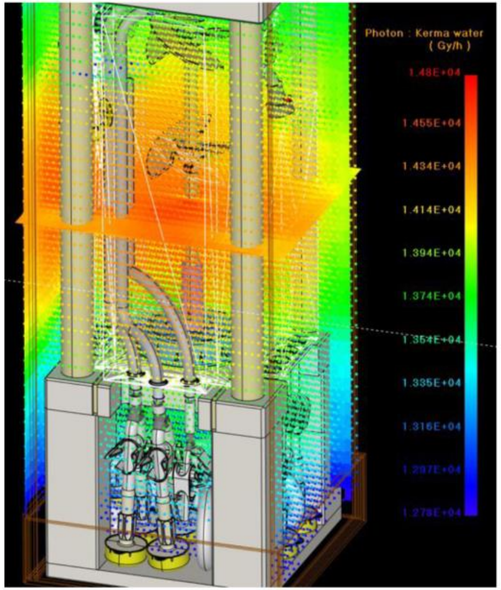
RayXpert

Monte Carlo Simulation
3D mapping

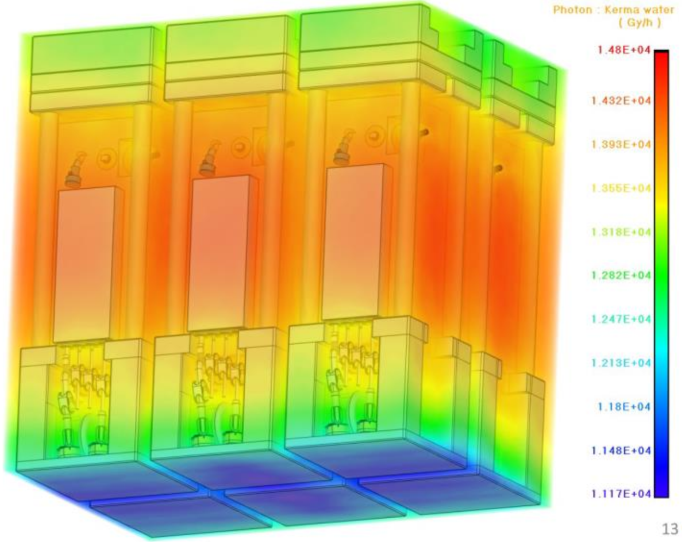


S.Dorey – L.Eychenne

Virtual mapping in all the product

Results for kerma water in ***Gy/h***

271 092 voxels in total



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Evaluation
of Monte Carlo simulation
in Radiation Processing

Samuel Dorey – *SARTORIUS* & Ludovic EYCHENNE – *TRAD Tests & Radiations*
Damien PRIEELS – IBA Industrial
Abbas NASREDDINE – AERIAL CRT
Florent KUNTZ - AERIAL CRT
Antoine GHILARDI – TRAD Tests & Radiations

Presented at Medical Device Sterilization:
From Possibilities to Practice
September 21-23, 2022
Fermilab

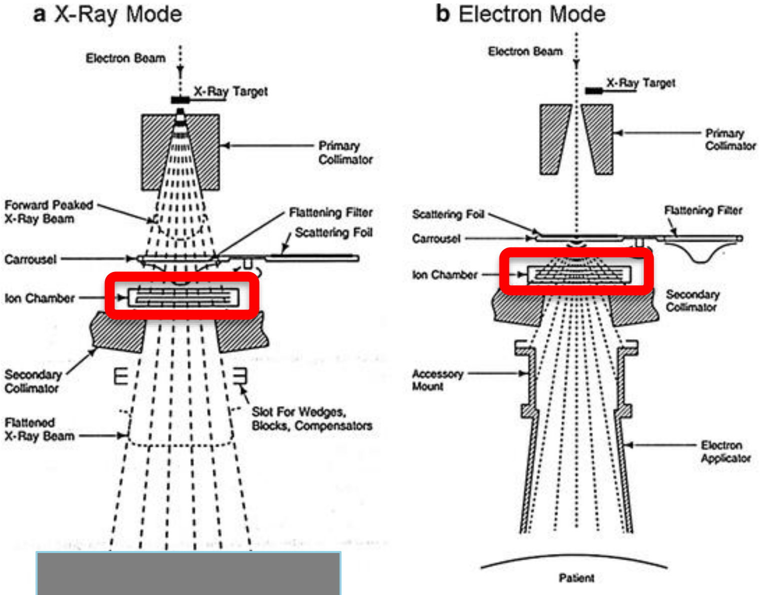
Salient Features

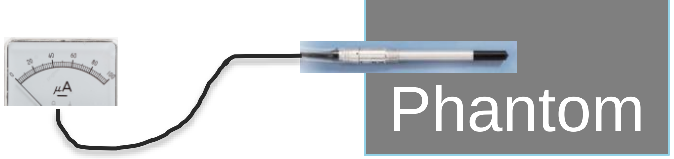
- PUFFIN
  - PENELOPE
    - Focus on DUR
    - Free
    - Local machine
- MCNP6
  - Complete simulation tool
  - ~$800 (export controlled)
  - Local machine
  - Large learning curve
- RayXpert
  - Geant4
    - Most complete simulation tool
    - Not free
    - Local machine
- Geant4
  - Complete simulation tool
  - Open source
  - Local machine
  - Large learning curve
  - Has extensive medical physics extensions
- DoseInsight
  - Geant4
    - Design for Sterilization/Packaging
    - Not free
    - Cloud based

Parametric Release

Radiation Oncology uses parametric release for all patients

- There is no external or internal dosimetry to monitor the dose given
  - Each morning the accelerator is calibrated to determine the ratio between ionization chamber that monitors the photon or electron fluence and the dose delivered to a standard phantom (measured by a precision separate ion chamber)
  - This ratio and the output of the monitoring ionization chamber (corrected for temperature and pressure) determine when the patient has received the prescribed dose.





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Thank you