Nuclear reactions in proton bean therapy

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June 2022

Introduction

In this work we present some calculations performed to investigate the relevance of nuclear reactions in proton beam therapy (PBT).

We have started by trying to reproduce with Geant4 Monte Carlo simulations the measurement results reported by **Verbeek** et al. in [Med. Phys. 48, 456 (2021)]. There they study the absorbed dose in a 40x40x40 cm^3 volume of water irradiated with **proton beams of 100, 160 and 225 MeV** at the **West German Proton Therapy Centre in Essen (WPE)**.

The measurements were performed with a 2D ionization chamber array which was moved along the water tank to take a 3D dose profile. The 2D array is made *of 1020 ionization chambers arranged in a square grid. The centers of the chambers are 0.7619 cm apart and the diameter of each cylindrical chamber is 0.42 cm.*

They try to reproduce the experimental results with simulations performed with different codes: **PENH** [link], an extension of PENELOPE [link] able to transport protons, including both electromagnetic and nuclear interactions; **TOPAS** [link], which is Geant4; and **RayStation** Monte Carlo (RS) [link].

Measurement

2D array is made of 1020 ionization chambers arranged in a square grid → Deposited energy

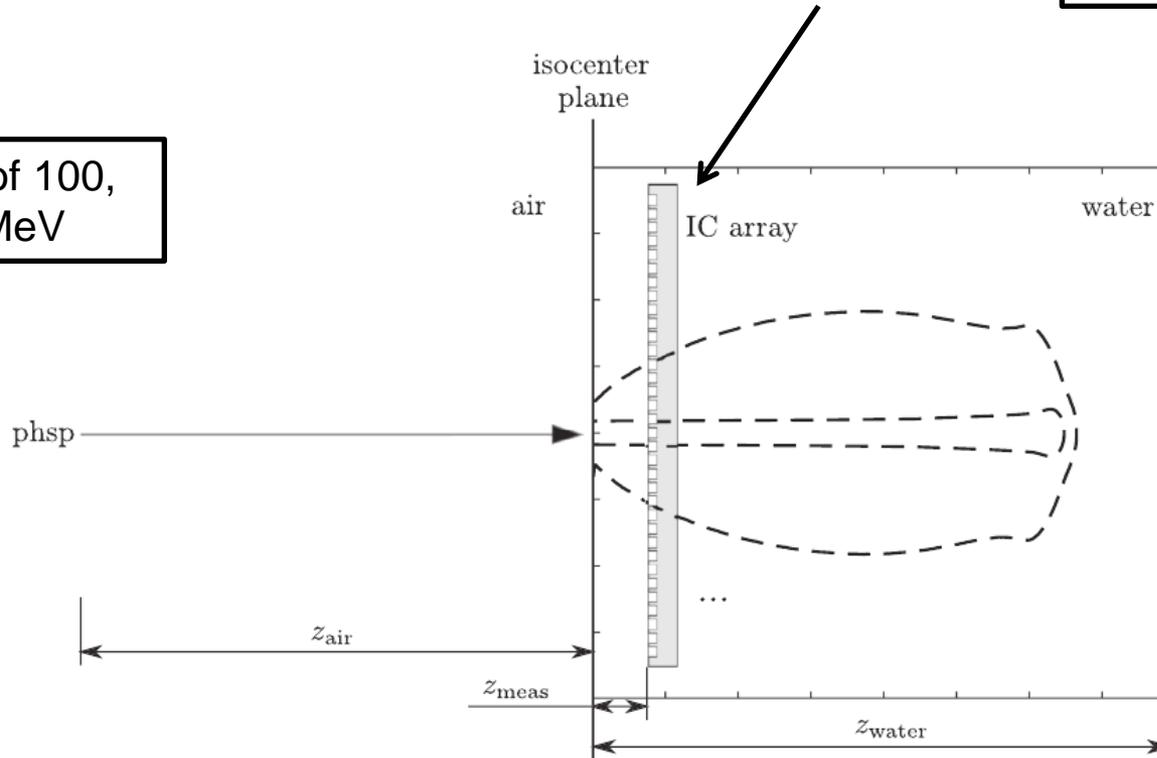40x40x40 cm³ water volume

Proton beam of 100, 160 and 225 MeV

Fig. 2 of Verbeek et al., Med. Phys. 48, 456 (2021)

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Measurement

- Source: they measure the source (protons) at some position in the *z-axis*, and they use this source in the MC simulations. (we found some inconsistencies here).

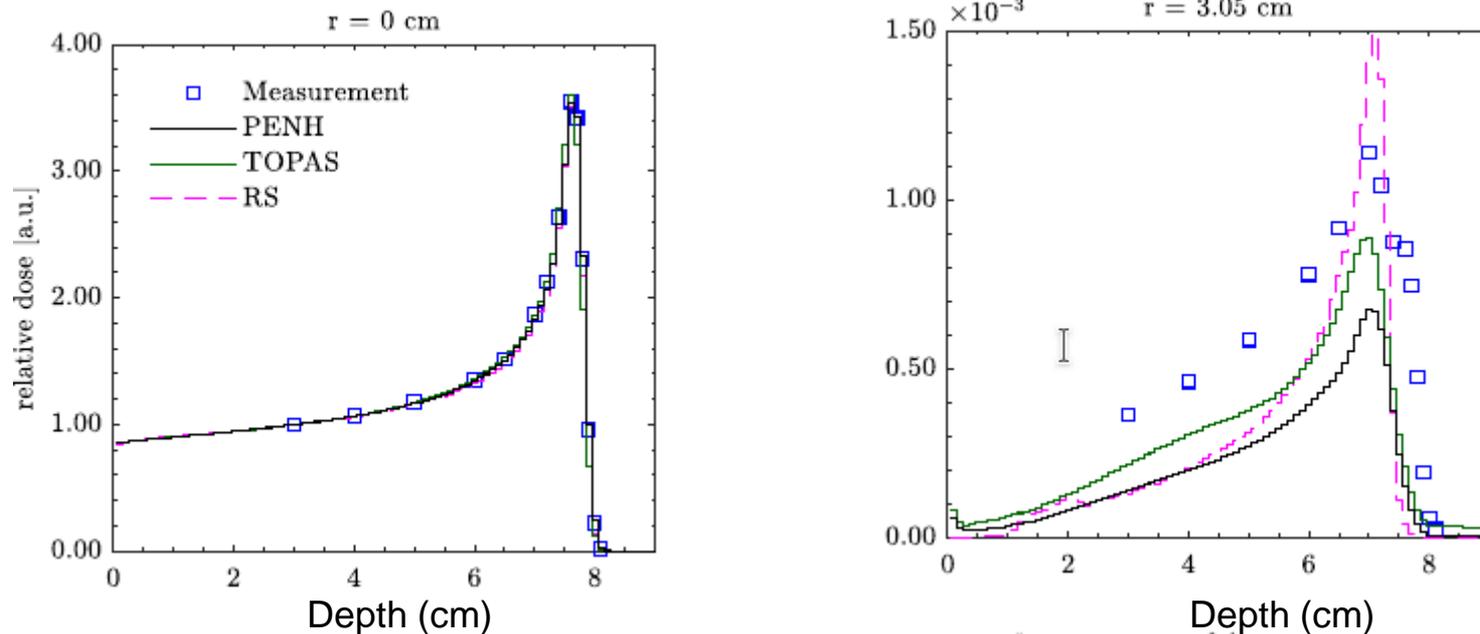- Simulations: PENH, TOPAS (Geant4) and RayStation

Figure from Fig. 3 of Verbeek et al., Med. Phys. 48, 456 (2021)

Who are we?

- Neutron physics

- Nuclear data measurements:
    - Neutron cross sections (n_TOF-CERN)
    - Neutron emission in radioactive decay (MONSTER)

- Nuclear instrumentation (see talk by Julio Plaza del Olmo)

- Data acquisition systems

- Monte Carlo calculations (MCNP & Geant4)
    - Members of the Geant4 collaboration → low energy neutron physics, data libraries (https://www-nds.iaea.org/geant4/).
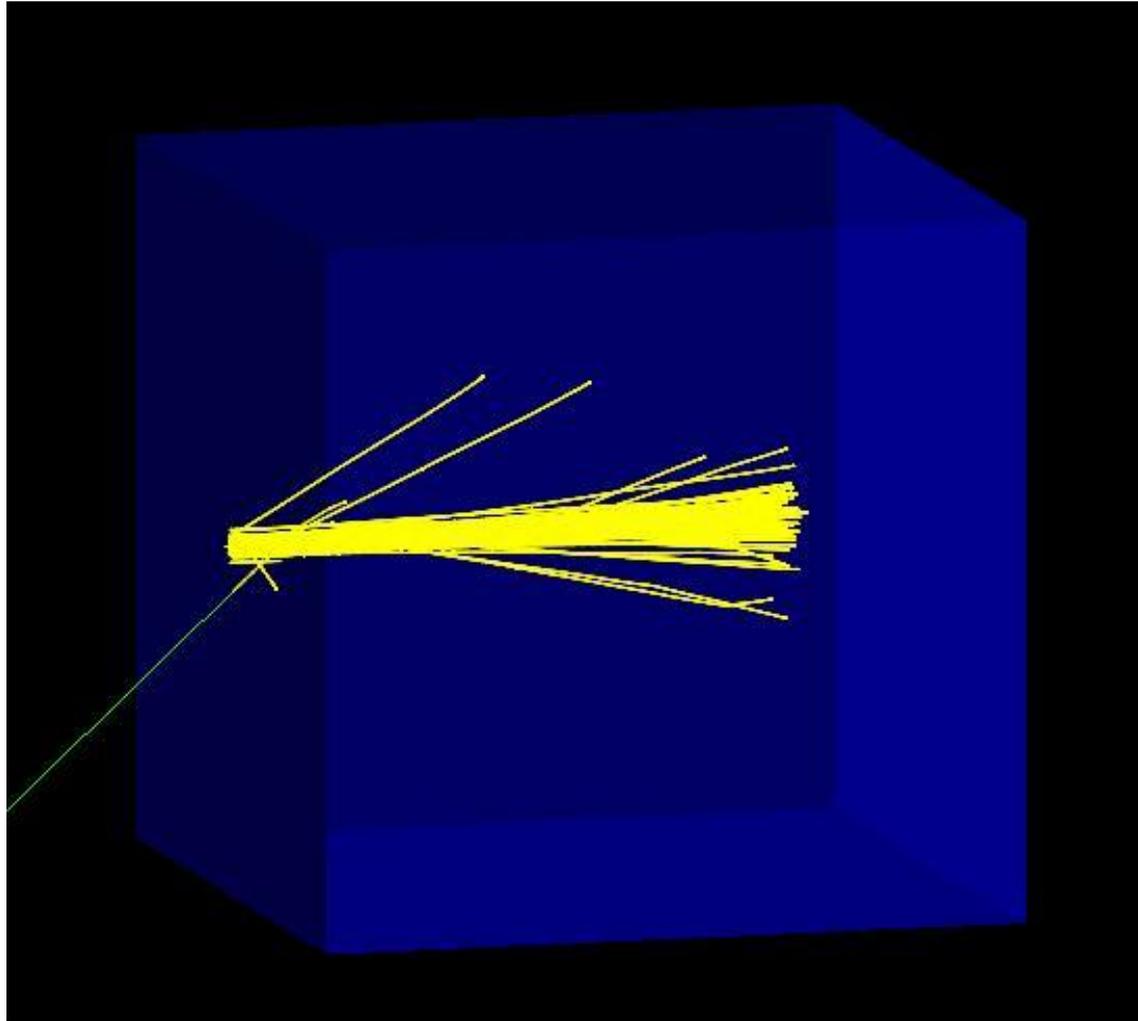
Summary of the work performed

We have tried to reproduce the same plots as in the Verbeek et al. publication, i.e. we have tried to reproduce the experimental data. In addition, we have investigated the following items:

1. **Cuts**: The dependence of the results on the production cuts.
2. **Interpolation**: The dependence of the results on the interpolation procedure to get the dose at some position.
3. **Source**: The dependence of the results on the source used in the simulation.
4. **Physics model**: The dependence of the results on the physics model used in the simulations.
5. **Partial contributions**: The partial contributions of the different secondary particles and reaction types to the dose, as a function of the position in the water tank.
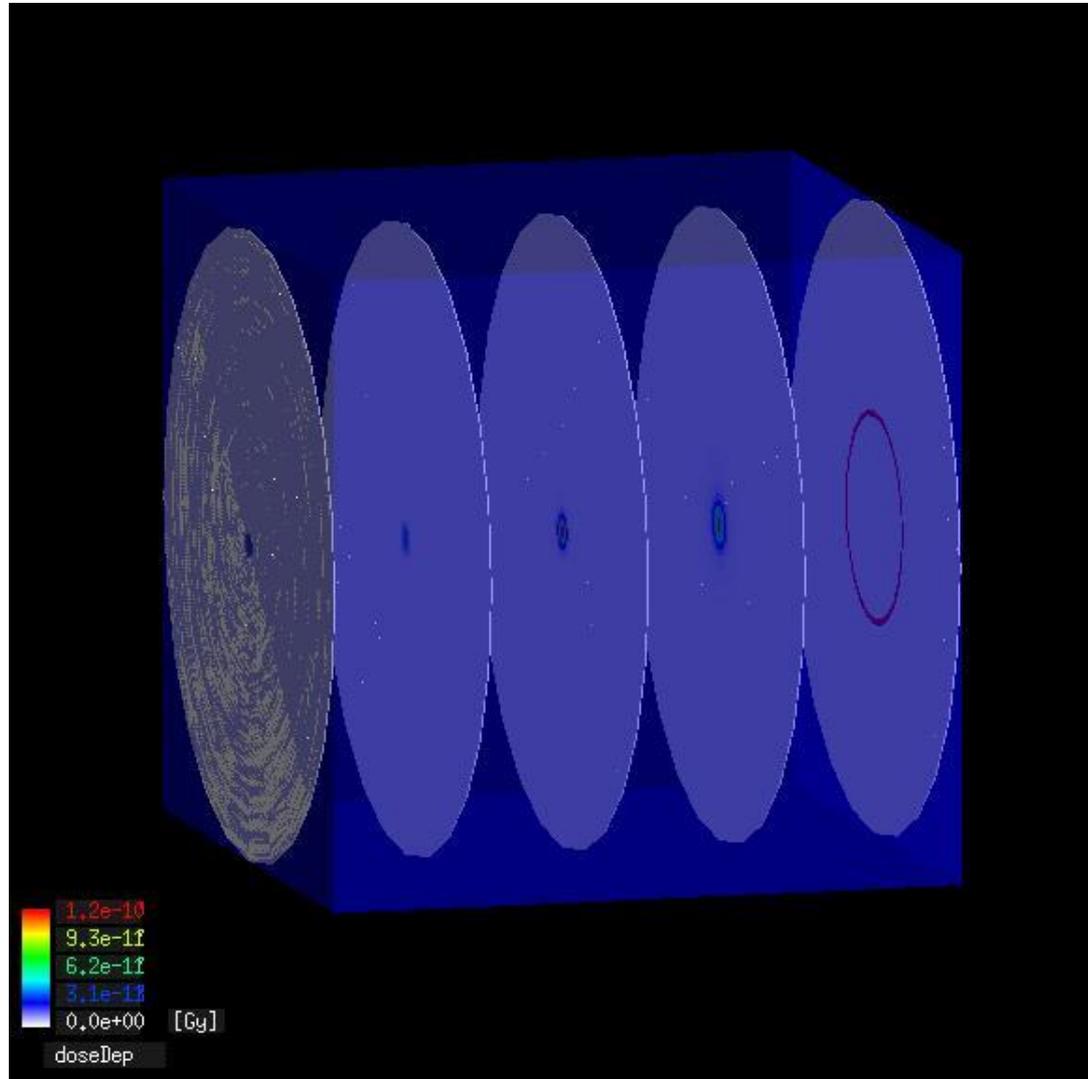
The simulations were performed using 10^7 source particles. We used geant4.10.6 version.

