Enhancing the efficiency of MC simulations of radiation transport

F. Salvat Pujol[1], M. Novak[1], S. Guatelli[2]

15th EURADOS School

Computational Methods in Dosimetry
State of the Art and Emerging Developments

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Overview

- **Convergence** of a Monte Carlo (MC) simulation

- **Figure of merit** (efficiency) of a MC simulation

- Focus on **essential physics** and **simulation parameters** ***FIRST***

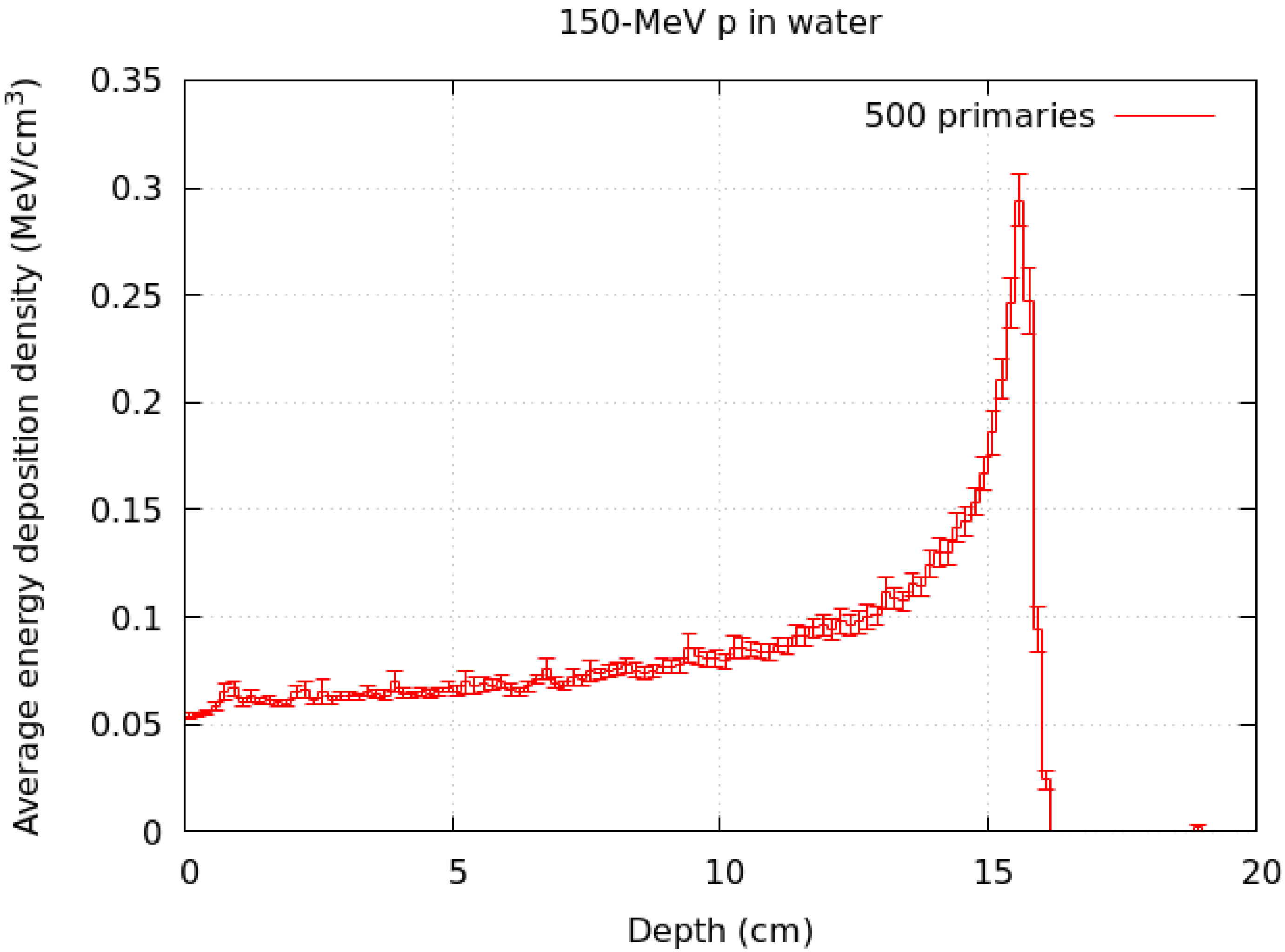
- Efficiency enhancement:
  - Software/algorithm side: **variance reduction/biasing** techniques
  - Hardware side: **distributed/parallel** MC runs

- Exploratory outlook
  - Applications of **GPUs** in MC simulations of radiation transport
  - Machine learning applications

Convergence and efficiency of a Monte Carlo simulation

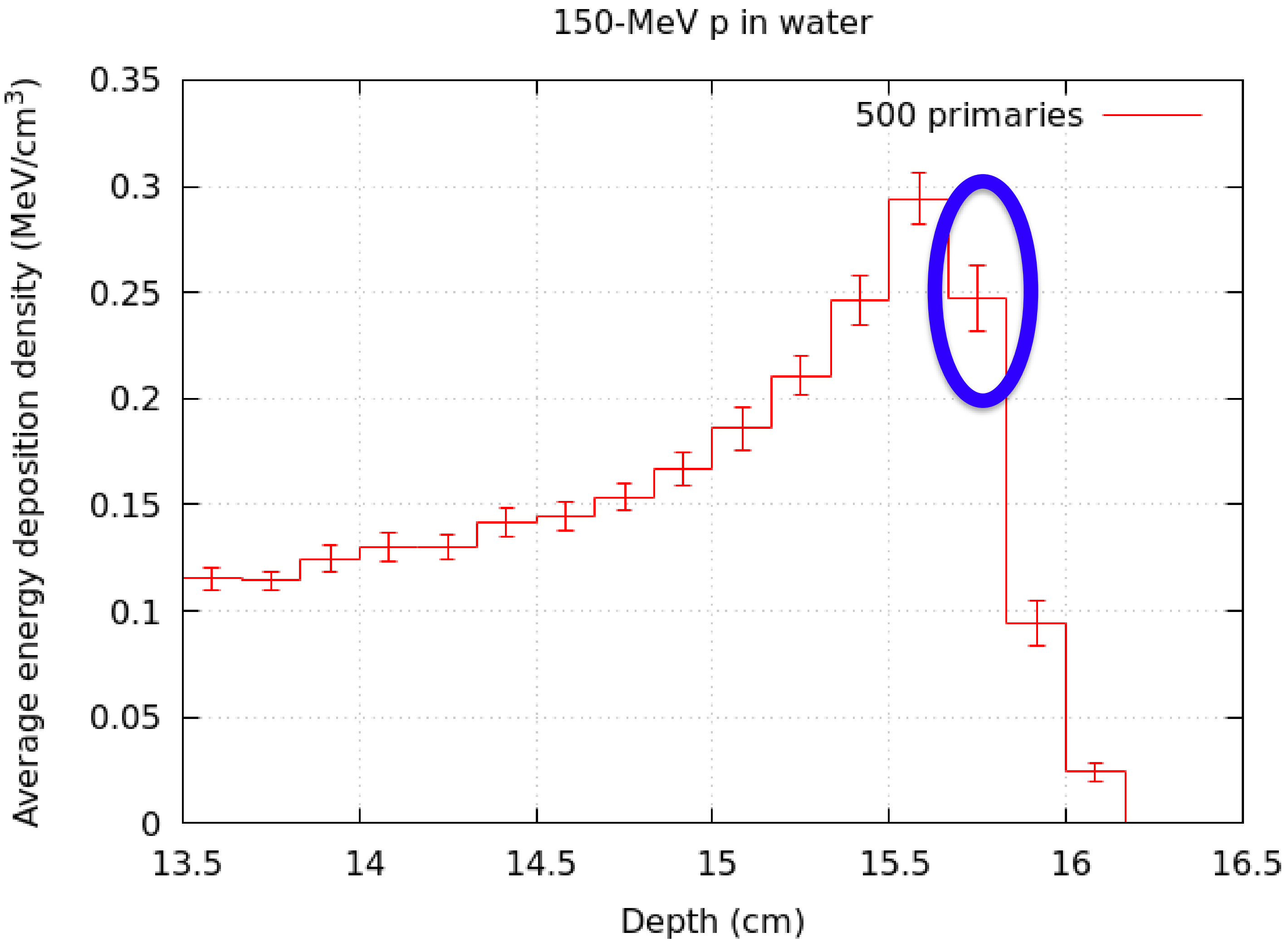
Statistical uncertainty in a MC simulation

- 150-MeV p beam impinging on water
- Scoring energy deposition density
- Averaged over transverse plane
- Displayed as a function of **depth**



