COMSOL Conference 2024 Florence

Monte-Carlo Model for Radiation Transport in Solid X-Ray Targets

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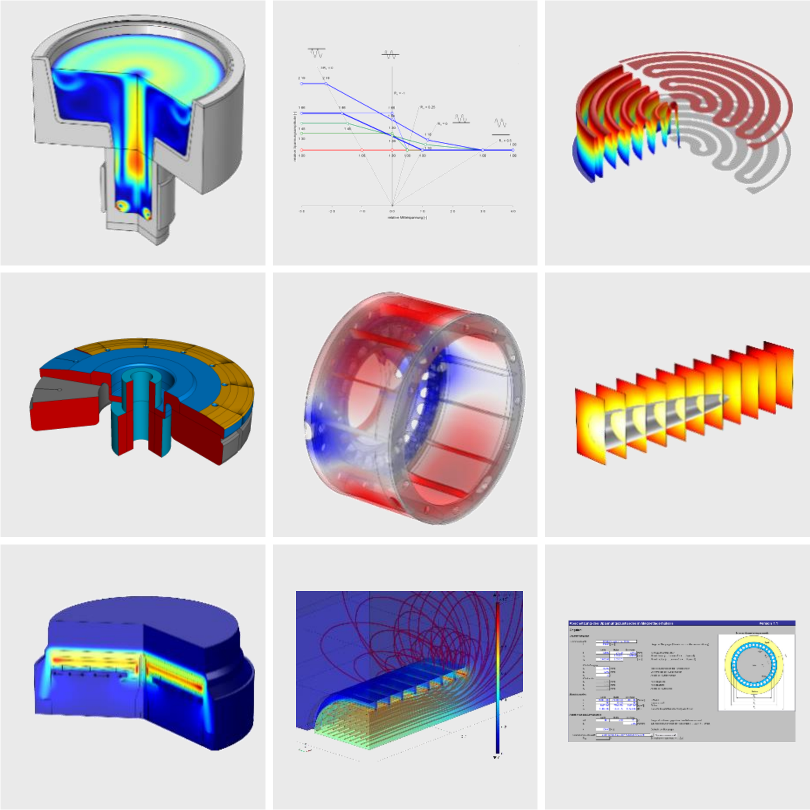
CENUMERICS

- engineering consultancy founded in 2005
- in Innsbruck, Austria
- mathematical modeling and numerical simulation
  - multiphysics modeling
  - component and process simulation
  - application and software development
    - COMSOL Application Builder
    - COMSOL Physics Builder
    - C/C++, Java



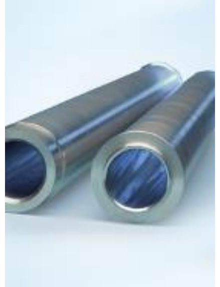
COMSOL Certified Consultant

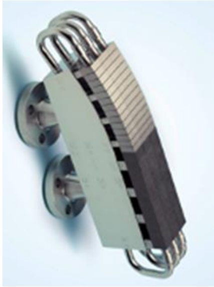
PLANSEE

- founded in 1921 for production of molybdenum (Mo) and tungsten (W) wires
- 1,000 MEUR turnover; 3,500+ employees worldwide (2023/24)
- world market leader in powder-metallurgical (P/M) production of refractory metals

- used in wide range of high-tech applications and industries





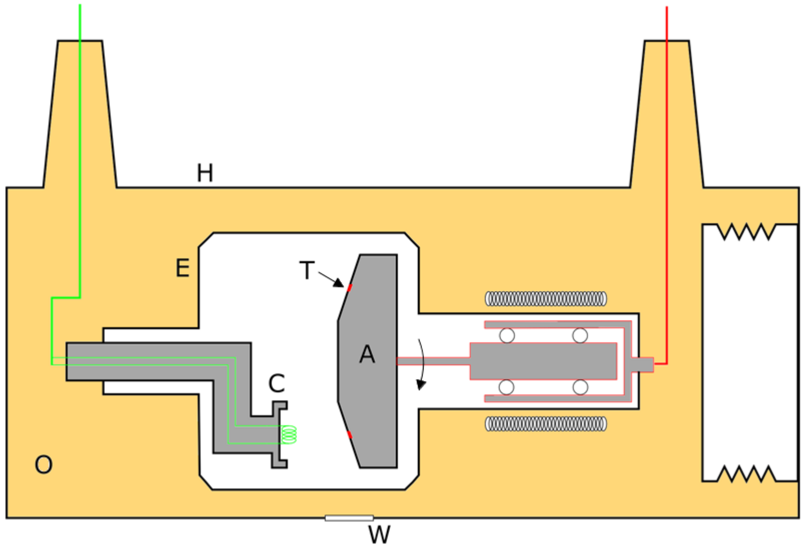

- unique combination of material properties
  - high melting point
  - excellent high temperature strength