→ **Master thesis** of **Francisco Belda Hériz**: *Simulación de la producción de neutrones en una instalación de protonterapia*, UCM, Septiembre de 2021.
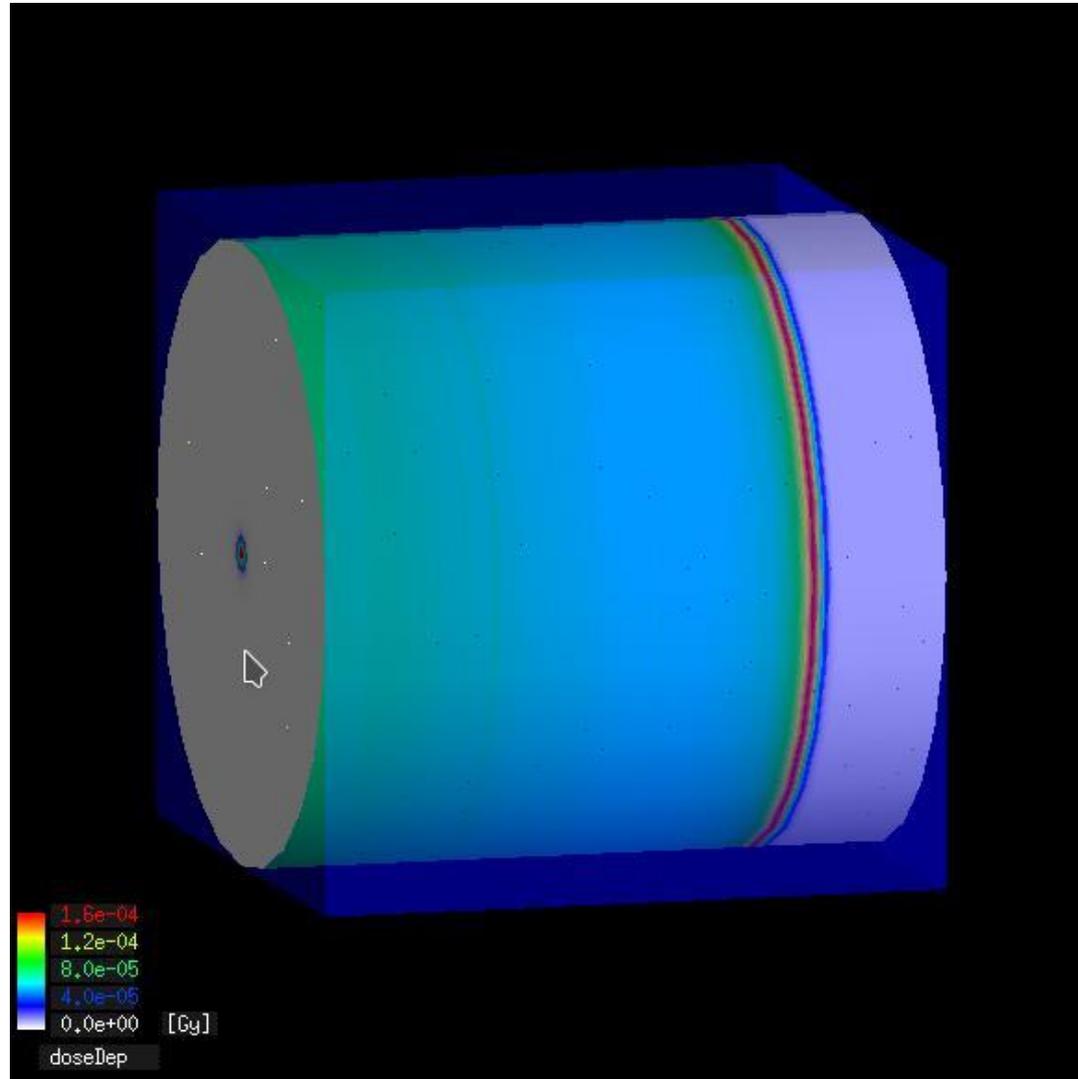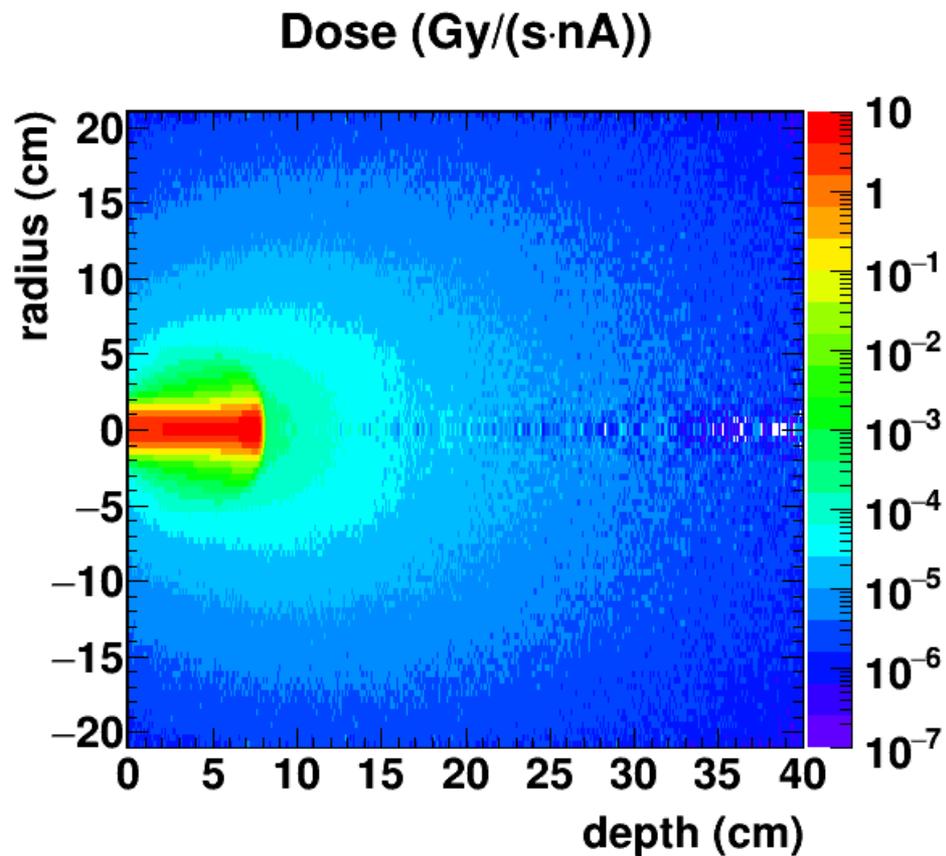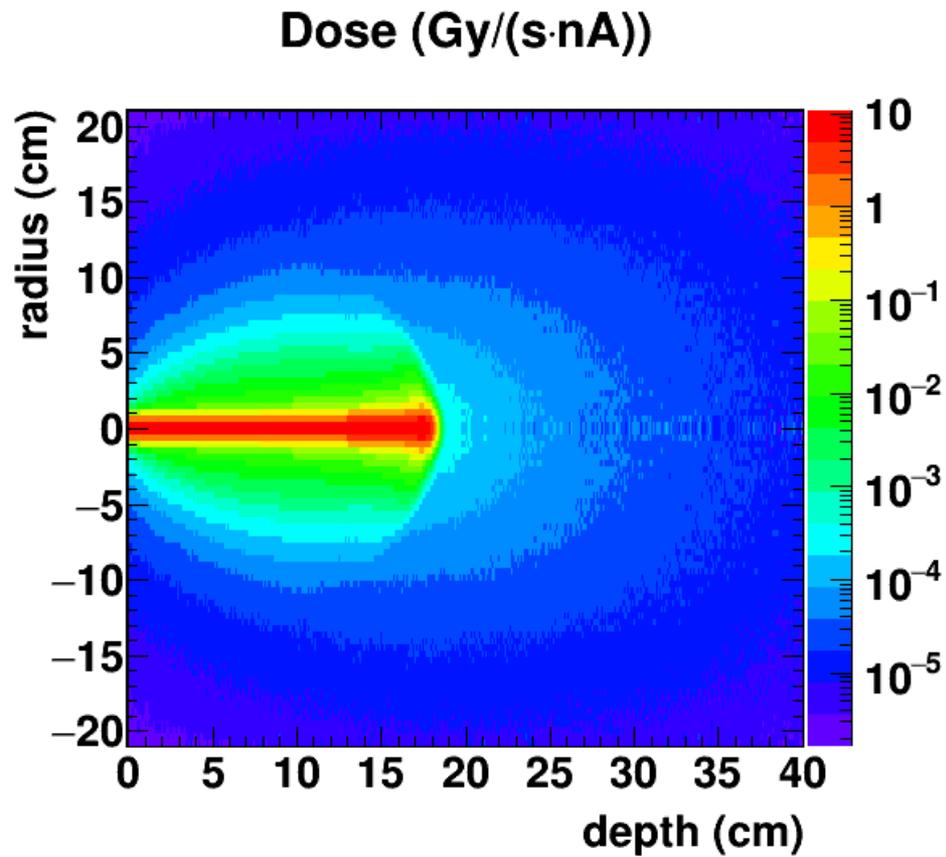
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Geant4 MC simulations

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Dose in the water tank – 100 MeV protons

Dose (Gy/(s·nA))