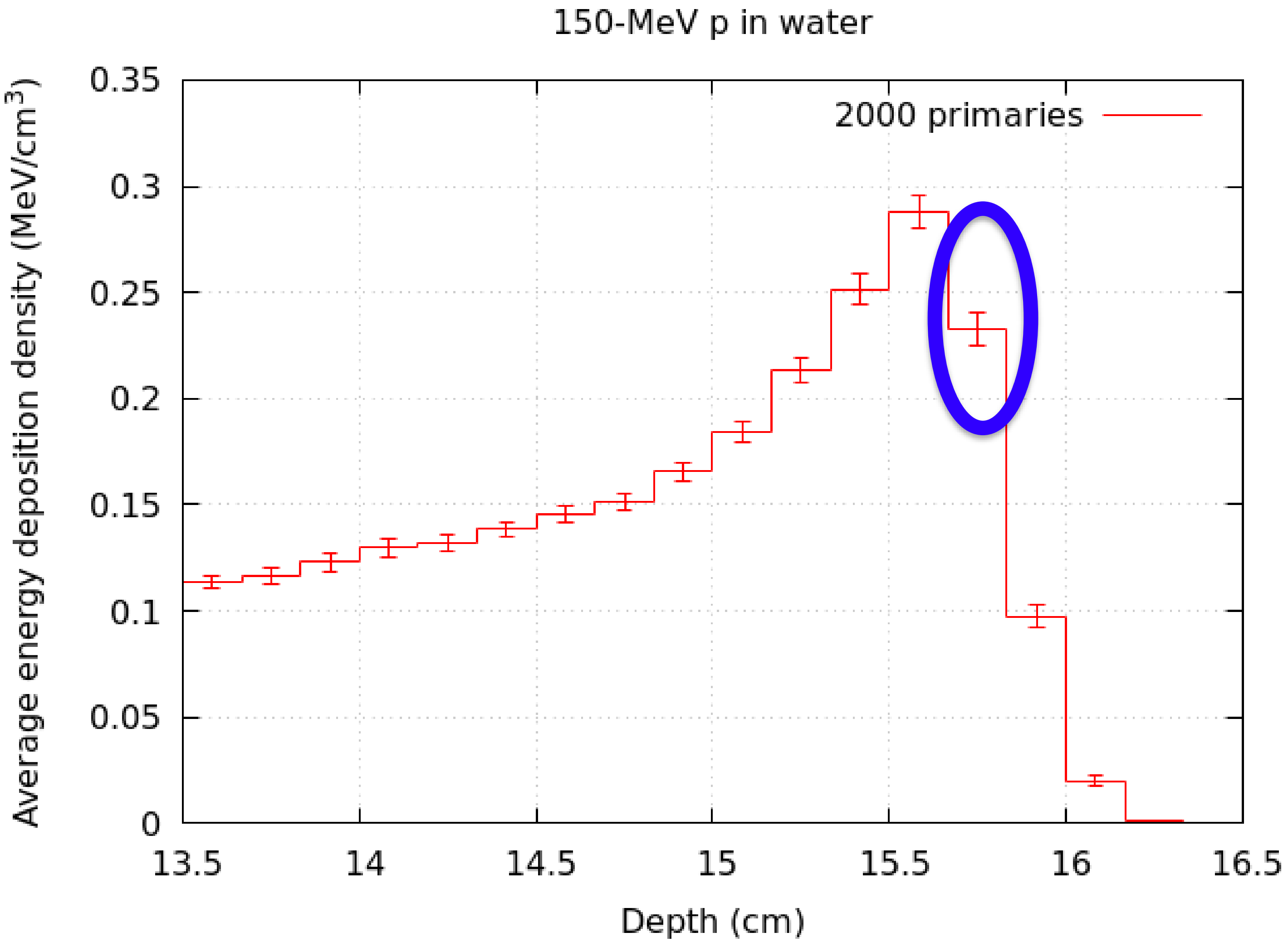
Statistical uncertainty in a MC simulation

- $N = N_0 = 500$ primaries
- CPU time: **$T_0 \sim 1$ s**
- **We focus on the indicated error bar**



Statistical uncertainty in a MC simulation

- $N=4N_0=2000$ primaries
- **$T \sim 4$ s $= 4T_0$**
- **Error bar has halved**



Statistical uncertainty in a MC simulation

- $N=16N_0 = 8000$ primaries
- **$T \sim 16$ s $= 16T_0$**
- **Error bar has halved again**

- The relative uncertainty of a MC estimator σ_f/f scales like

$$\sigma_f/f \sim 1/\mathrm{sqrt}(N)$$

- The CPU time scales like

$$T \sim N$$

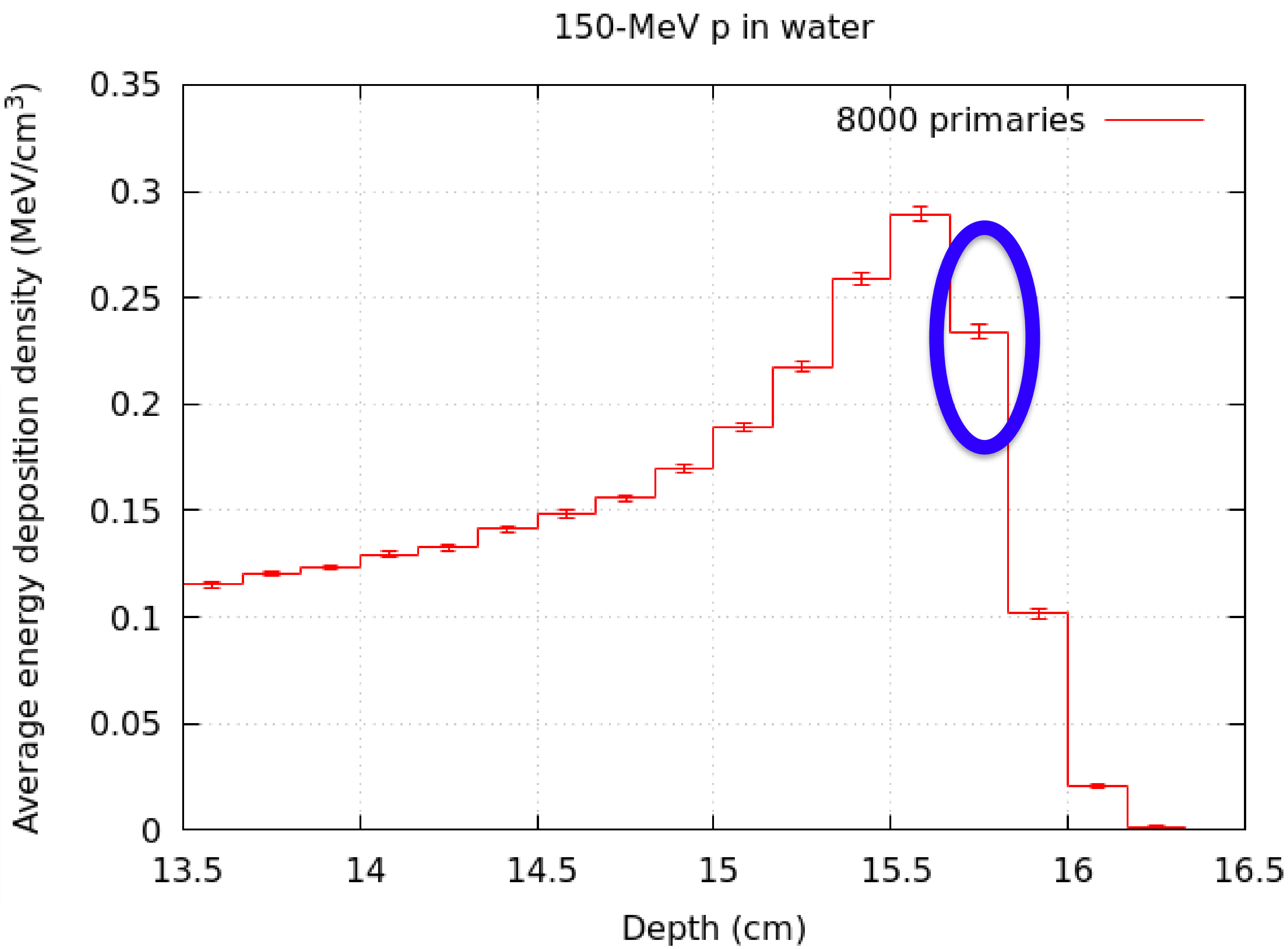


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Figure of merit of a MC simulation algorithm

- Figure of merit (efficiency)

$$\epsilon = \left(\frac{\overline{f}}{\sigma_f}\right)^2 \frac{1}{T}$$

CPU time

Relative statistical uncertainty (squared)

- Scaling with N:
  - $\sigma_f/f \sim 1/\mathrm{sqrt}(N)$ and $T \sim N$
  - For a given MC simulation problem, ϵ is independent of N **(when ~converged!)**

- ϵ is a relative measure of how well computational time is spent towards convergence

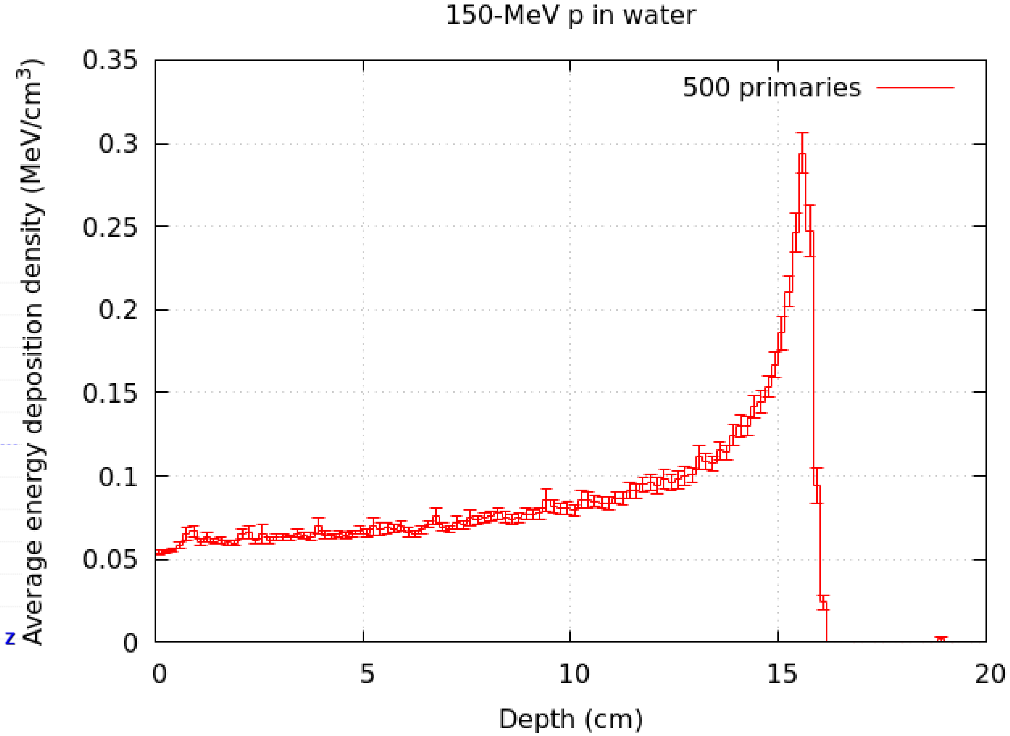
- For simulation problems with pathologically slow convergence / low efficiency, one wishes to have techniques to lower T and/or σ, overall **increasing ϵ**