High-energy electromagnetic radiation

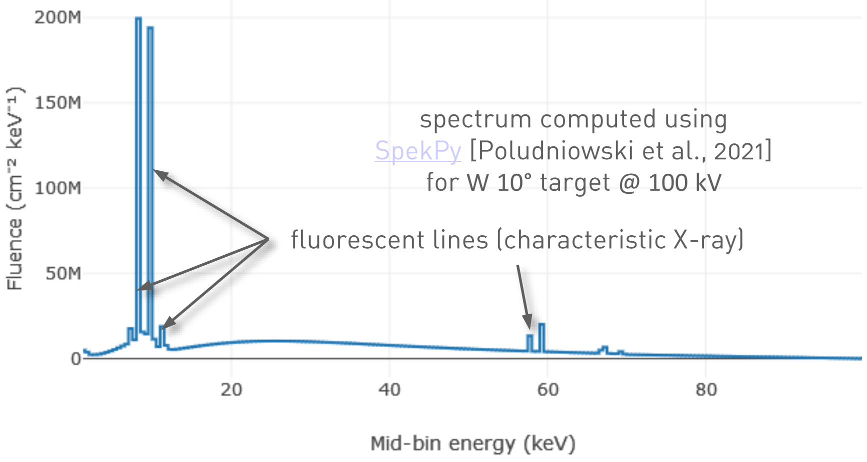
- discovered 1895 by CONRAD RÖNTGEN
- energy range above UV light
- good penetration of solid matter ($\rho \approx 0$)
- widely used in medical diagnostics and material testing

Production using high-vacuum X-ray tubes

- electrons e⁻ thermionically emitted from cathode (C)
- accelerated to anode (A), voltage $10^1 \ldots 10^2$ kV, formation of e-beam
- impact on target or focal track (T)
- cascade of atomic interactions within target material
- emission of X-ray photons γ as:
  (1) bremsstrahlung → continuous spectrum
  (2) characteristic X-rays → discrete spectrum
- escaping by tube window (W) → utilizable radiation



Ref: wikipedia:User:ChumpusRex, X ray tube in housing, Accessed: 2024-08-28



Low efficiency, high heat dissipation

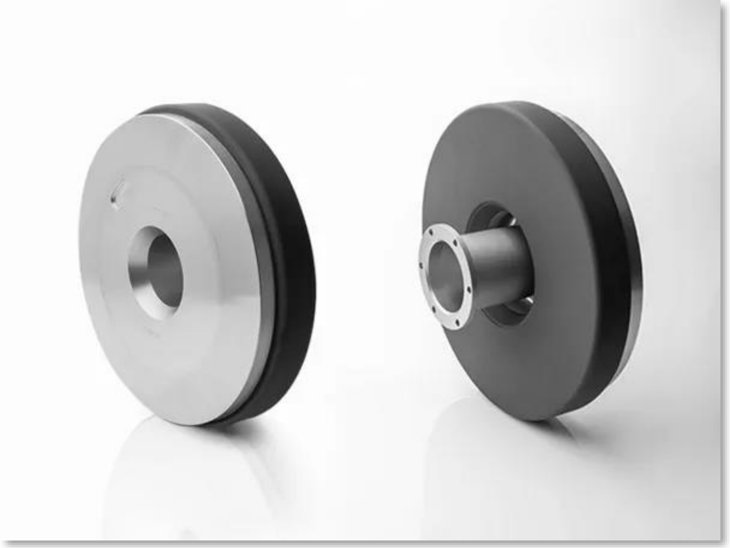
- only 0.1…1% as photon emission
- significant thermo-mechanical loads

Concepts for increased power

- active cooling of stationary anodes
- rotating anodes
- rotating envelope anode
- line-focus-principle (target inclination, stretched beam)