Dose in the water tank – 160 MeV protons

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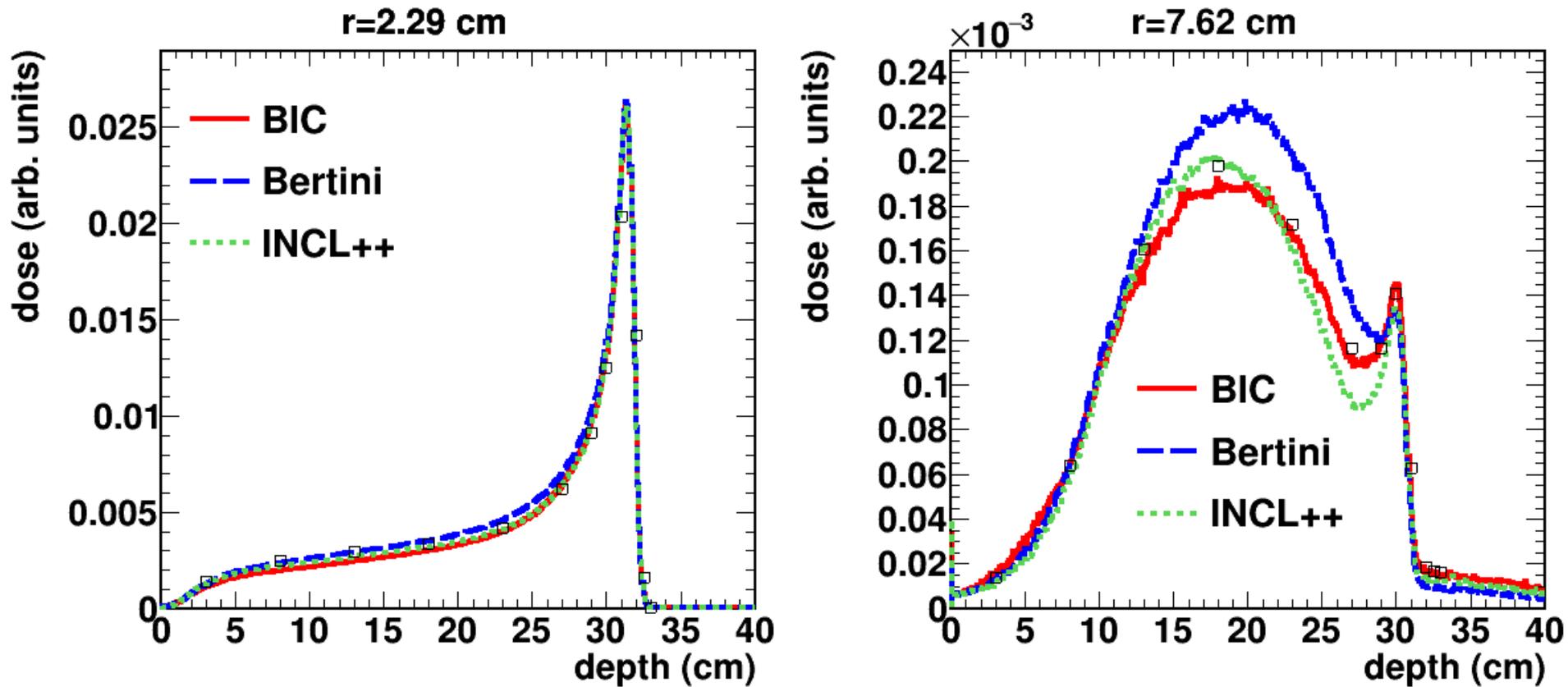# Dose in the water tank – 225 MeV protons
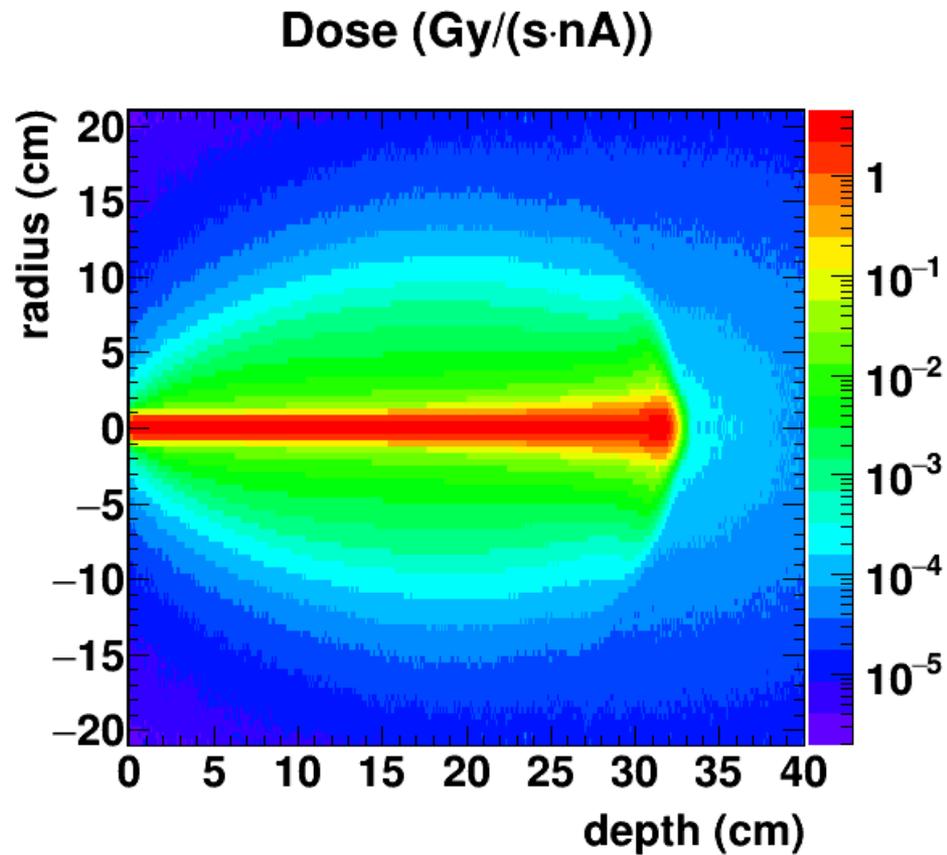
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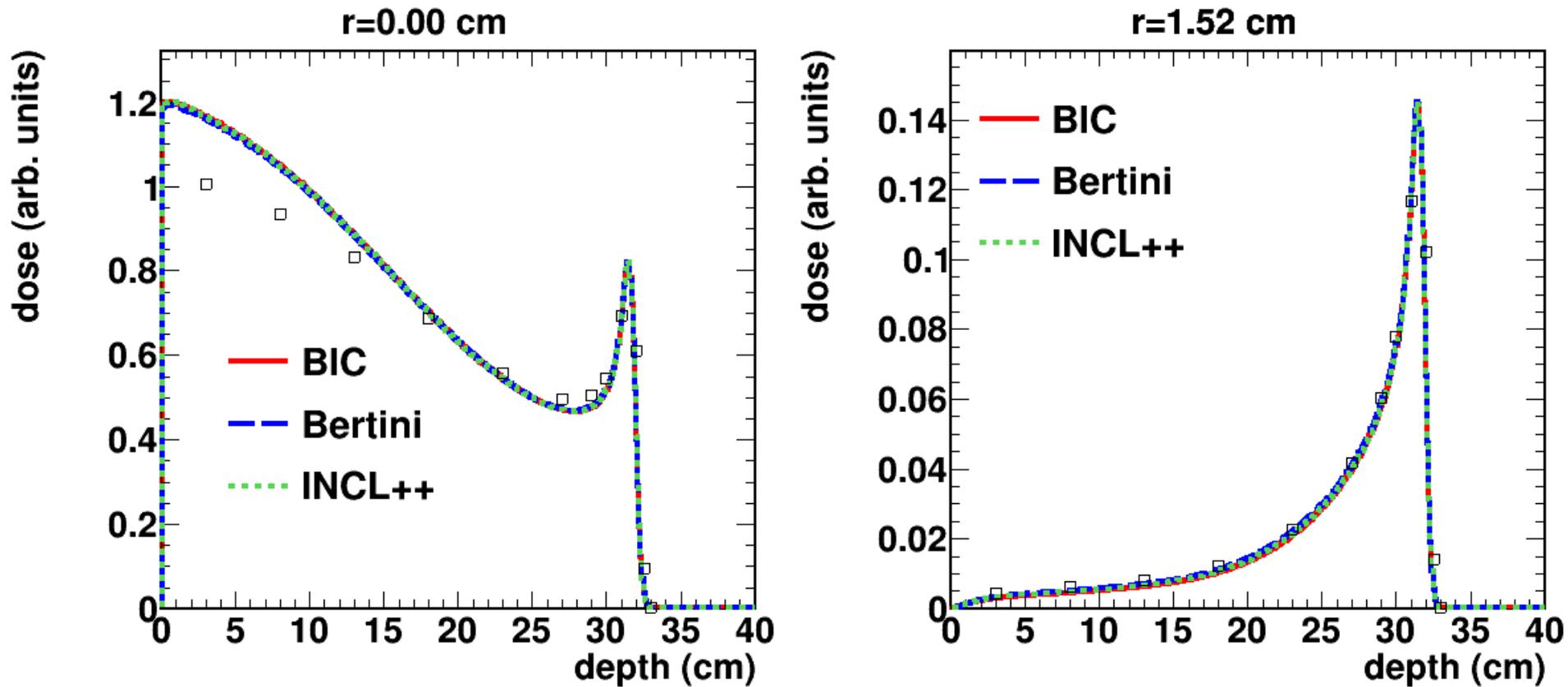
Depth-dose profiles 225 MeV

Depth-dose profiles (225 MeV protons), at different distances to the center of the beam, for different Geant4 physics models.
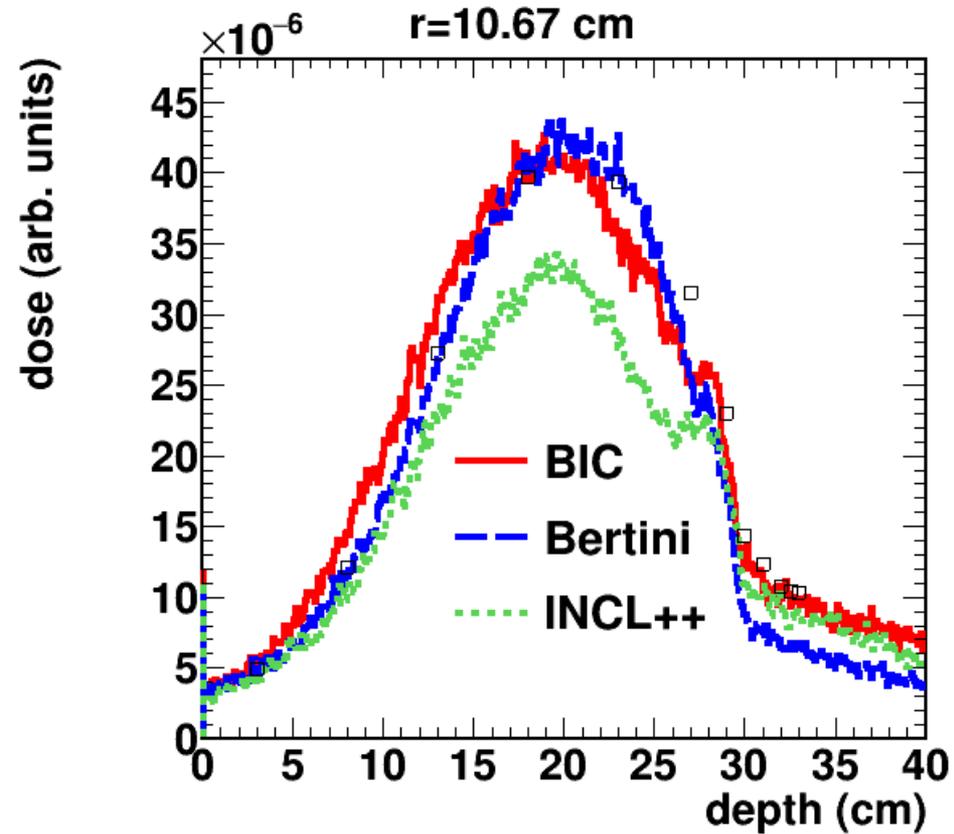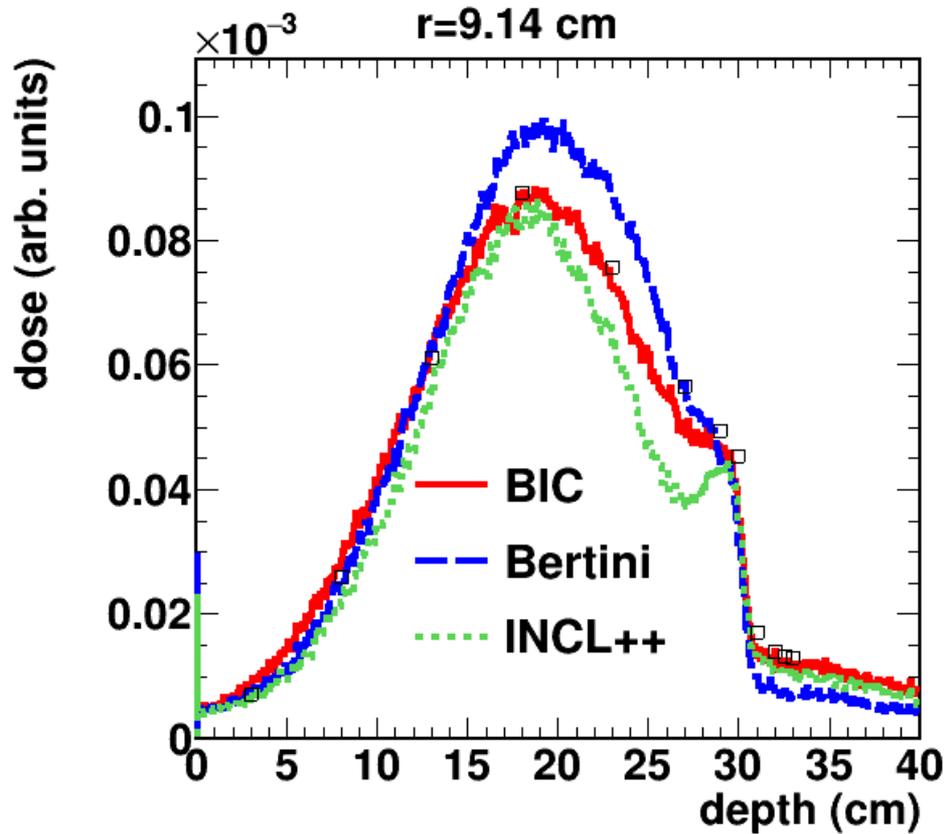
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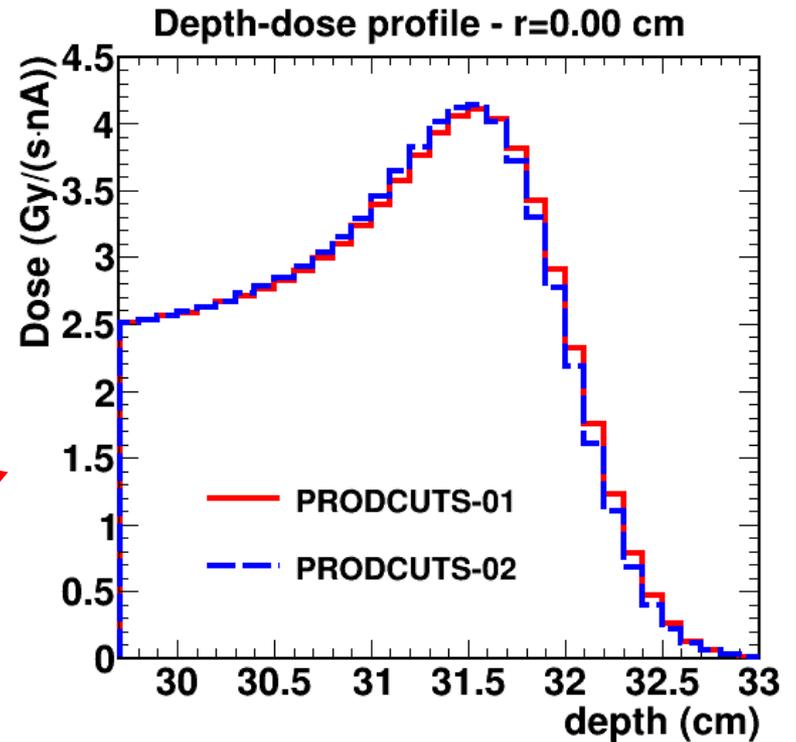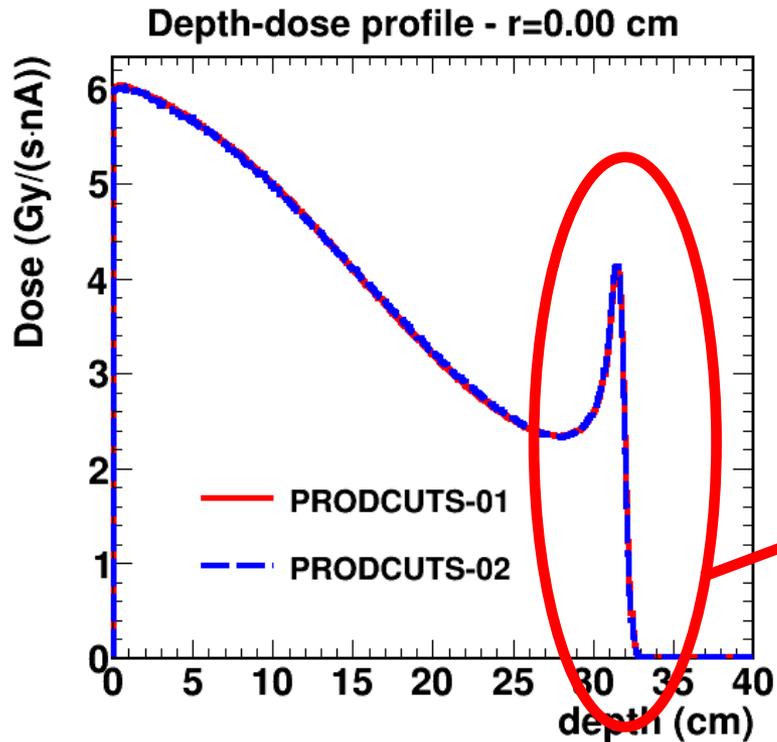
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Production cuts

Depth-dose profile - r=0.00 cm (left plot, PRODCUTS-01 red, PRODCUTS-02 blue dashed)