Before “fancy/sophisticated” attempts to enhance the efficiency of MC simulations, one better have a reasonable grasp of

- Underlying physics
- Monte Carlo simulation parameters

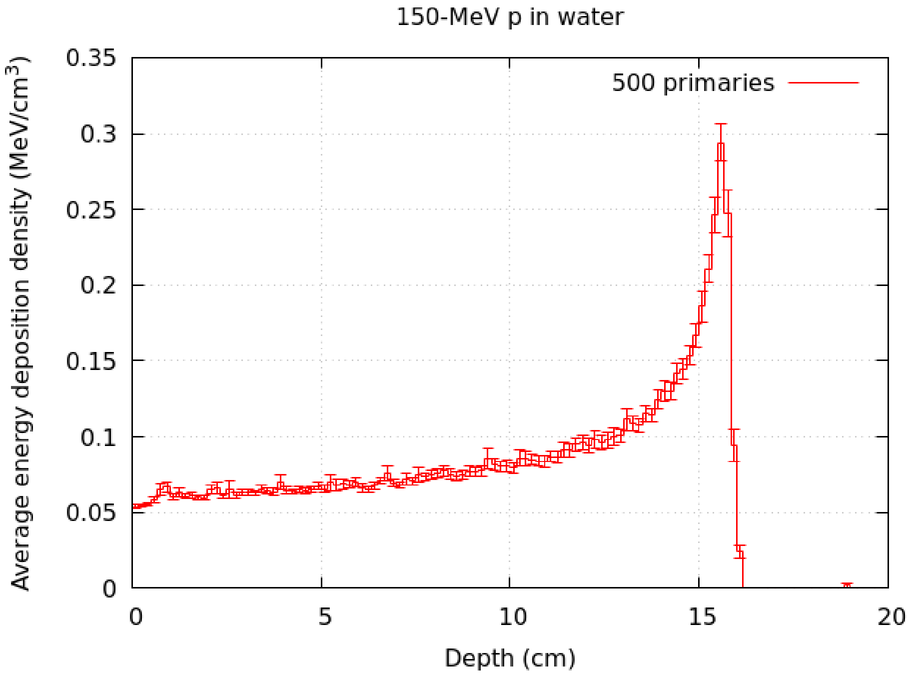
Example: Setting particle transport thresholds

- Energy deposition by 150-MeV protons in water
  - Dominated by **proton ionization losses** (collisions with target e-)
  - Mean free path for nuclear inelastic scattering of 150-MeV p in water: **106.8 cm**
    (a few protons undergo a nuclear reaction -> n production -> contribute mostly to tails of the distribution, modulate a bit the intensity of the Bragg peak)
  - Simulation bottleneck**: e- production/transport threshold**
    i.e. **condensed (dE/dx)** vs **detailed delta-ray simulation**



Threshold settings

e- transport threshold (keV)	CPU time (s)
100	3
50	8
10	72
5	176
1	3000



- **Exponential increase** of CPU time as one lowers e- thresholds
- An e- threshold of 100 keV is OK if one cares just about a coarse depth-dose curve:
  - CSDA range of 100 keV e- in water: ~**0.014 cm**
  - Histogram spatial resolution: ~**0.16 cm -> we could have used even higher e- thresholds!**
- **Factor 1000 speed-up** just for being minimally aware of what governs the problem

Particle transport/production thresholds

- MC codes typically provide **default threshold values**, but they are **not guaranteed to be meaningful for your problem**

- Following e-/e+ to energies lower than one really needs is a ruthless time-intensive **CPU eater**

- **It pays off to set transport threshold such that residual range is small compared to geometry / scoring mesh dimensions (and such that you don't cut out any relevant physics process…)**

Enhancing the MC simulation efficiency in problems with strong attenuation

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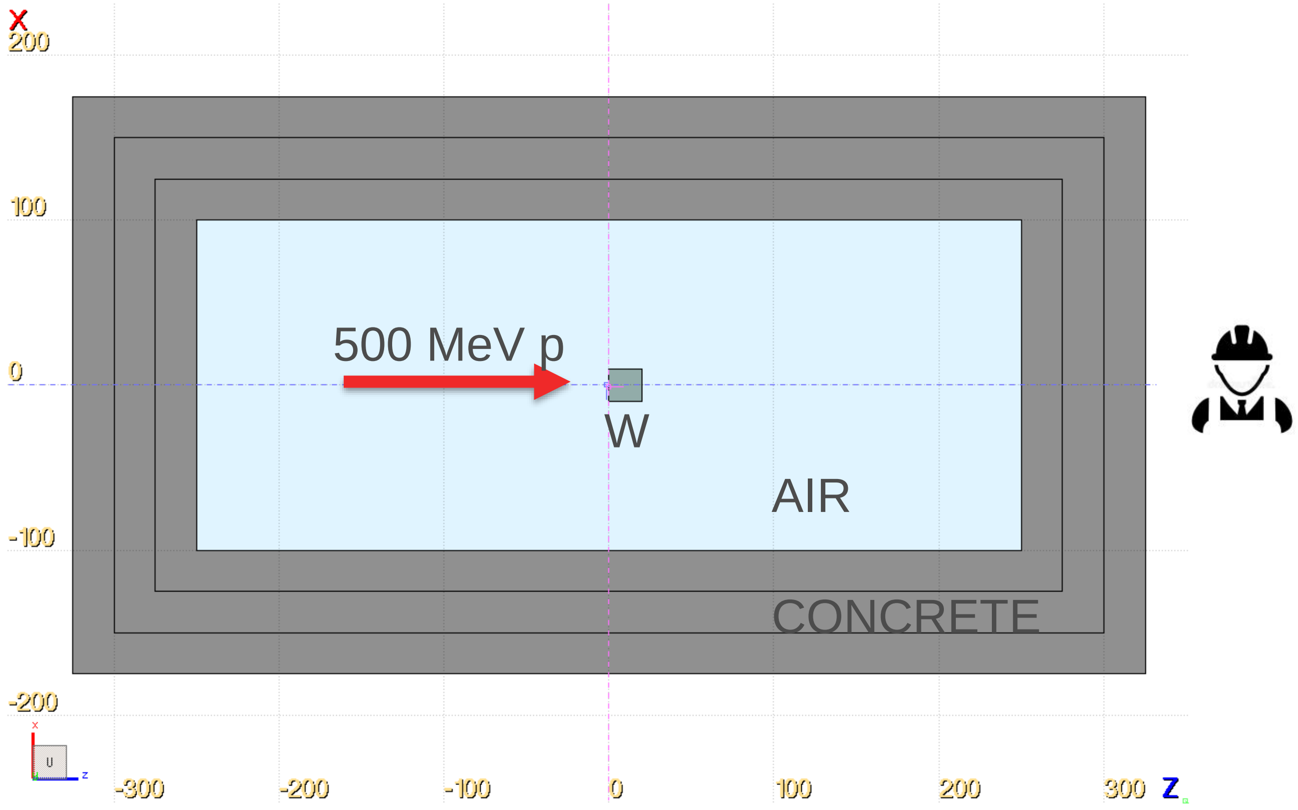
Region importance biasing

Shielding example

- 500-MeV p beam
- 20 cm W target in air
- Concrete shielding, 3 layers of 25 cm width
- Estimate H*(10) ambient dose equivalent outside shielding



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The basic physics

- Proton undergoing nuclear inelastic interactions, mostly in W

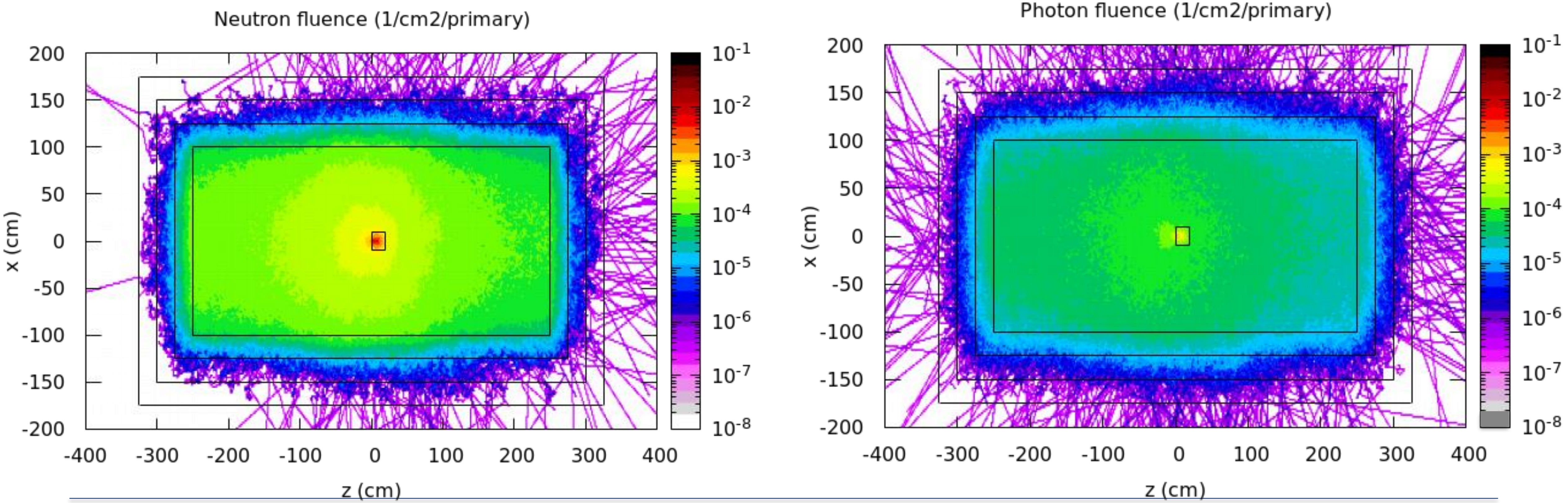
- Secondaries produced per incident proton (tallied with FLUKA):
  - **10.8 n** -> undergo inelastic interactions mostly in target and concrete
  - **7.4 photons**
  - **1.6 p**
  - **<0.5: d, t, 3He, 4He**