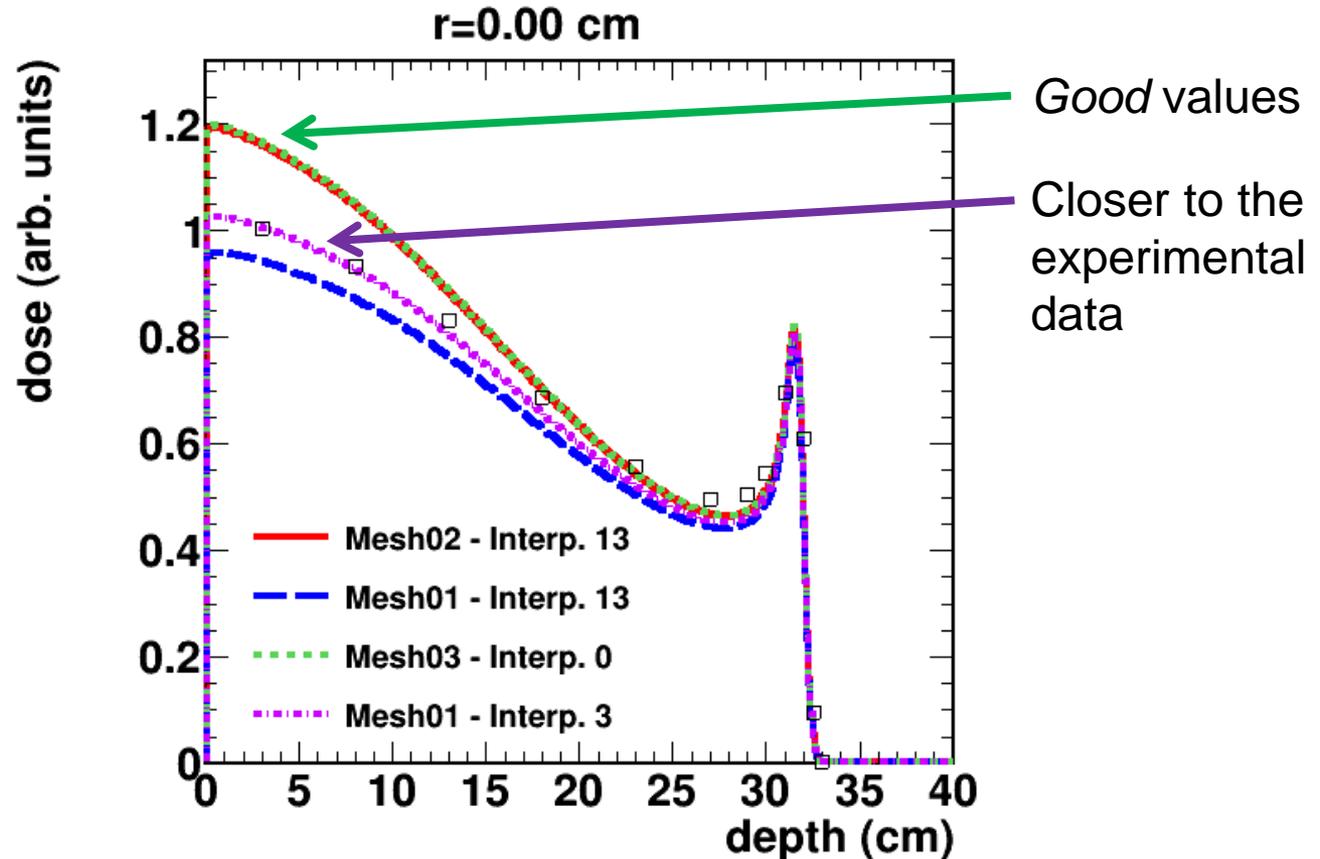Depth-dose profile - r=0.00 cm (right plot, zoomed on Bragg peak, PRODCUTS-01 red, PRODCUTS-02 blue dashed)

We have tested different production cuts:
- PRODCUTS-01: 0 cm protons and 0.07 cm gammas, e+ and e- → **cuts used in this work**
- PRODCUTS-02: 0 cm protons and 0.0005 cm gammas, e+ and e- (10-20 times slower)
→ **Very similar results**. Only Small differences in the Bragg peak (the difference comes from the 0.0005 cm cut in gammas, e+ and e-).
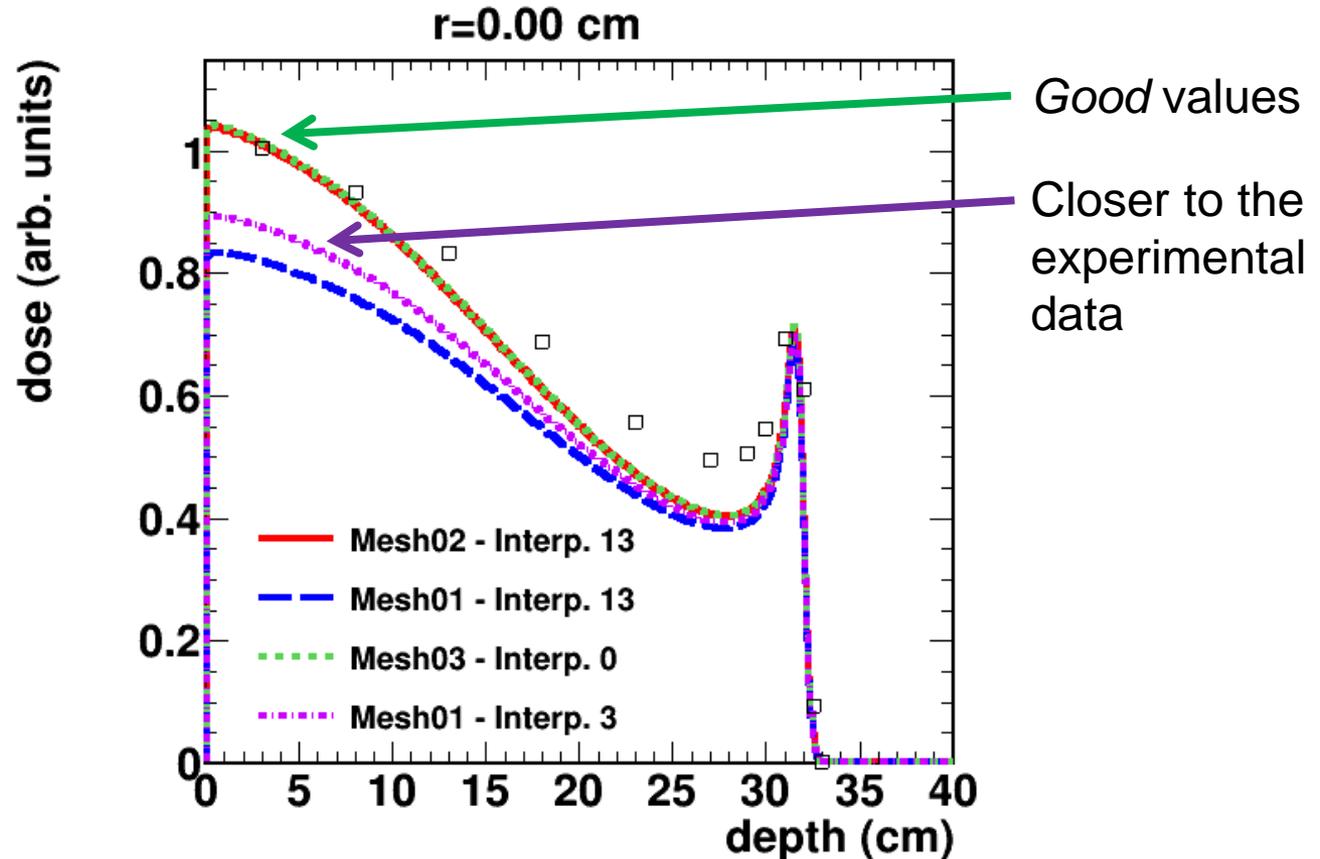→ Differences are not much bigger for other proton energies or other radial distances.

The interpolation issue

r=0.00 cm

Good values

Closer to the experimental data

Legend:
- Mesh02 - Interp. 13
- Mesh01 - Interp. 13
- Mesh03 - Interp. 0
- Mesh01 - Interp. 3

Comparison of the dose obtained with different interpolation types with the experimental data (225 MeV protons at r=0). The values in purple are closer to the experimental points, but in principle the *correct* ones are the values in green.

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The interpolation issue

r=0.00 cm

Good values

Closer to the experimental data

Same plot, alternative normalization

Mesh02 - Interp. 13
Mesh01 - Interp. 13
Mesh03 - Interp. 0
Mesh01 - Interp. 3

Comparison of the dose obtained with different interpolation types with the experimental data (225 MeV protons at r=0). The values in purple are closer to the experimental points, but in principle the *correct* ones are the values in green.

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# The interpolation issue

Conclusions:

- The dose at radial distances closer to 1-2 cm from the center of the beam depends on how the interpolation or the integration is performed.

- In Verbeek et al. they say that they use a cylindrical mesh with dimensions similar to the detectors used to measure the dose and then a 2D-Spline is used to interpolate between the obtained values.

→ normalization to the experimental data not straightforward (in Verbeek et al. they say that they normalize at z=3 cm and r=0 cm, where the differences between interpolations are large).

Source

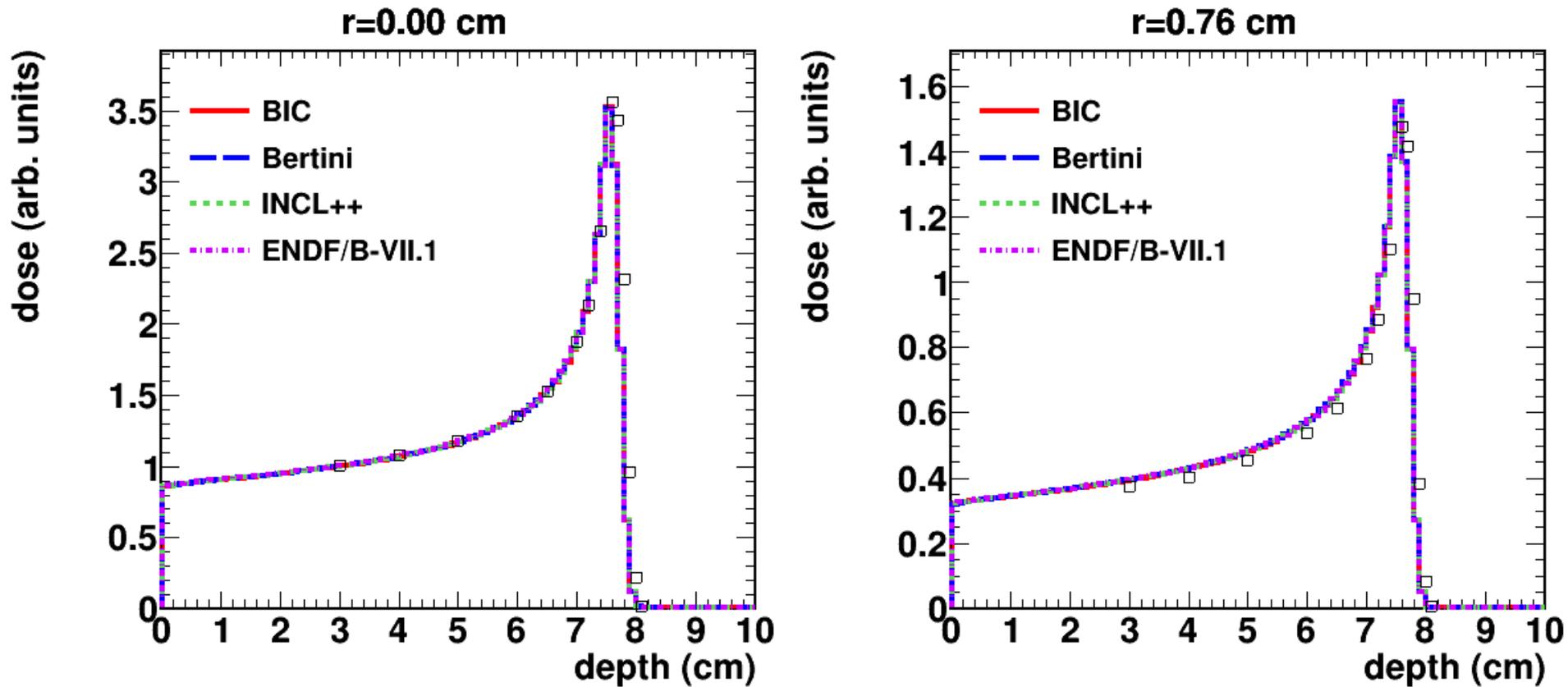→ Some discrepancies come from a *non-complete* description of the source.
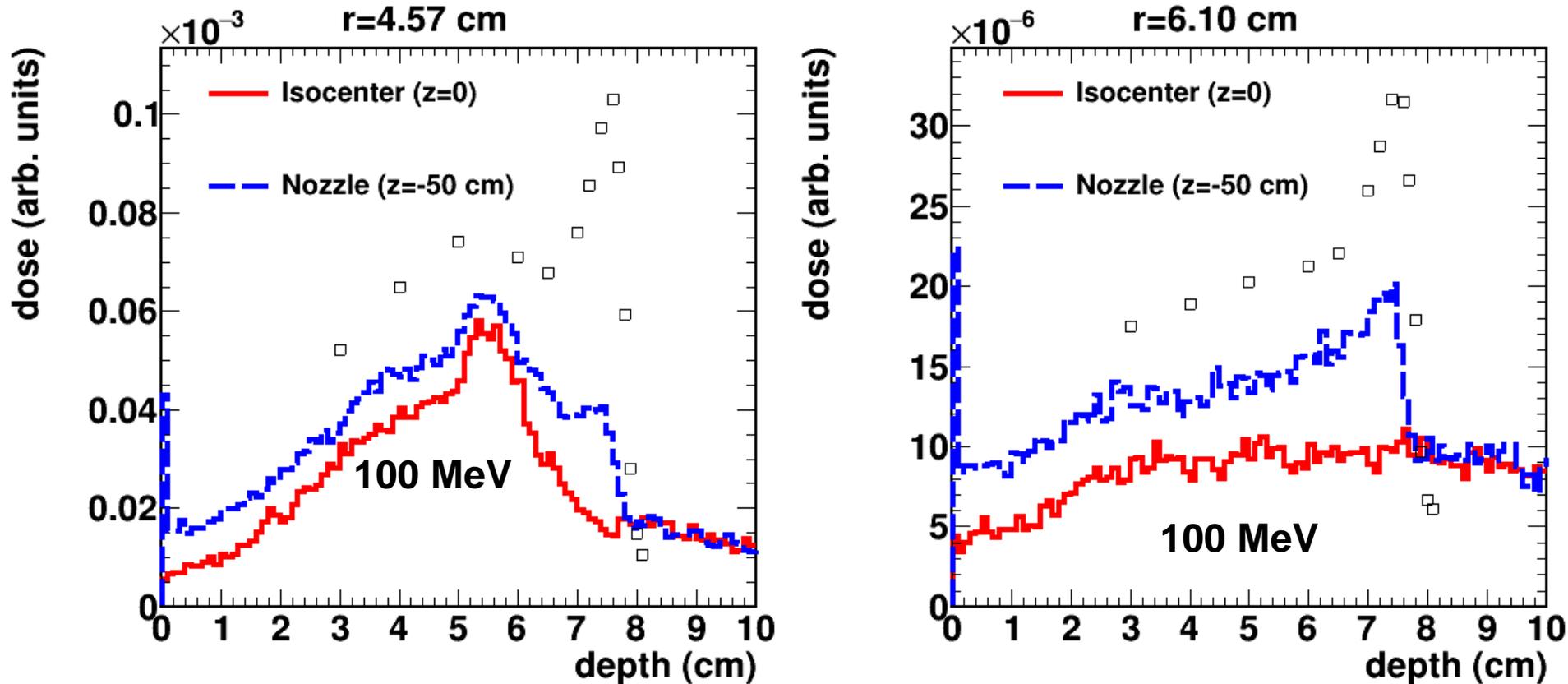
Depth-dose profiles (100 MeV protons), at two different distances from the center of the beam, for the source emitted from the isocenter and from the nozzle.

Physics model

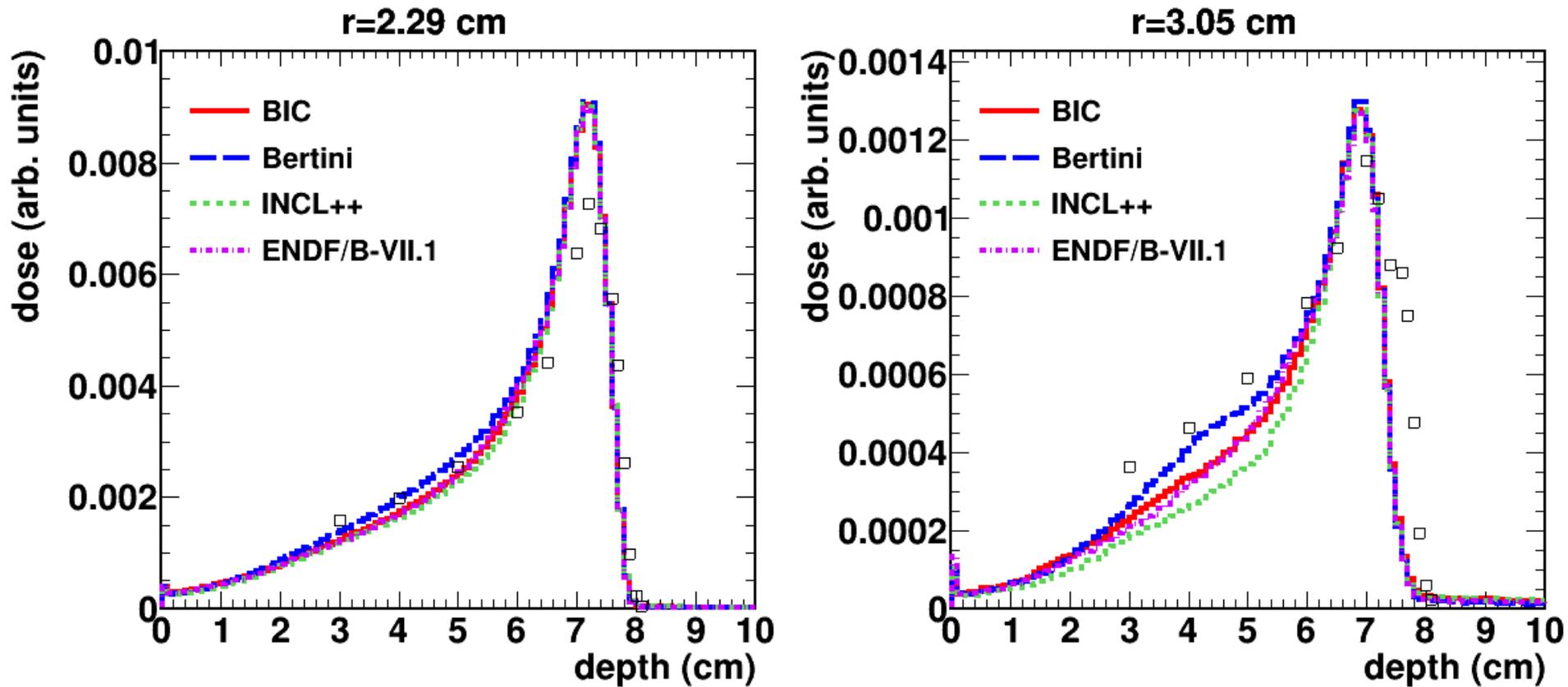The following physics lists available in Geant4 have been considered:

- EM: G4EmStandardPhysics_option4 (the *best* one).

- Hadron elastic: G4HadronElasticPhysicsPHP, which means

  - Protons: G4BGGNucleonElasticXS cross sections (Barashenkov parameterization below 100 GeV) + G4ChipsElasticModel.

  - Neutrons: thermal data libraries (water) up to 4 eV + HP model (JEFF-3.3) up to 20 MeV + G4NeutronElasticXS with G4ChipsElasticModel above 20 MeV.

- Hadron inelastic: G4HadronPhysicsFTFP_BERT_HP + G4IonPhysics (but we change the physics for protons), which means

  - Protons: different physics,

    - **Binary cascade model (BIC)**

    - **Bertini**

    - **INCL++**

    - ParticleHP with G4TENDL data (which is **ENDF/B-VII.1** for ^{16}O) $\rightarrow$ this model can be used only below 150 MeV (i.e. for the 100 MeV protons).

  - Neutrons: HP model (JEFF-3.3) up to 20 MeV + NeutronHPInelasticXS with Bertini model above 20 MeV.

- Radioactive decay

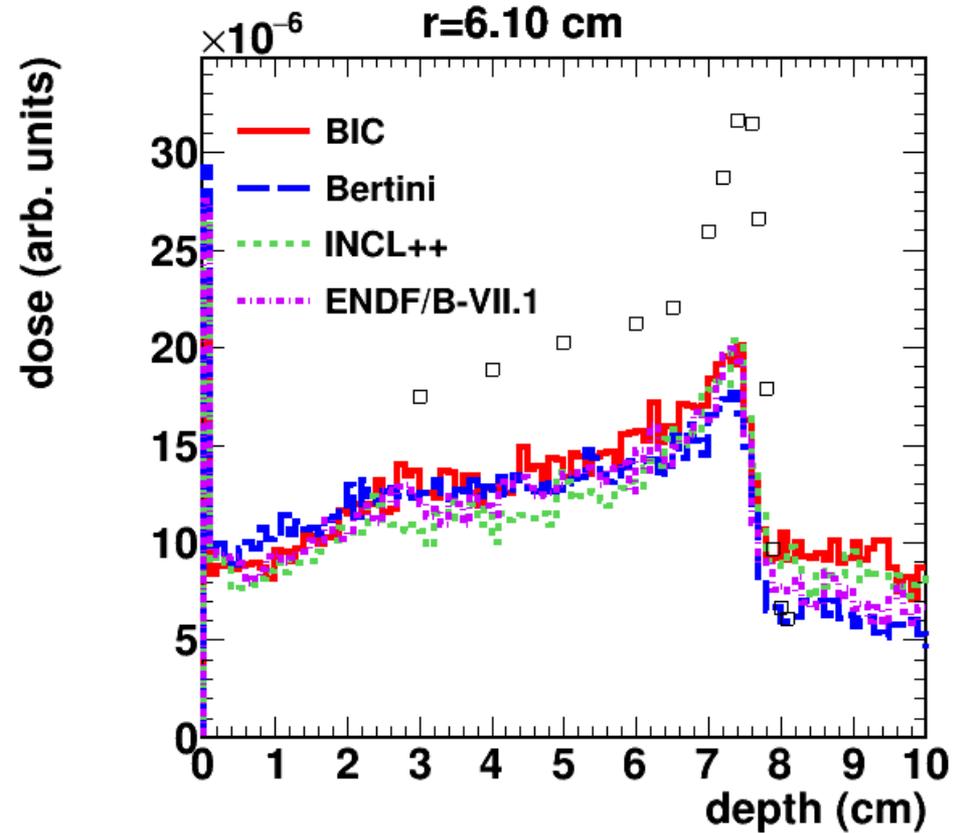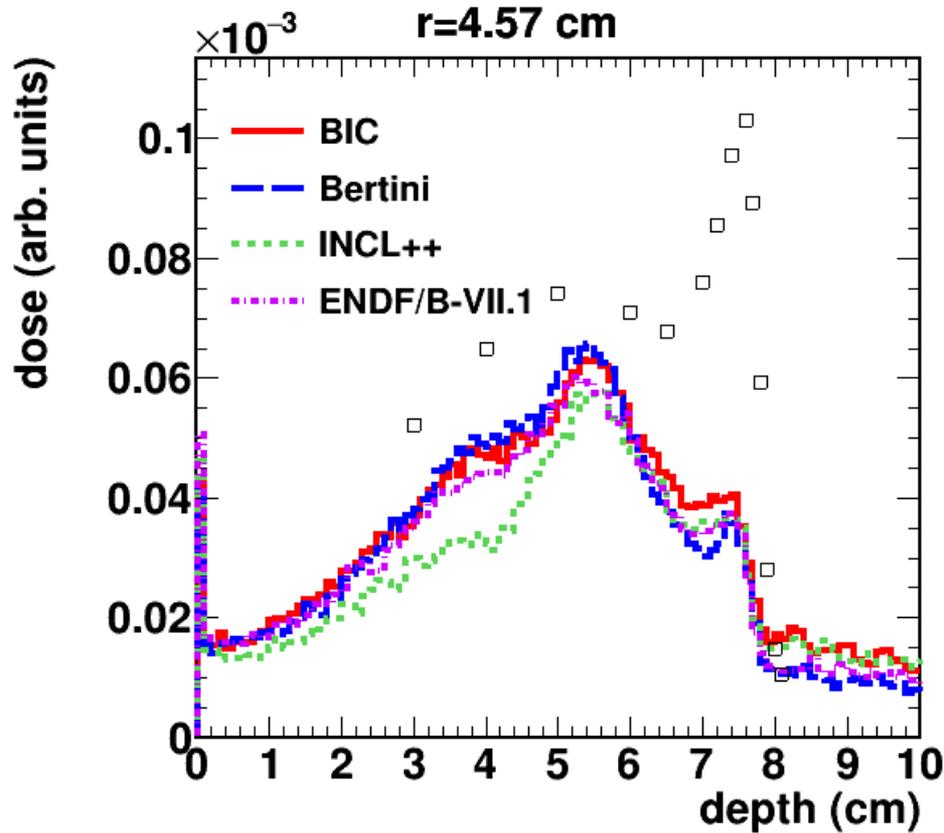- Stopping   physics