  By and large stopped in concrete

- n and photons might manage to make it through the shielding and contribute to the H*(10) ambient dose outside

Neutron and gamma fluence

- Particle fluence past shielding is **dominated by neutrons and photons**
- Neutron and photon fluence is gradually **attenuated** by the shielding
- But we still want a statistically significant estimate of the dose outside of the shielding

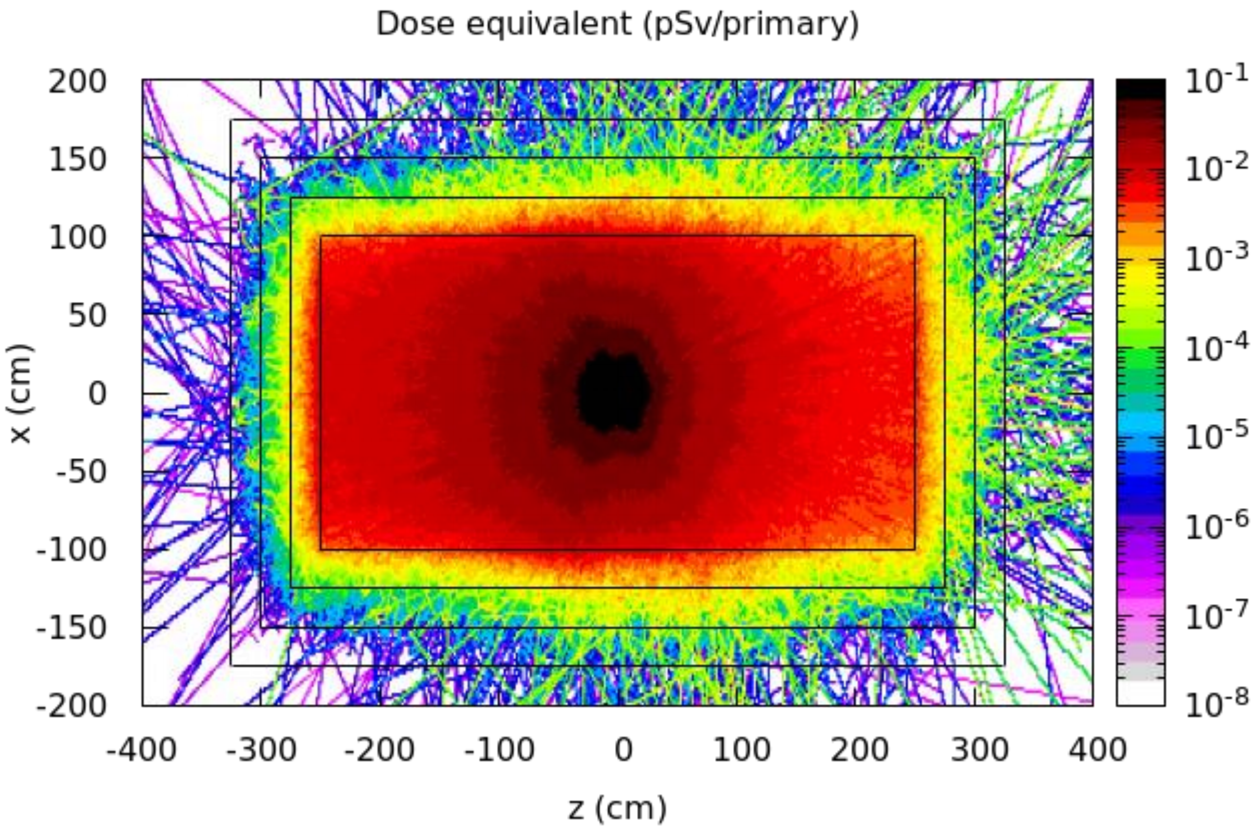


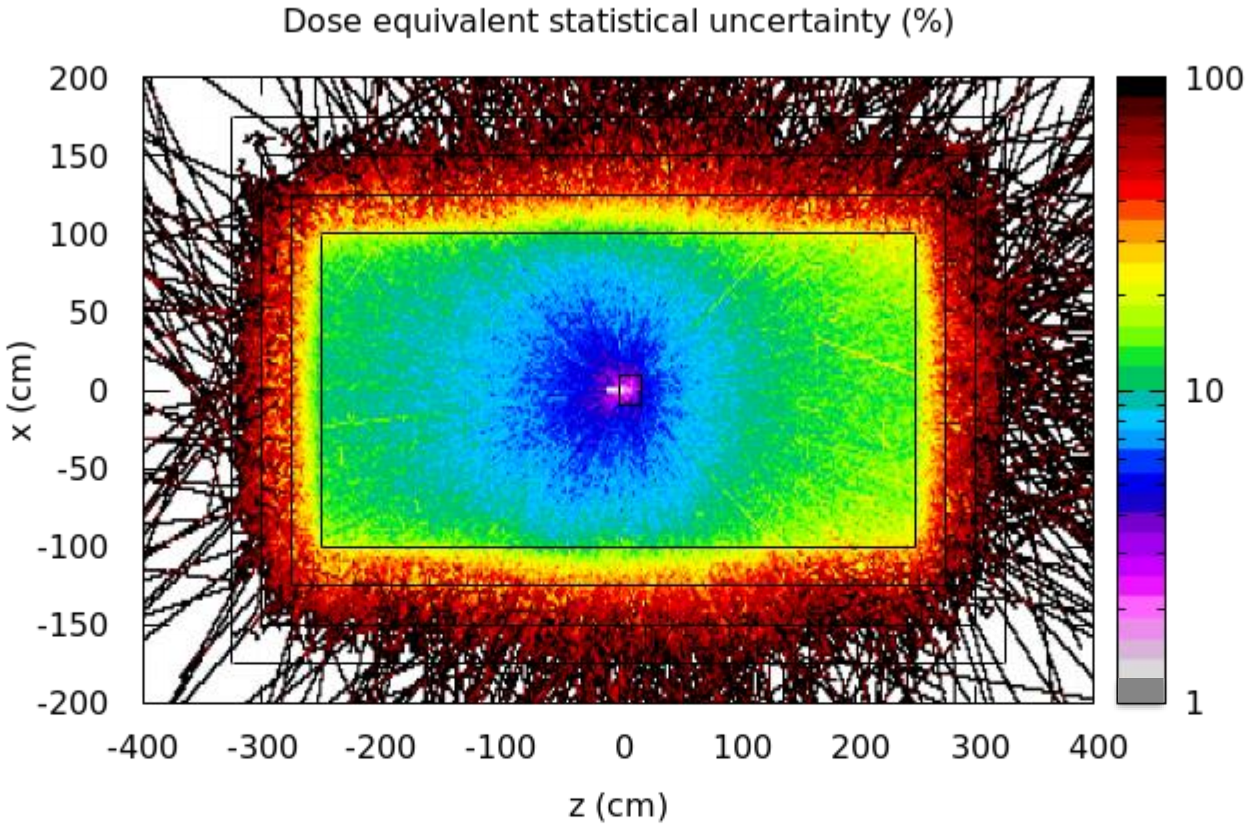
H*(10) ambient dose equivalent

NOTE: only meaningful in air/outside shielding…

- **N_{prim}= 4000**
- **T_{CPU}= 43 seconds**

$\epsilon \sim (0.8^2 \times 43)^{-1} \sim 0.03\ s^{-1}$

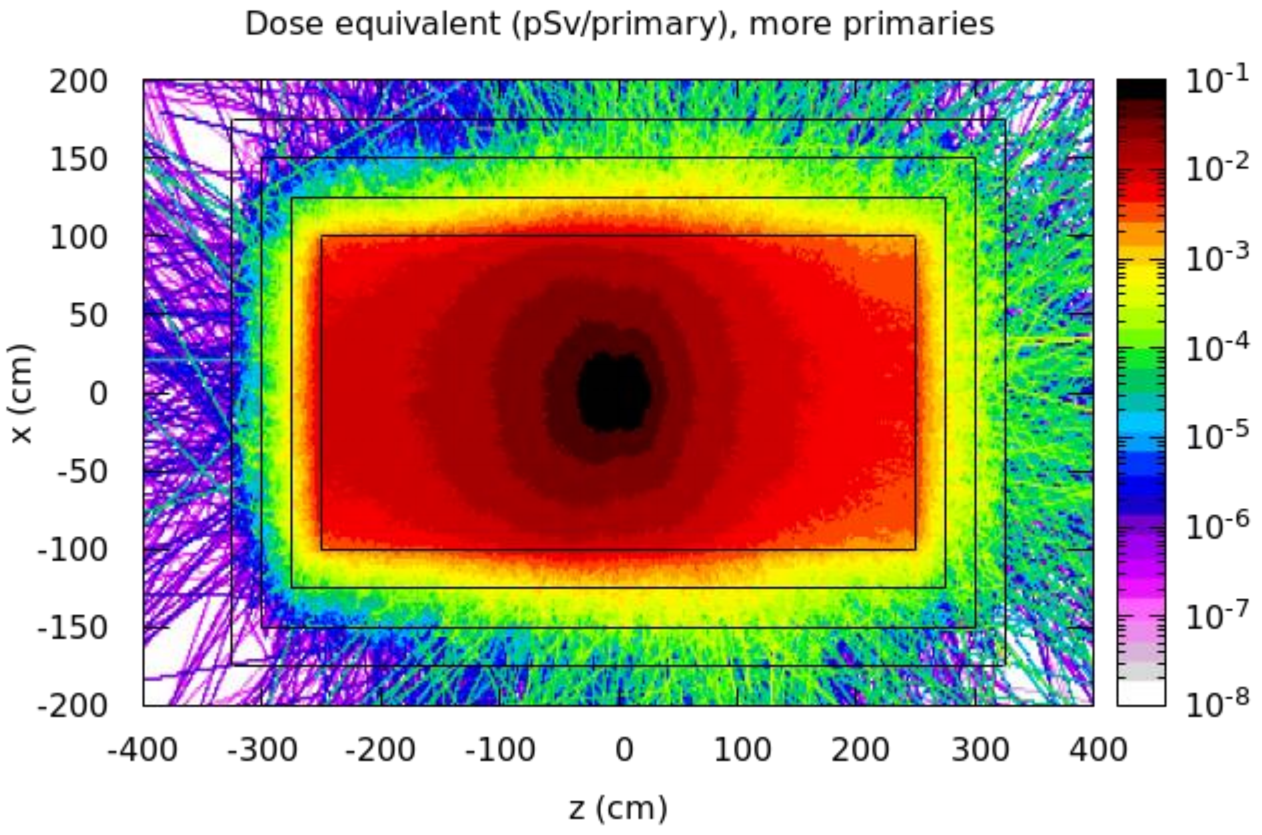


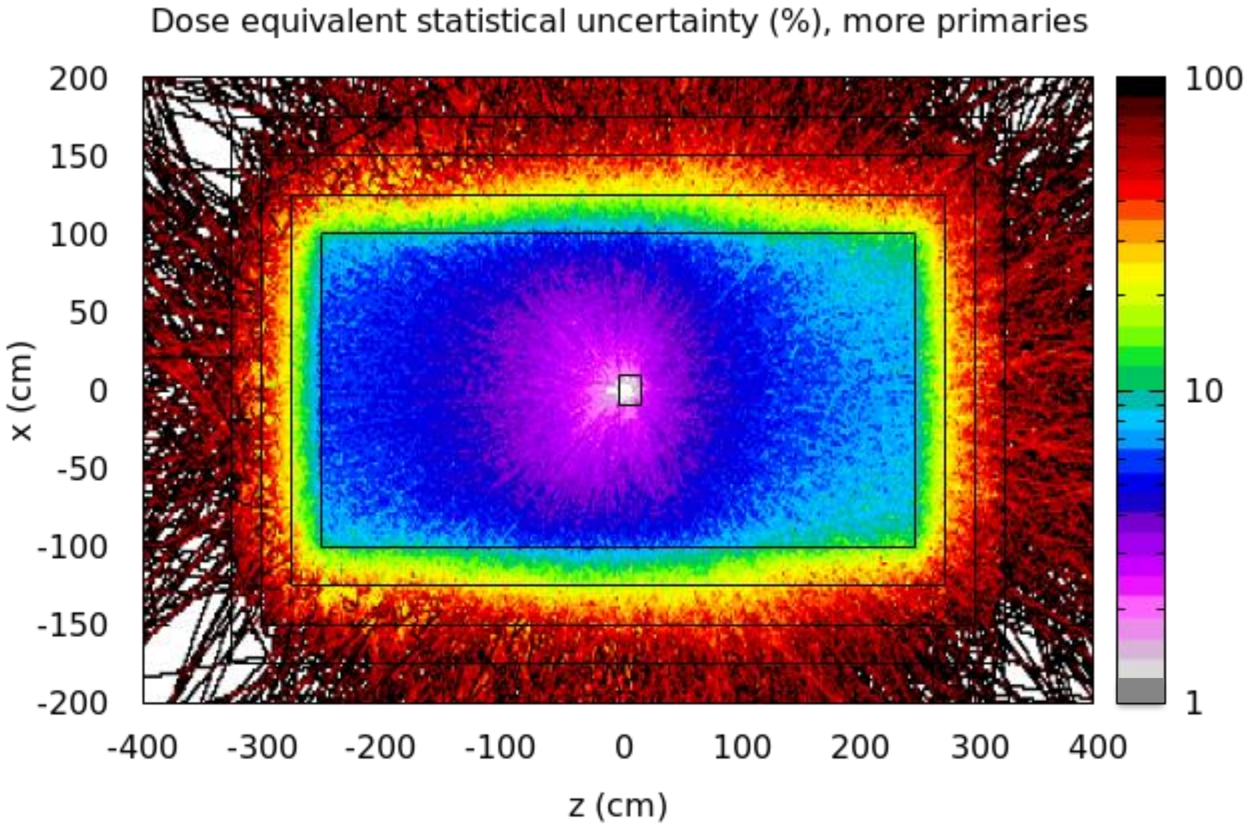


H*(10) ambient dose equivalent, 4x more primaries

- N_{prim}= 16000
- T_{CPU}= 171 seconds

$\epsilon \sim (0.4^2 \times 171)^{-1} \sim 0.03\ s^{-1}$





Biasing

- Figure of merit of a Monte Carlo simulation:

$$\epsilon = \left(\frac{\overline{f}}{\sigma_f}\right)^2 \frac{1}{T}$$

Simulation time

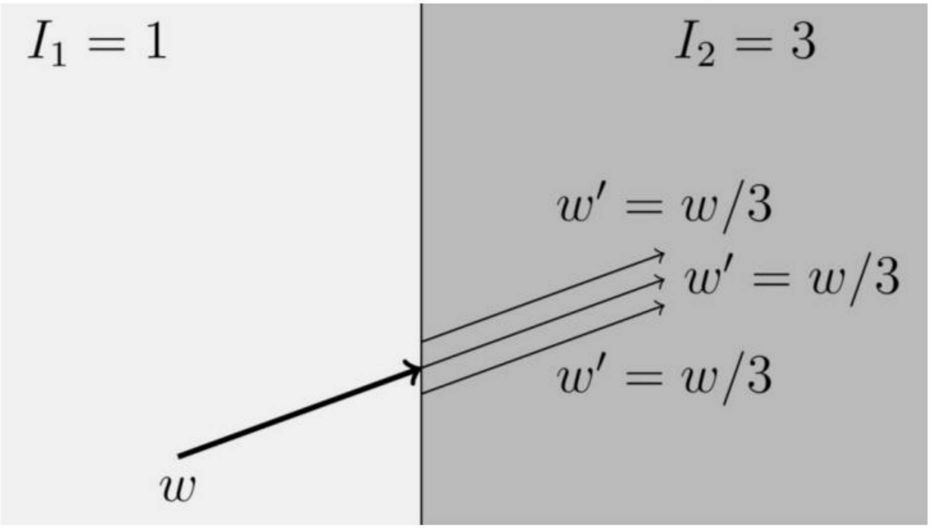
Relative statistical uncertainty (squared)

- **Convergence** of desired physical observable might be **slow**, e.g.:
  - Problems with strong **attenuation** of relevant particle fluence
  - Processes with **low cross section** (e.g. photonuclear interactions)
- Biasing techniques aim at **enhancing the simulation efficiency**:
  - Reduce the variance and/or CPU time
  - Leading to an overall larger ϵ