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Depth-dose profiles 100 MeV

Depth-dose profiles (100 MeV protons), at different distances to the center of the beam, for different Geant4 physics models.
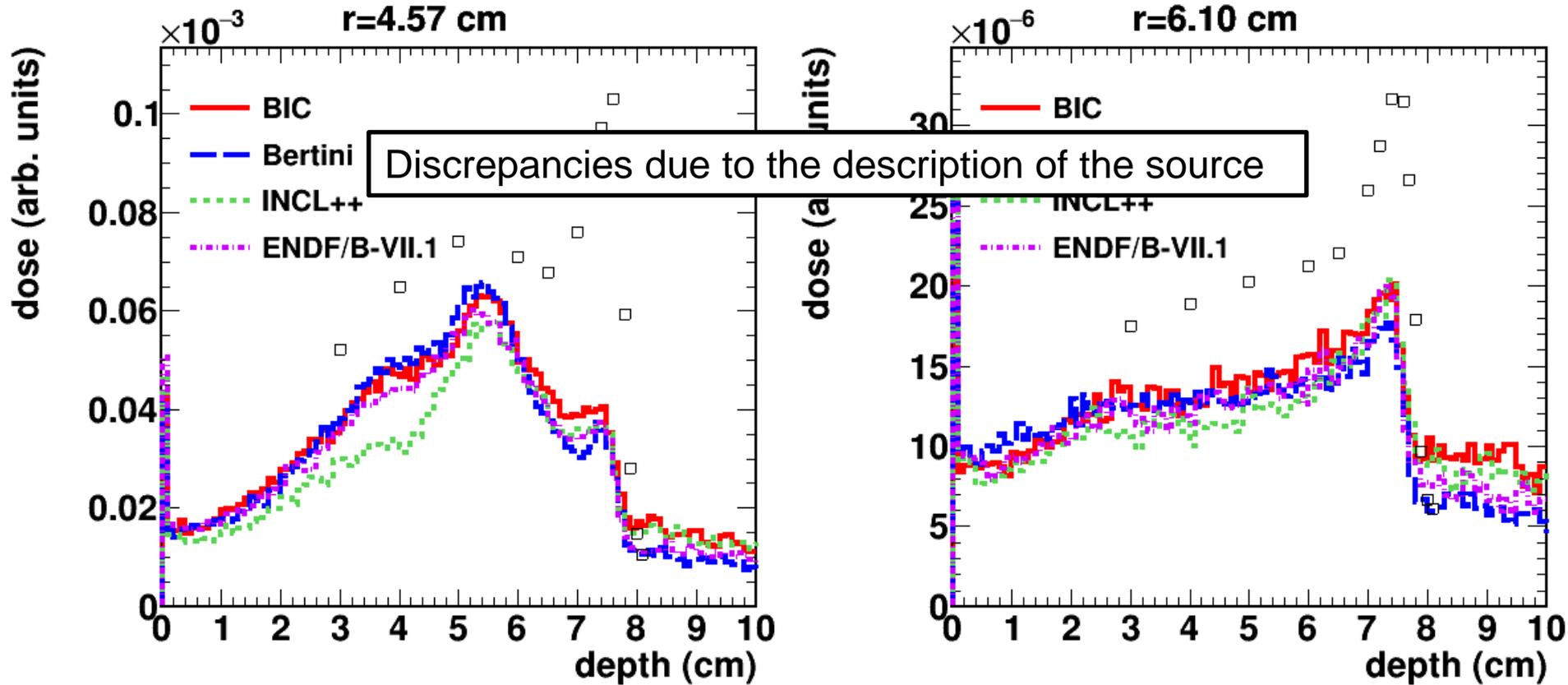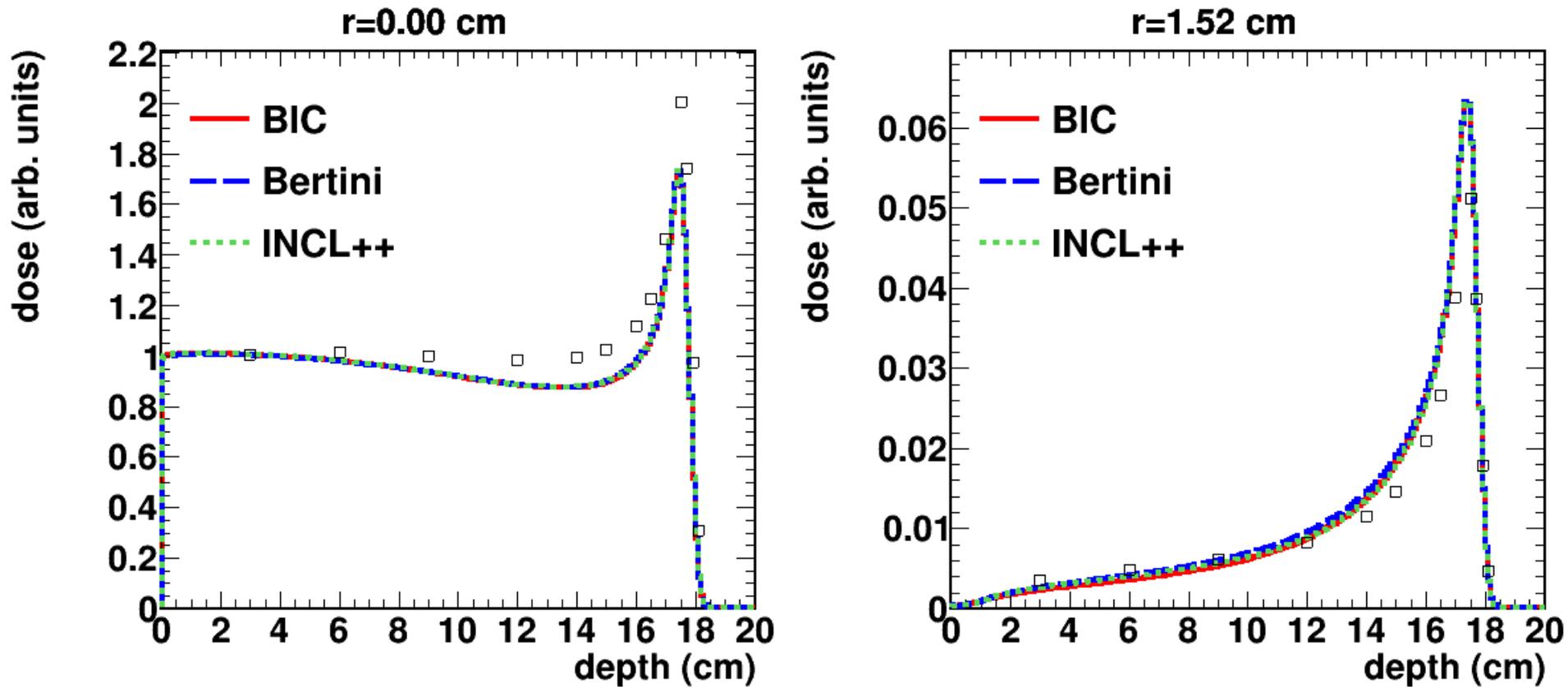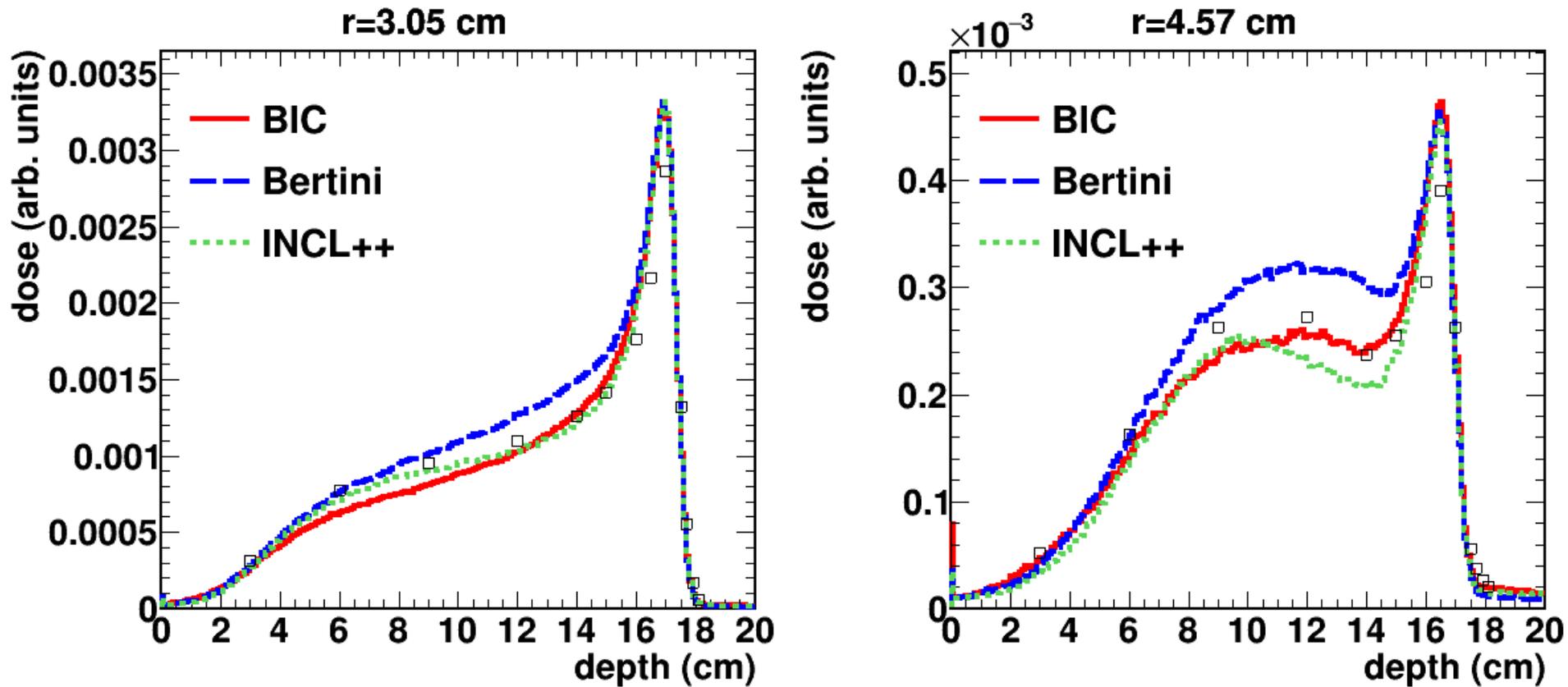
Depth-dose profiles 100 MeV

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Depth-dose profiles 100 MeV

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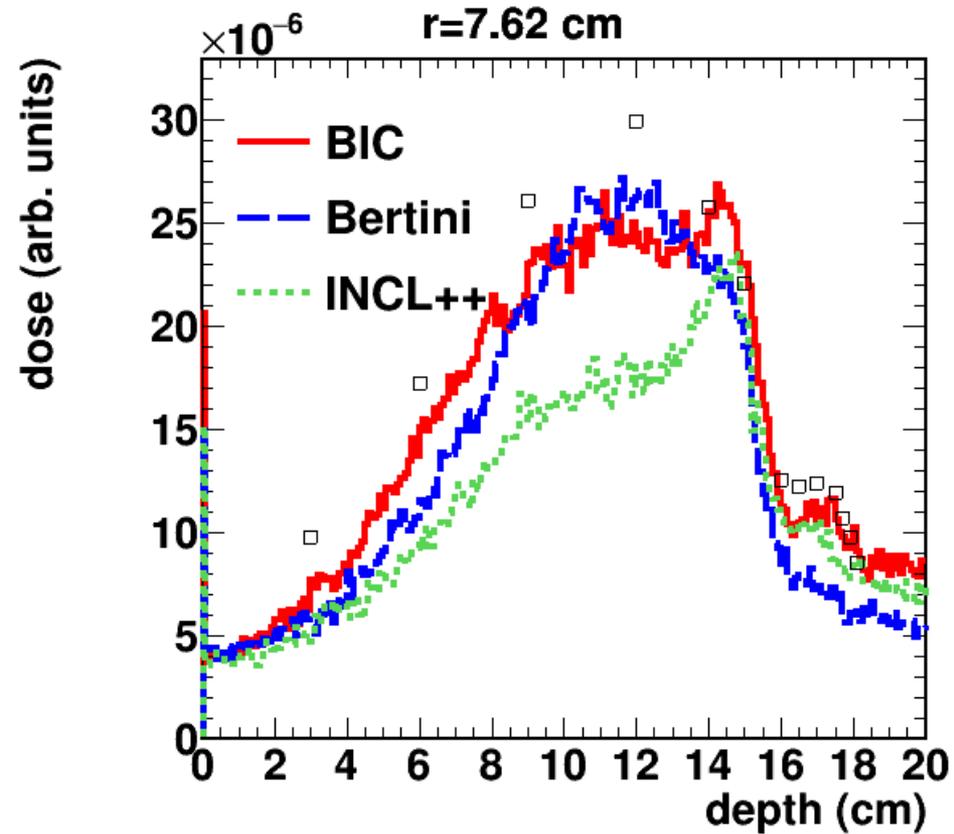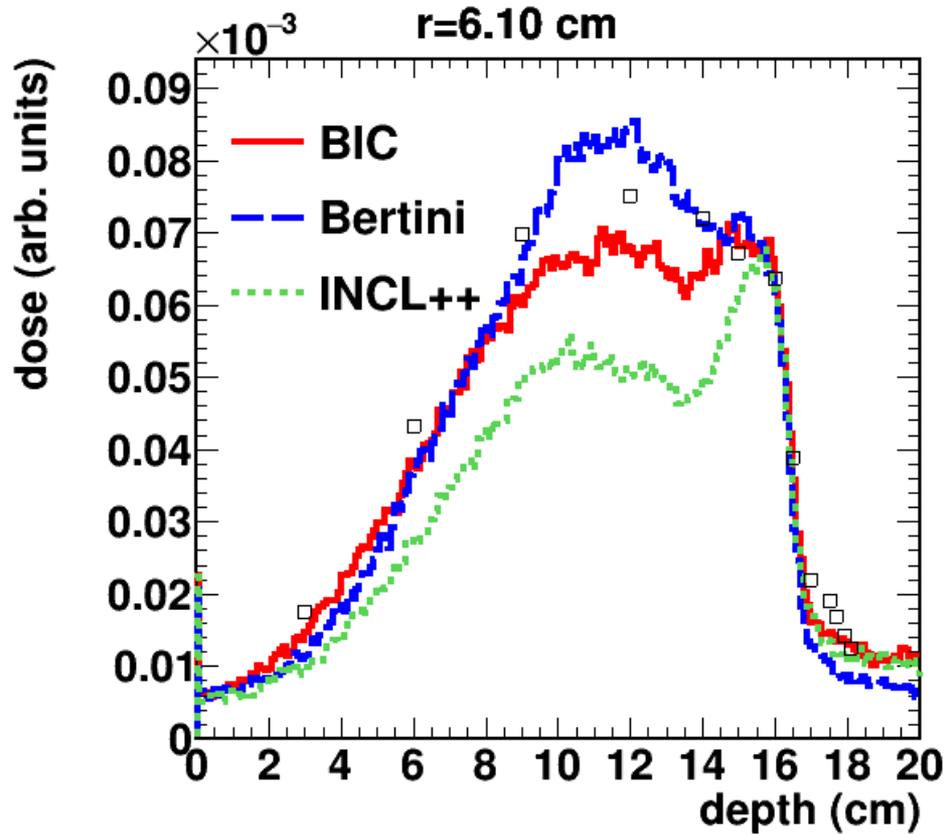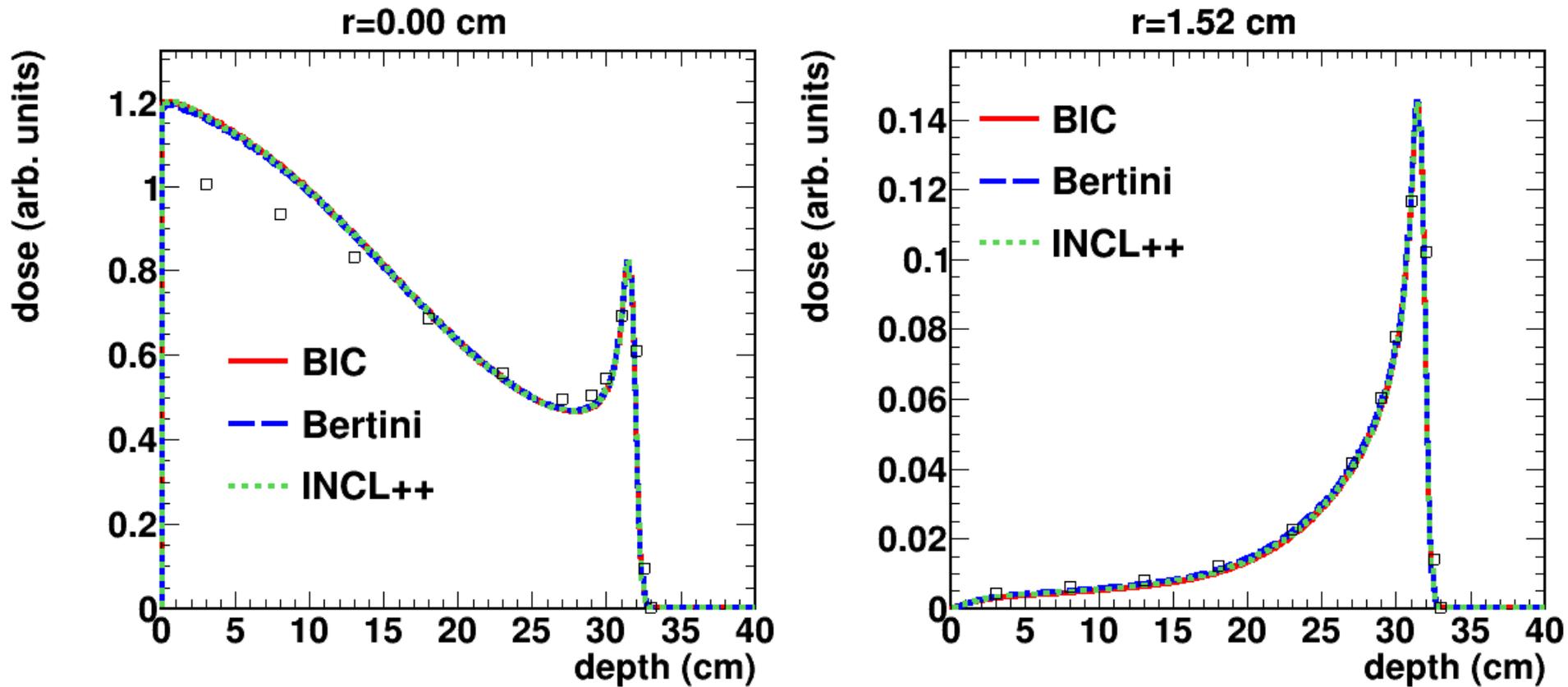
Depth-dose profiles 160 MeV

Depth-dose profiles (160 MeV protons), at different distances to the center of the beam, for different Geant4 physics models.