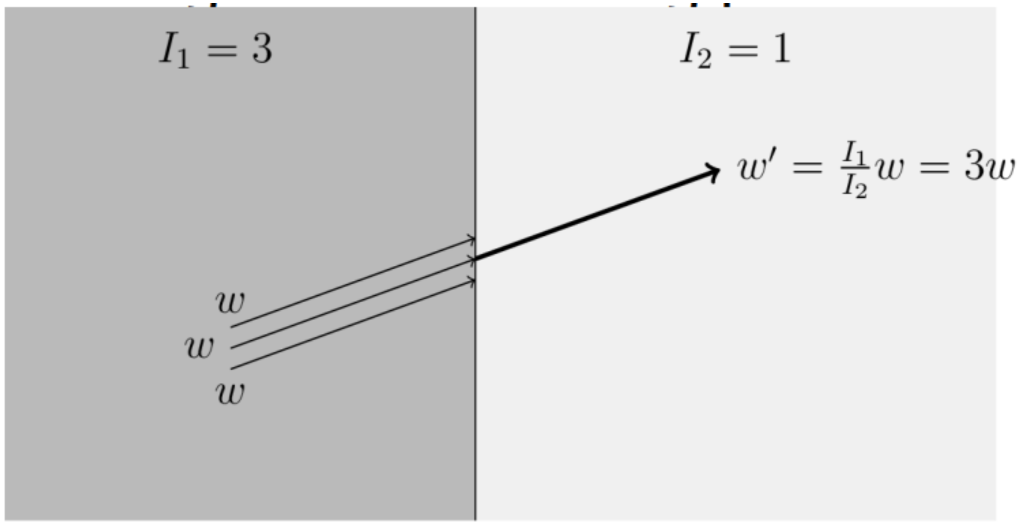
Region importance biasing

- Assign numerical **importance** to regions in your geometry

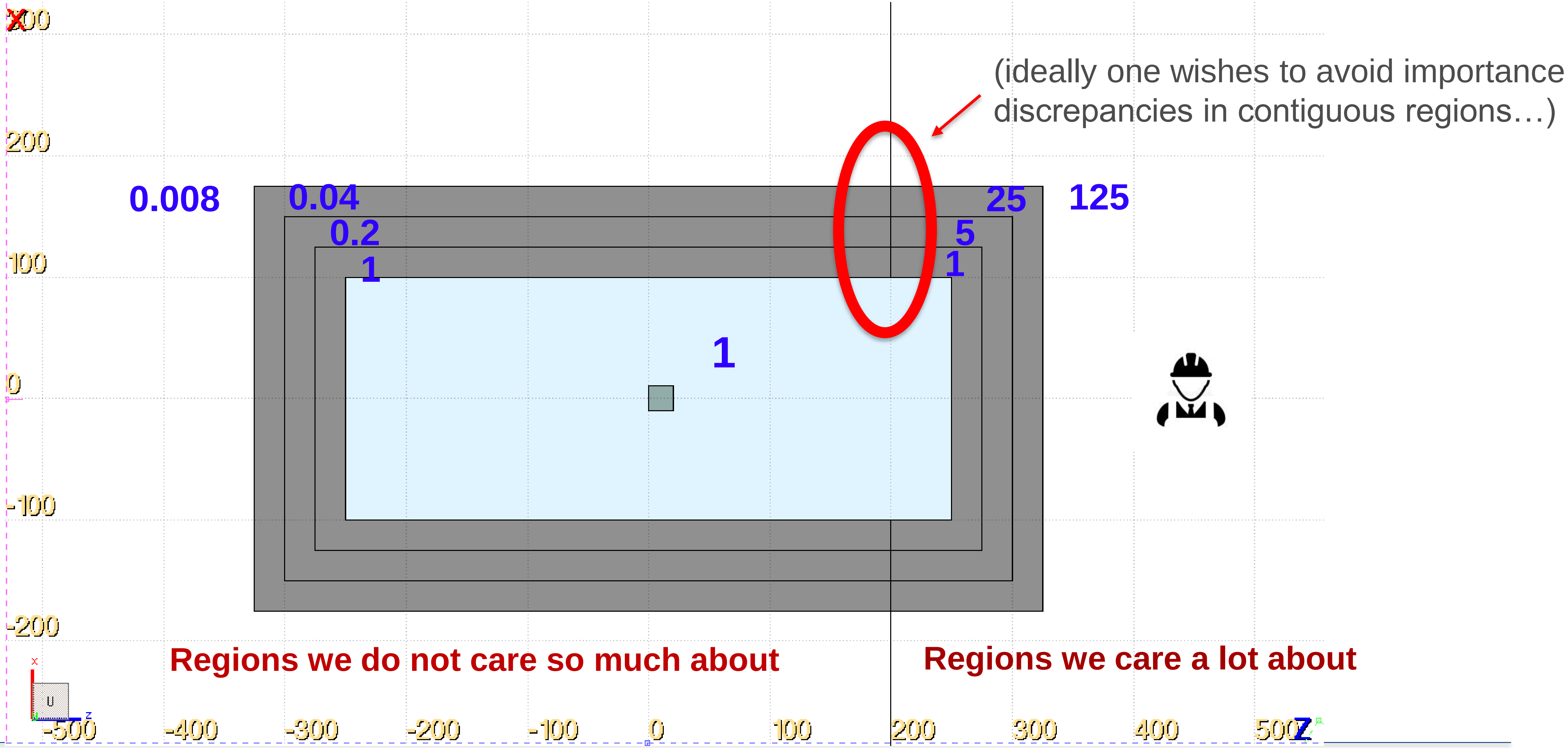
- **Splitting**
  - Crossing into region with **larger** importance
  - Particle split into I_2/I_1 particles
  - Reduced statistical weight



- **Russian roulette**
  - Crossing into region with **lower** importance
  - Particle reduced to I_2/I_1 particles
  - Enhanced statistical weight



Region **importance** biasing for our shielding problem

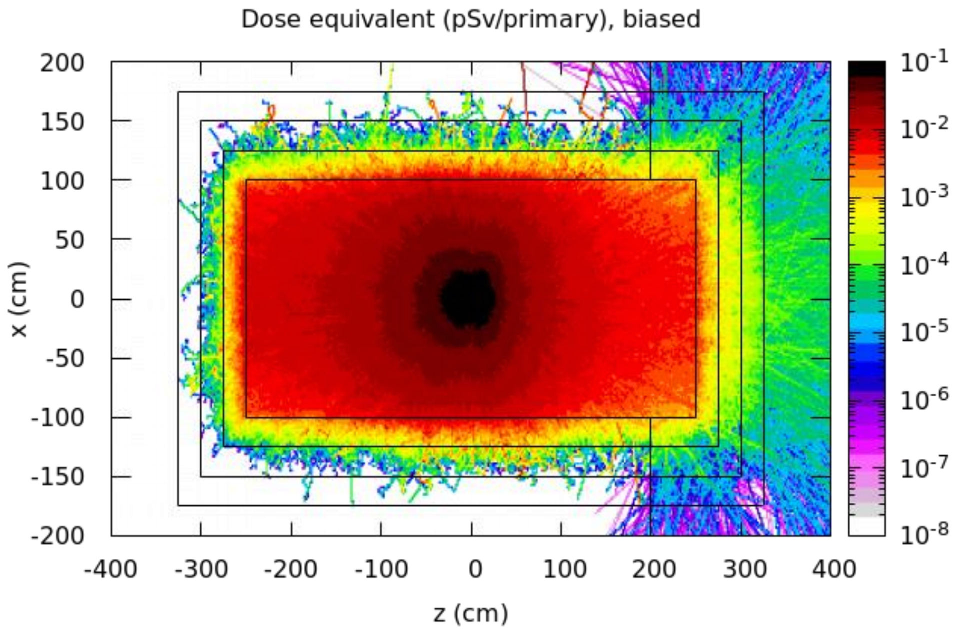


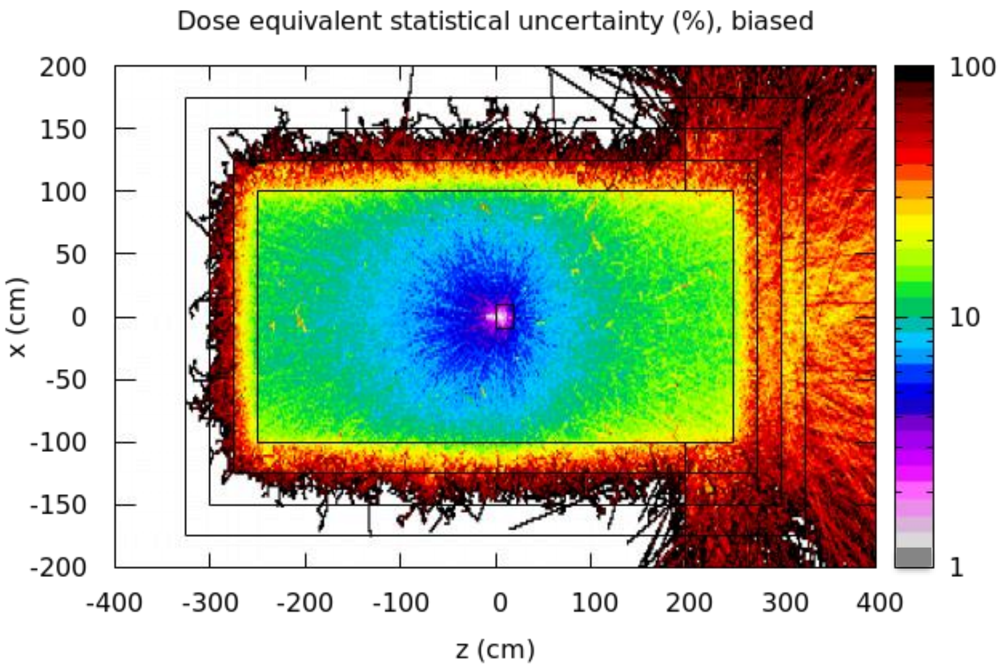
H*(10) ambient dose equivalent, original N_{prim}, biased

- N_{prim} = 4000
- T_{CPU} = 42 seconds

$\epsilon \sim (0.2^2 \times 42)^{-1} \sim 0.6\ s^{-1}$

(efficiency increased by a factor ~20!)





- Particle population is maintained (suppressed) in regions of high (low) importance
- Efficiency **enhancement in the right-hand regions** comes at the **detriment of left-hand regions**
- 20% uncertainty is still a bit far from convergence -> from now on it's a matter of running for more primaries

A word of caution

- Biasing techniques effectively concentrate simulation effort in desired regions of the geometry / phase space
- **It's the user's responsibility to ensure no contributions from relevant regions are left out by a too careless biasing scheme**
- Particle shower correlations are lost*: no event-by-event analyses