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Depth-dose profiles 160 MeV

Depth-dose profiles (160 MeV protons), at different distances to the center of the beam, for different Geant4 physics models.

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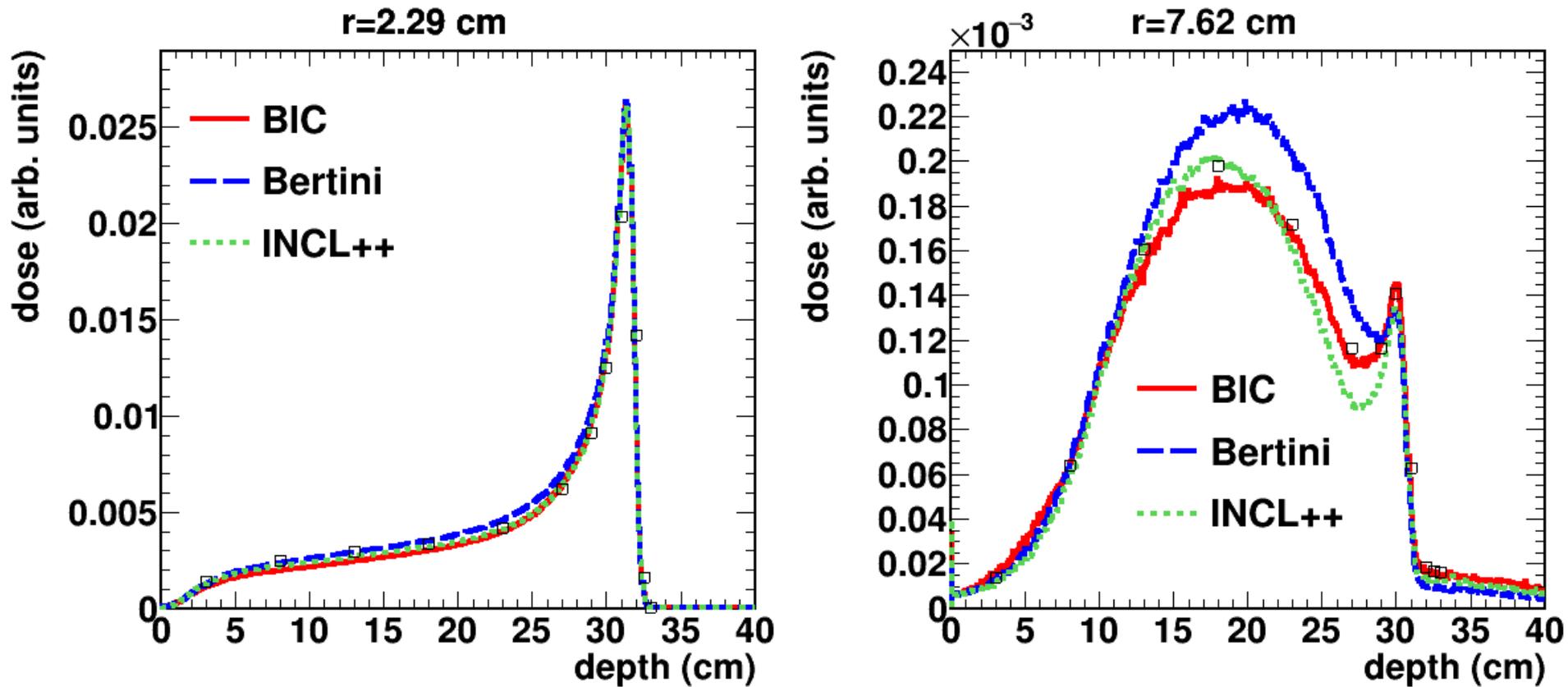*June 2022*

Depth-dose profiles 160 MeV

Depth-dose profiles (160 MeV protons), at different distances to the center of the beam, for different Geant4 physics models.
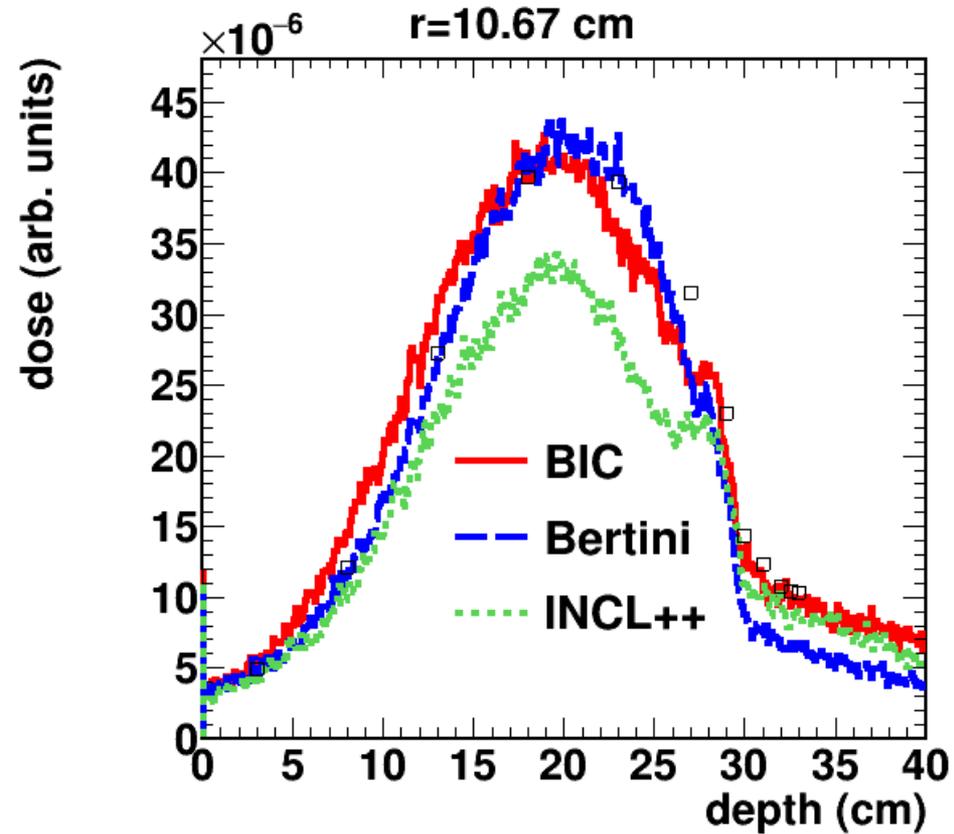
Depth-dose profiles 225 MeV

Depth-dose profiles (225 MeV protons), at different distances to the center of the beam, for different Geant4 physics models.

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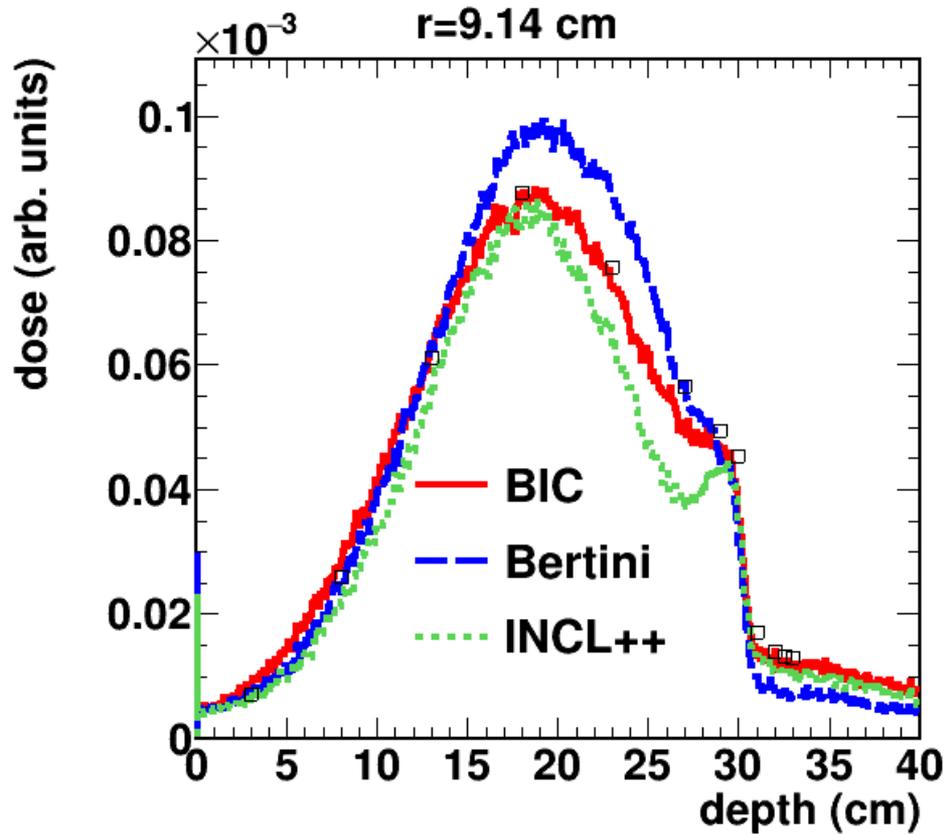
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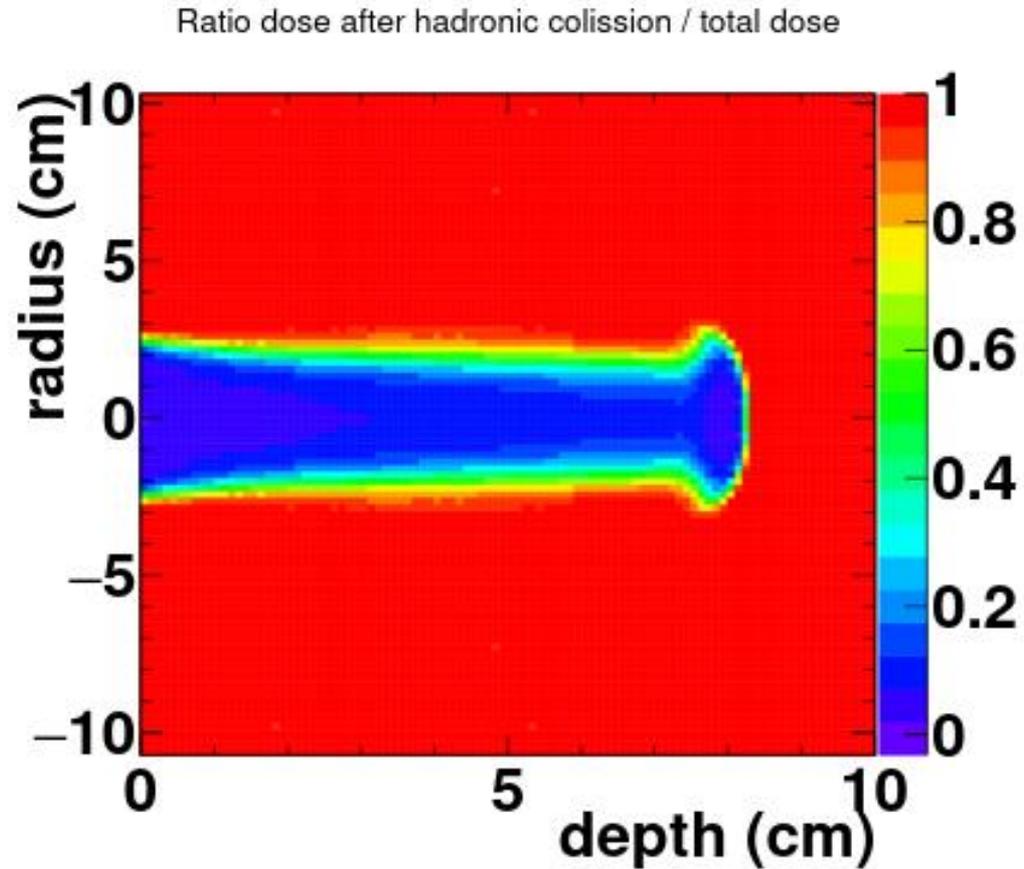
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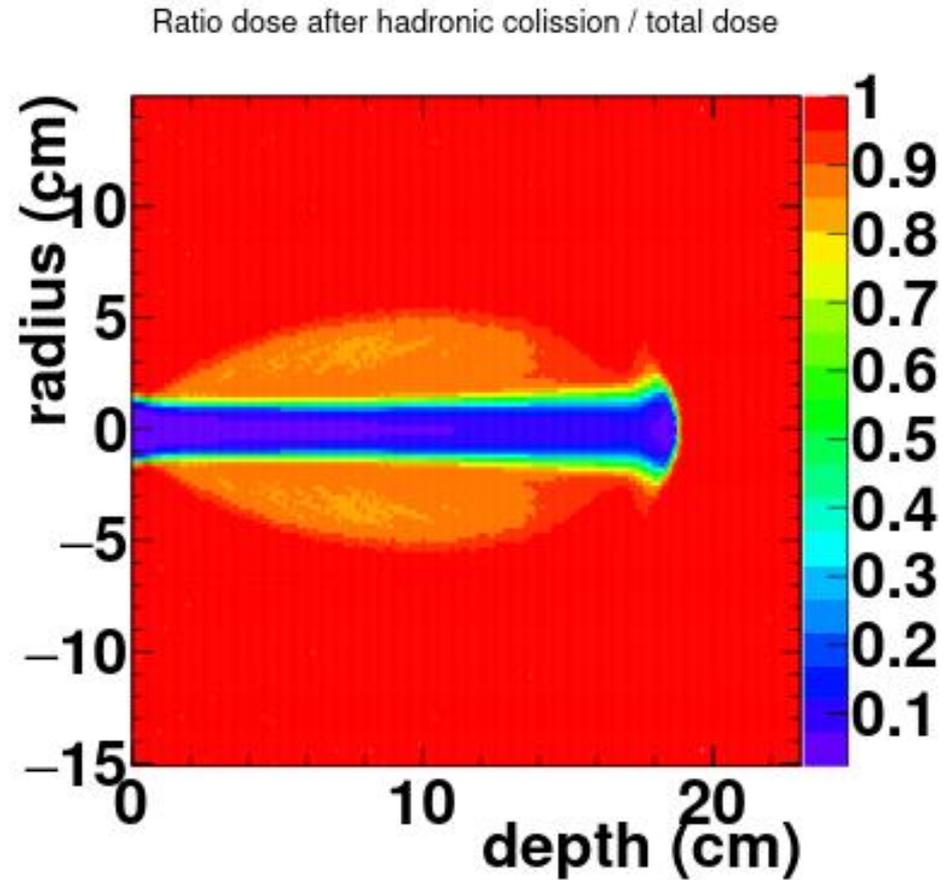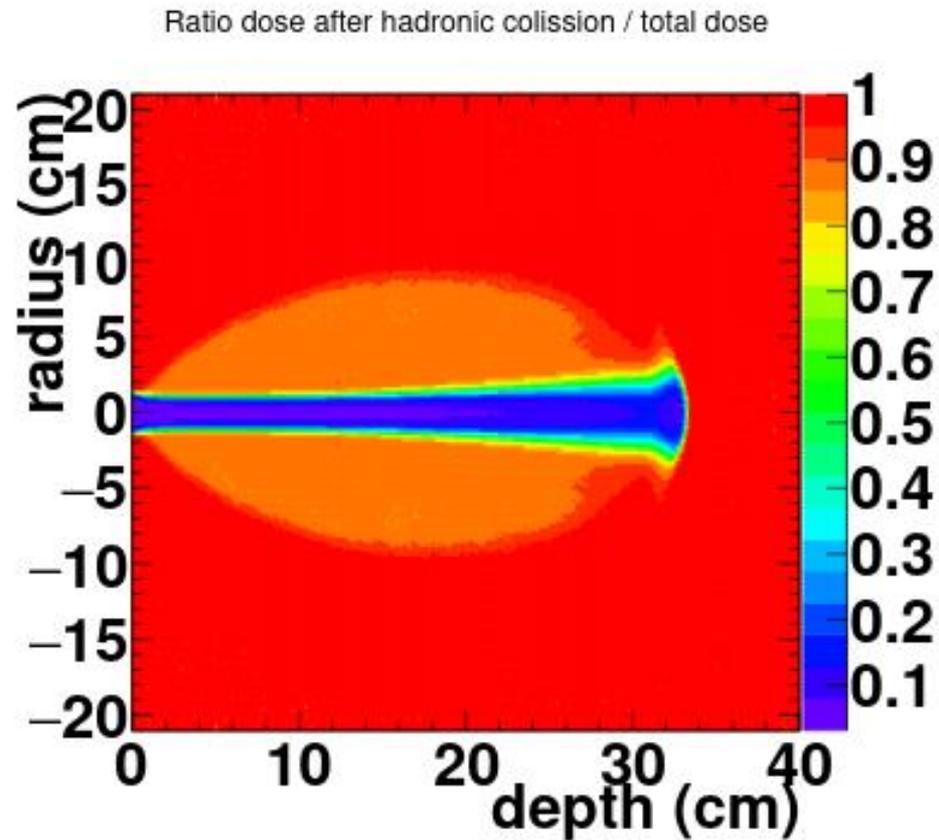
Partial contributions

Dose after hadronic reaction – 100 MeV

Ratio dose after hadronic colission / total dose

Dose after hadronic reaction – 160 MeV

Ratio dose after hadronic colission / total dose

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Dose after hadronic reaction – 225 MeV

Ratio dose after hadronic colission / total dose

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Partial contributions to the depth-dose profiles (225 MeV protons), at different distances to the center of the beam (BIC model for the proton induced inelastic reactions).

Partial contributions to the depth-dose profiles (225 MeV protons), at different distances to the center of the beam (BIC model for the proton induced inelastic reactions).
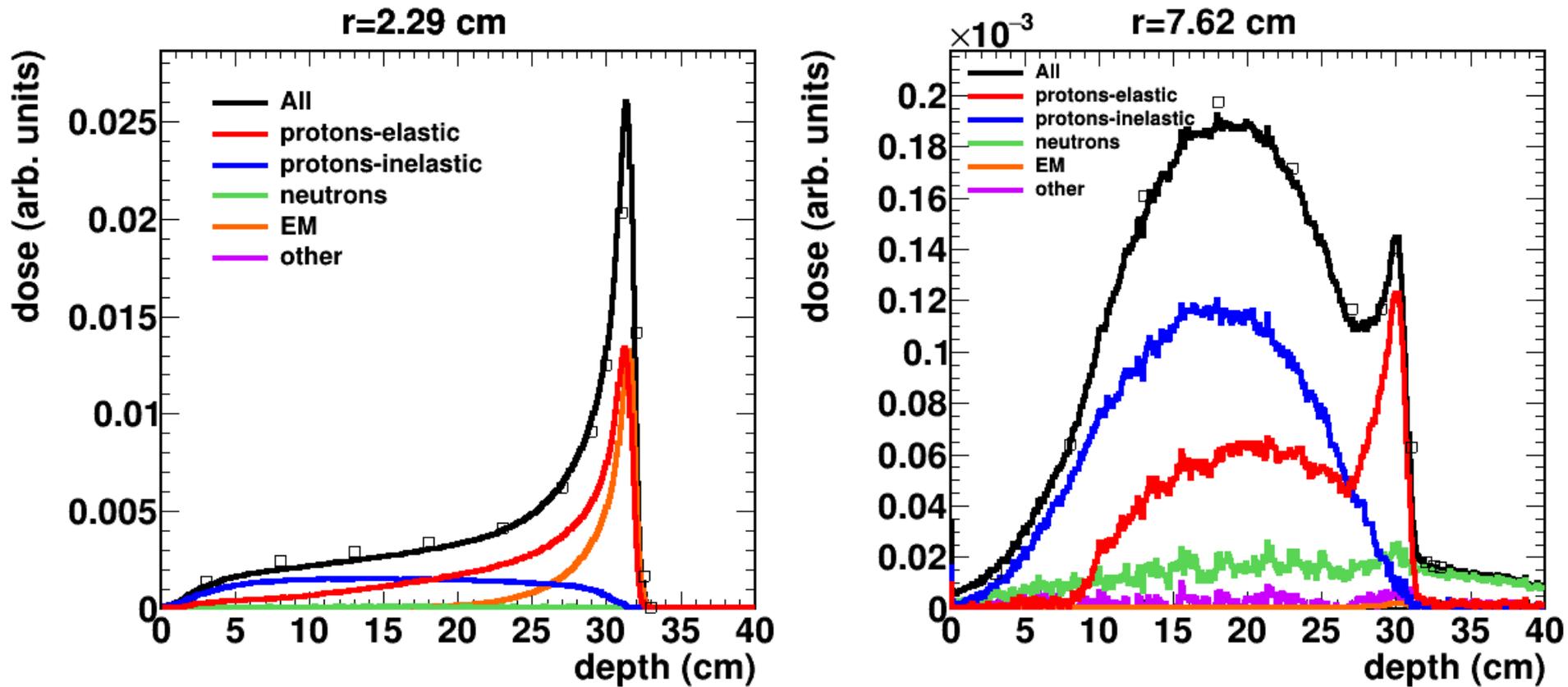
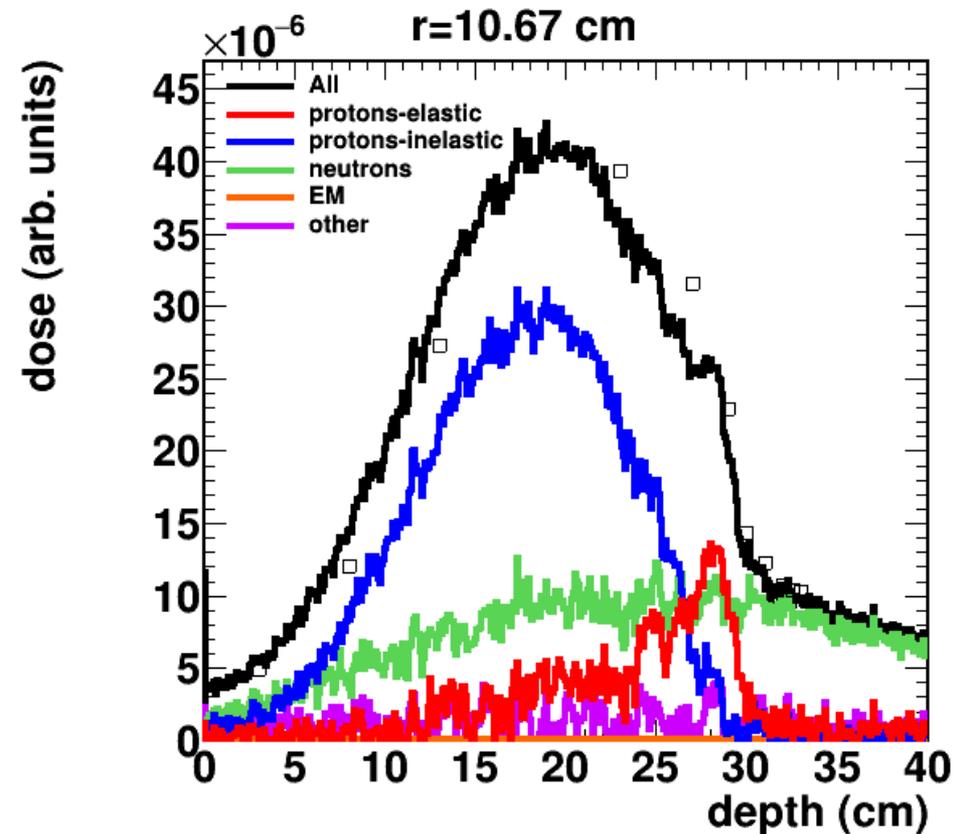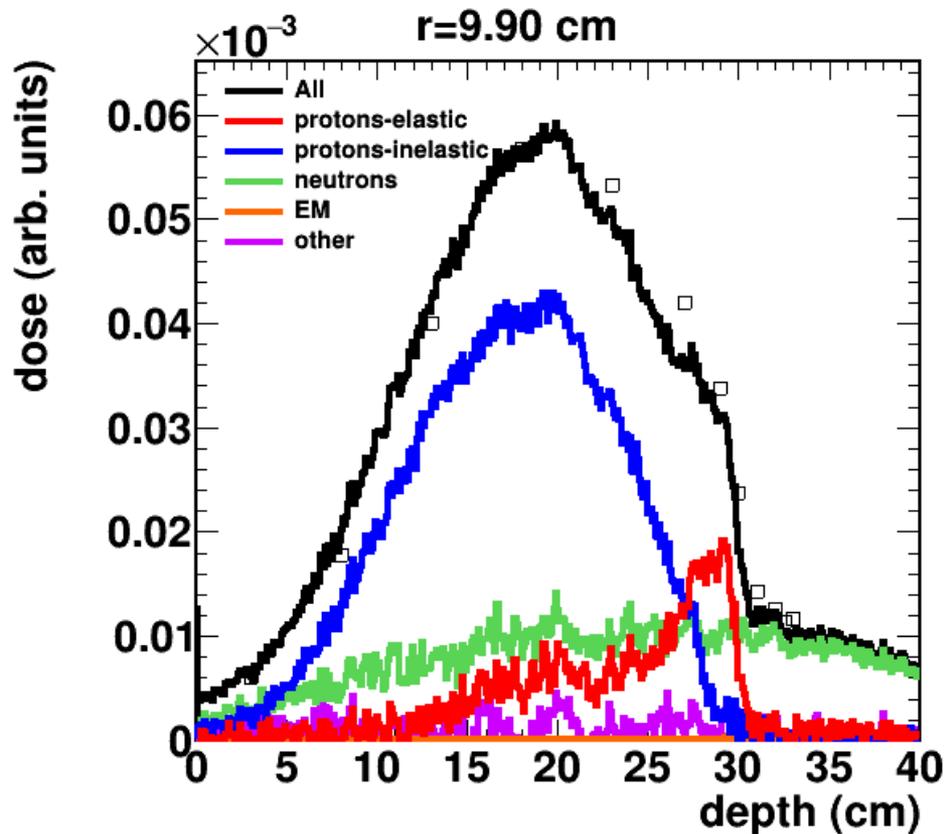# Partial contributions to the depth dose profiles - 225 MeV

Partial contributions to the depth-dose profiles (225 MeV protons), at different distances to the center of the beam (BIC model for the proton induced inelastic reactions).

Conclusions

- We have found that the comparison between simulations and experimental results not straightforward → interpolation + source.

- We have performed simulations with different nuclear reaction models, and compared the obtained results with the experimental data → different results, but there isn't any model working much better or much worse than the others.

- We have also quantified the contribution of different processes (p,xp), (p,xn), (p,xγ) … reactions to the dose → the most relevant hadronic processes are, in this case elastic scattering and (p,xp), (p,xn) reactions.

Future work

We can improve the data driven models implemented in Geant4 (ParticleHP), i.e. those which use nuclear data libraries to model the nuclear reactions.

Present situation:

– Neutrons: data driven models operate for elastic and non-elastic reaction **up to 20 MeV.**

– Protons (and also d, t, ^{3}He and α): data driven models operate for non-elastic reactions only, **up to 200 MeV**. The library distributed together with the code (G4TENDL) have some data with an upper limit below 200 MeV (e.g. ^{16}O for protons → 150 MeV, since it comes from ENDF/B-VII.1 instead of TENDL).

– In all the cases, **models and data libraries cannot be used at the same time** in the same energy range → if a library contain a limited number of isotopes, it is not possible to make a simulation using data for these isotopes and models for the isotopes not present in the library.

Proposed improvements:

– **Extend ParticleHP** so that it can be used for neutrons, protons .. **up to higher energies** (a few GeV).

– **Improve ParticleHP** so that **models and data libraries can be used at the same time** and in the same energy range.

– Extend the capabilities of ParticleHP so that **several data libraries can be used at the same time**, in different energy ranges (e.g. for neutrons JEFF-3.3 below 20 MeV and JENDL/HE-2007 above).

– Creation of the data libraries (from ENDF-6 format files) + verification process (indeed, ParticleHP has not been validated much for incident charged particles).

Acknowledgments

We would like to express our gratitude to Lorenzo Brualla and Nico Verbeek, from the West German Proton Therapy Centre Essen WPE (Essen, Germany) for sharing with us their experimental data, their time, and for their very kind support along all our study.

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