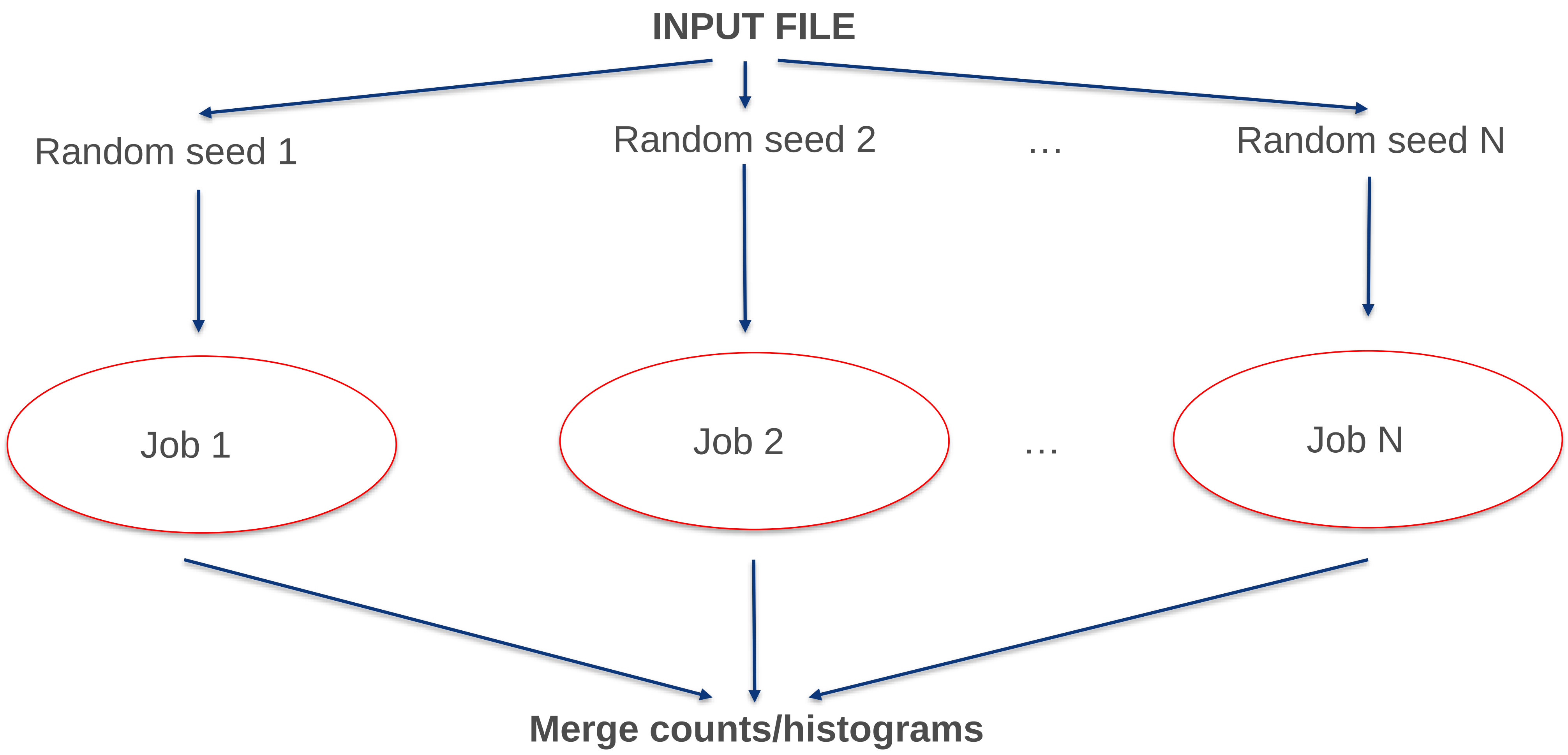
Standard biasing techniques

- **Region importance biasing**
- Mean free path biasing
- Weight windows
- Ant colony algorithm
- …

- Ref: S. Garcia-Pareja et al., *Front. Phys.* **9** 718873 https://doi.org/10.3389/fphy.2021.718873

Hardware acceleration

MC as a naturally distributed calculation



Efficiency enhancement from distributed runs

- MC simulation efficiency:

$$\epsilon = \left(\frac{\overline{f}}{\sigma_f}\right)^2 \frac{1}{T}$$

Simulation time

Relative statistical uncertainty (squared)

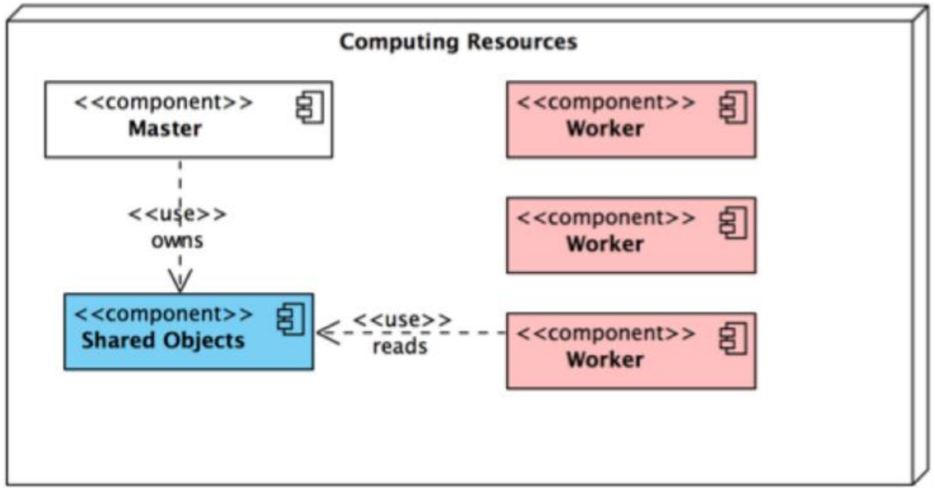
- For a fixed number of primaries N distributed in n jobs running at the same time, the cumulative CPU time T is the same, but if one takes T as a **walltime**, the simulation **efficiency is enhanced by a factor of nearly* n**

- Negligible coding overhead, no synchronization issues

[Possible bottleneck for large memory requirements]

- n distributed runs → n x memory

- **Each instance replicates its own memory** for geometry, cross section, scoring, etc.
- Extreme limit (complicated geometry + e.g. plenty of low-energy neutron cross sections to load + very dense scoring meshes), insufficient memory e.g. if running 16 threads on one CPU
- Codes like e.g. Geant4 allow for **shared memory** (cross sections and geometry) among threads
- A bit of coding overhead / thread synchronization



- Ref: https://indico.cern.ch/event/776050/contributions/3240673/attachments/1788898/2913542/Multithreading1.pdf

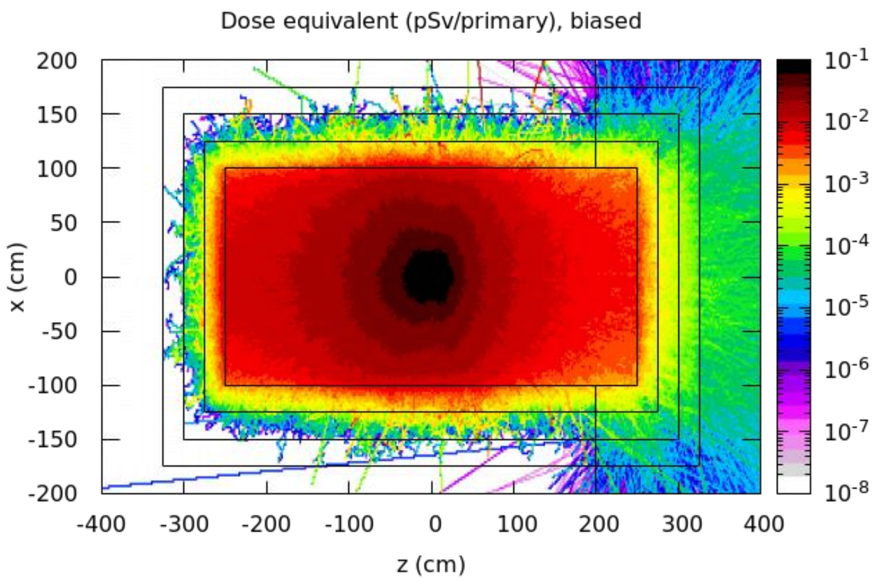
Best of both worlds: **exploit both** biasing and distributed/parallel runs!

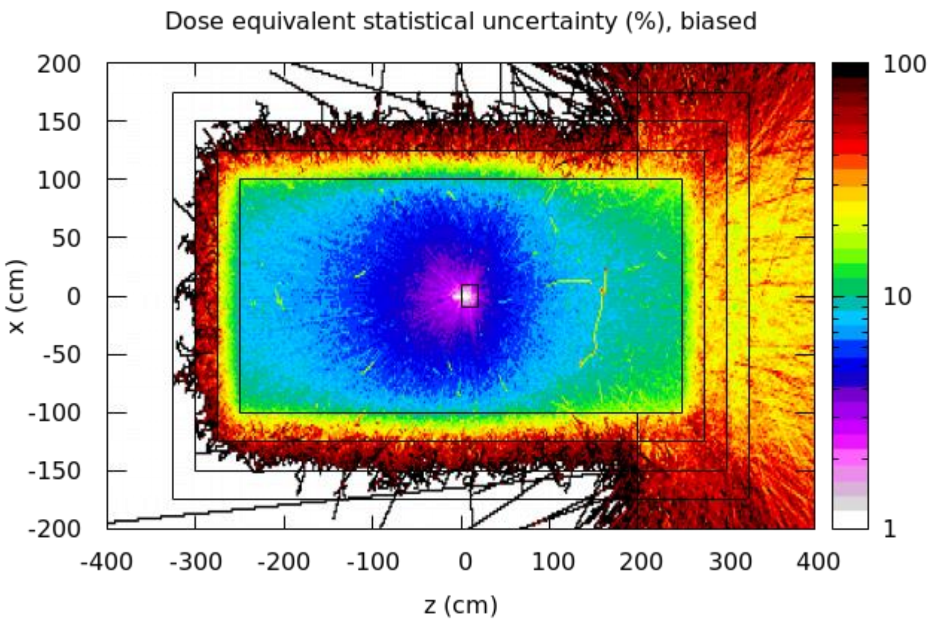
Twice as many jobs now, leading to:

- **N_{prim}= 8000**
- **T_{wall}= 42 seconds**

$\epsilon \sim (0.14^2 \times 42)^{-1} \sim 1.2\ s^{-1}$

(efficiency increased by a factor ~40 wrt to the initial efficiency)





- **For a vast majority of practical situations, a combination of biasing + distributed runs suffices**

Exploratory outlook (hardware): GPUs

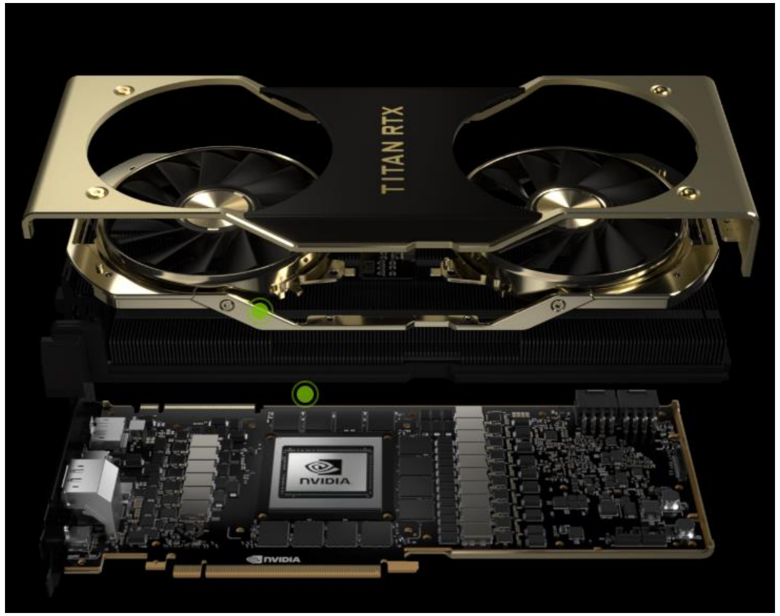
GPUs

- **GPU: graphics processing unit**
  - Parallel processing of thousands of computational threads

- **Naturally advantageous scenarios:**
  - Tasks requiring millions of ***identical*** operations (problem reducing to linear algebra)
  - ***Direct, uniform, contiguous memory access***

- **Challenging scenarios:**
  - Tasks with ***thread divergence*** and ***random memory access***
    (…as in a MC simulation of radiation transport!)

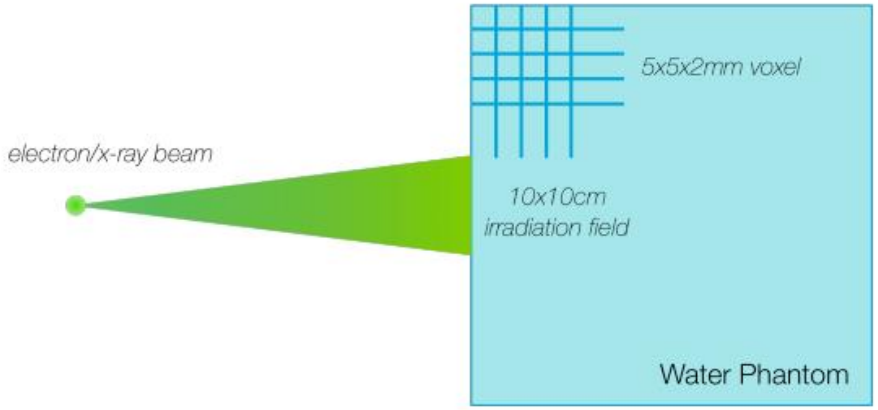
- **Requires heavy recoding of MC simulation (CUDA programming model)**



nVidia Titan RTX GPU

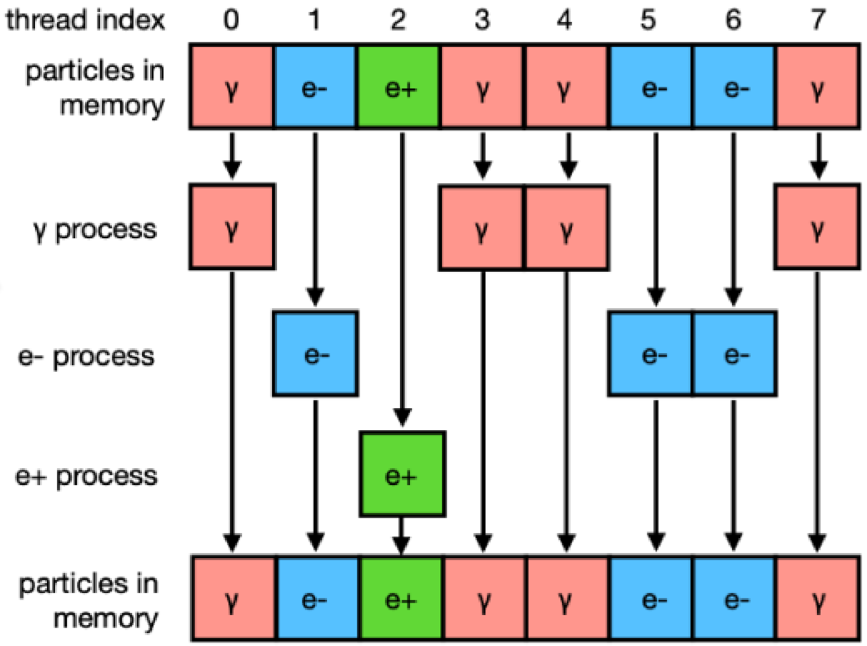
MPEXS

- KEK-based tool for radiotherapy:
  - Limited set of physics: e-,e+,gamma
  - Simple geometry (infinite medium)
  - Water-equivalent material



- Process thousands of independent particle histories in parallel

- Thread divergence: **~50% (!!)**
- Nevertheless, speed-up factor of ~400 attainable against single-core CPU.



- Ref: https://indico.cern.ch/event/921244/contributions/3870624/attachments/2045775/3427426/HSF-200527-MPEXS.pdf

High-energy-physics community

- Electromagnetic interactions + geometry are among the most CPU time consuming aspects for HEP detector simulations
- Ongoing R&D attempting to cast HEP particle transport problem to benefit from massive parallelization on GPU architectures
- **AdePT**:
  - Workload balancing, reduce impact of shower tails, maximize number of tracks in flight, etc
  - Speed-up observed in simple geometries, pending real geometry (ATLAS/CMS calorimeters)
- **Celeritas:**
  - Targetting EM+hadronic pysics, re-implementation of subset of G4 physics for GPU, focusing on EM showers

- **Refs (talks and git repos):**
  https://indico.cern.ch/event/1156147/contributions/4854699/attachments/2444243/4188160/HSFGPU_report.pdf
  https://github.com/apt-sim/AdePT
  https://github.com/celeritas-project/celeritas

Exploratory outlook (algorithms): Machine learning attempts

Material kindly provided by Florian Mentzel

Do not miss Habib Zaidi’s interesting talk at 16h!

MC+ML attempts for medical physics applications

- Main ongoing lines of applications of ML to MC simulations:
  - Convolutional neural networks for dose estimation in radiotherapy and imaging
  - Dose denoising from low statistics Monte Carlo simulations,
  - Detector modelling
  - Event selection
  - Replacing particle sources / phase space modelling with generative models

Application	Input type	Refs (among others)	Main ML types
Dose computation	image	[49, 63, 79, 85, 90, 104, 116, 117, 147]	CNN, U-net
Dose denoising	image	[43, 59, 71, 101, 103, 111, 131, 153][1]	CNN, U-net
SPECT scan-time reduction	image	[82, 119, 121]	CNN, U-net
CBCT scatter modelling	image	[27, 58, 60, 75, 79, 84, 87, 88, 140, 145, 152, 155]	CNN, U-net
PET attenuation/scatter correction	image	[6, 97]	CNN, U-net
Detector response modelling	particles	[126, 144]	GAN, MLP
Source + phase space modelling	particles	[108, 125, 127]	GAN
Event selection	particles	[8, 12, 40, 46, 93, 98, 100, 102, 107, 157][2]	MLP, CNN
Interaction position in scintillators	various	[23, 33, 37, 99, 109, 110, 122, 150, 154]	MLP, CNN

[1] *http://hdl.handle.net/11603/19255*
[2] *http://hdl.handle.net/2078.1/thesis:14550*

https://www.frontiersin.org/articles/10.3389/fphy.2021.738112/full

Overview of ML applications in MC simulations (~medical)

- Dose estimation with neural networks:
  - Mentzel et al., **Fast and accurate** dose predictions for novel radiotherapy treatments in heterogeneous phantoms using conditional 3D-UNet generative adversarial networks. *Medical Physics* 2022;1–16. **https://doi.org/10.1002/mp.15555**
  - Oscar Pastor-Serrano et al., **Millisecond speed** deep learning based proton dose calculation with Monte Carlo accuracy. *Physics in Medicine and Biology,* in press. https://doi.org/10.1088/1361-6560/ac692e
- Low-statistics Monte Carlo enhancement
  - X. Xudong et al., Cone Beam CT (CBCT) Based Synthetic CT Generation Using Deep Learning Methods for Dose Calculation of Nasopharyngeal Carcinoma Radiotherapy, *Technology in Cancer Research and Treatment* 2021; 20: 15330338211062415 https://doi.org/10.1177/15330338211062415
  - Z. Peng et al., MCDNet – A Denoising Convolutional Neural Network to Accelerate Monte Carlo Radiation Transport Simulations: A Proof of Principle With Patient Dose From X-Ray CT Imaging. *IEEE Access* (7) 76680 – 76689, 2019. https://doi.org/10.1109/ACCESS.2019.2921013
- Replacing particle sources with generative models
  - D. Sarrut et al., Generative adversarial networks (GAN) for compact beam source modelling in Monte Carlo simulations. *Physics in Medicine and Biology* 64 215004, 2019. https://doi.org/10.1088/1361-6560/ab3fc1
  - D. Sarrut et al., Modeling complex particles phase space with GAN for Monte Carlo SPECT simulations: a proof of concept. *Physics in Medicine and Biology* 66 055014, 2021. https://doi.org/ https://doi.org/10.1088/1361-6560/abde9a

A sobering comment

- D. Sarrut *et al*., *Front. Phys.* ***9*** *738112 (2021)*

  "For the moment, even if it is envisioned that deep learning can improve simulations, it does not seem certain that it can always replace Monte Carlo."

Summary

Summary

- Basic **understanding** of **underlying physics** and code **simulation parameters** can already lead to orders of magnitude enhancement of simulation efficiency wrt a careless run
- **Biasing techniques** as natural methods to enhance simulation efficiency e.g. in desired regions of interest in geometry:
  - Further orders-of-magnitude enhancement, but user responsible for not cutting out relevant corners of phase space
- MC **naturally distributed** computational problem
  - Truly parallel codes can reduce memory requirements
- Exploratory outlook onto applications of **GPUs and ML** to MC
- Even beyond: field programmable gate arrays (FPGAs), MC on a chip (MCoaC)
  - Speedups of factor ~90 for TOPAS https://doi.org/10.1016%2Fj.ejmp.2019.06.016
  - Less power (~30 W) than CPUs (~100 W) or GPUs (~300 W)
  - Promising applications and speed-ups for condensed matter spin system simulations (Ising model): https://arxiv.org/pdf/1602.03016.pdf
- MC code developers share the blame:
  - Efficiency of interaction/transport/sampling algorithms is on us! Physics performances 1st, optimization 2nd.

Thank you very much for your attention!

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