Motivation for study

- numerical model for radiation transport in X-ray target
- gain insight into performance of target, emitted spectrum, heat dissipation, influence of main design parameters



Ref (top, bottom): PLANSEE

Modeling of radiation transport

- transport of high-energy electrons and photons (particles) through matter (medium)
- interaction with atoms and molecules
- energy transfer and secondary particle emission (cascade, particle shower)
- energy deposition within medium

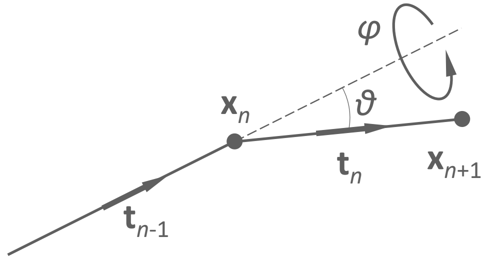
Monte Carlo method

- particle-based approach
- history of particles discretized as random sequence of

  (1) free „flights“ (sampled from mean free path length)

  (2) subsequent particle-interactions (sampled from relative interaction probability)
    - change of flight direction and energy
    - possible emission of secondary particles

  tracked until energy absorption



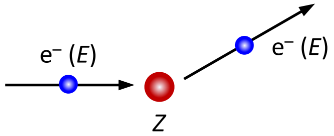
$$s(E) = -\lambda_{\mathrm{T}} \log \xi\,, \qquad \xi \in [0,1]$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + s\,\mathbf{t}_n\,; \qquad \mathbf{t}_n = \mathbf{T}(\theta,\varphi)\,\mathbf{t}_{n-1}\,; \qquad \theta = f(E,\ldots)\,, \quad \varphi = 2\pi\xi$$

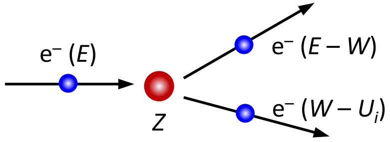
Relevant atomic interactions

- electrons

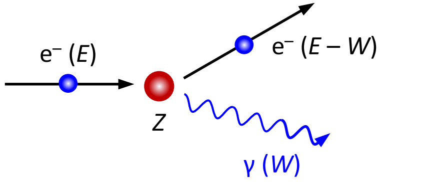
elastic scattering



inelastic scattering

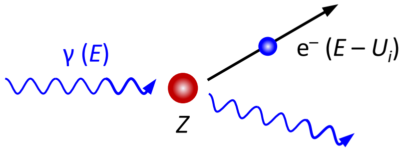


bremsstrahlung emission

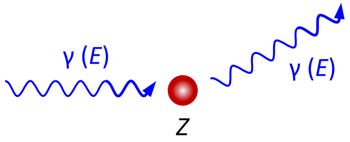


- photons

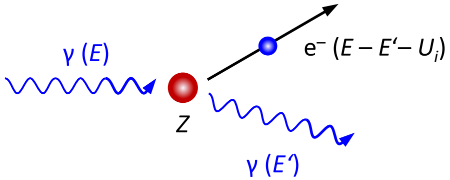
photoelectric absorption



coherent (Rayleigh) scattering



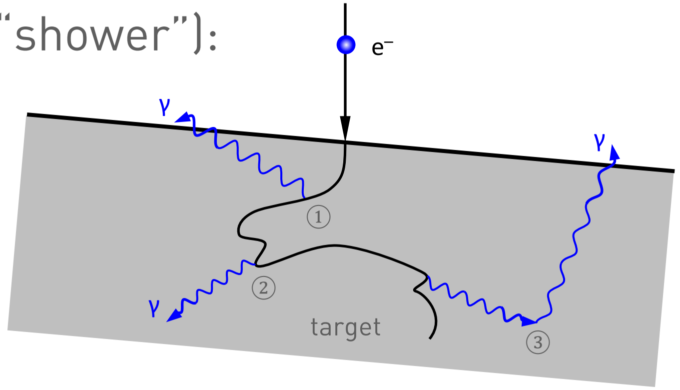
incoherent (Compton) scattering



- X-ray production from combined electron and photon interactions ("shower"):

① bremsstrahlung emission
② electron ionization
③ photon-atom interaction

② and ③ → characteristic X-ray emission through radiative transitions

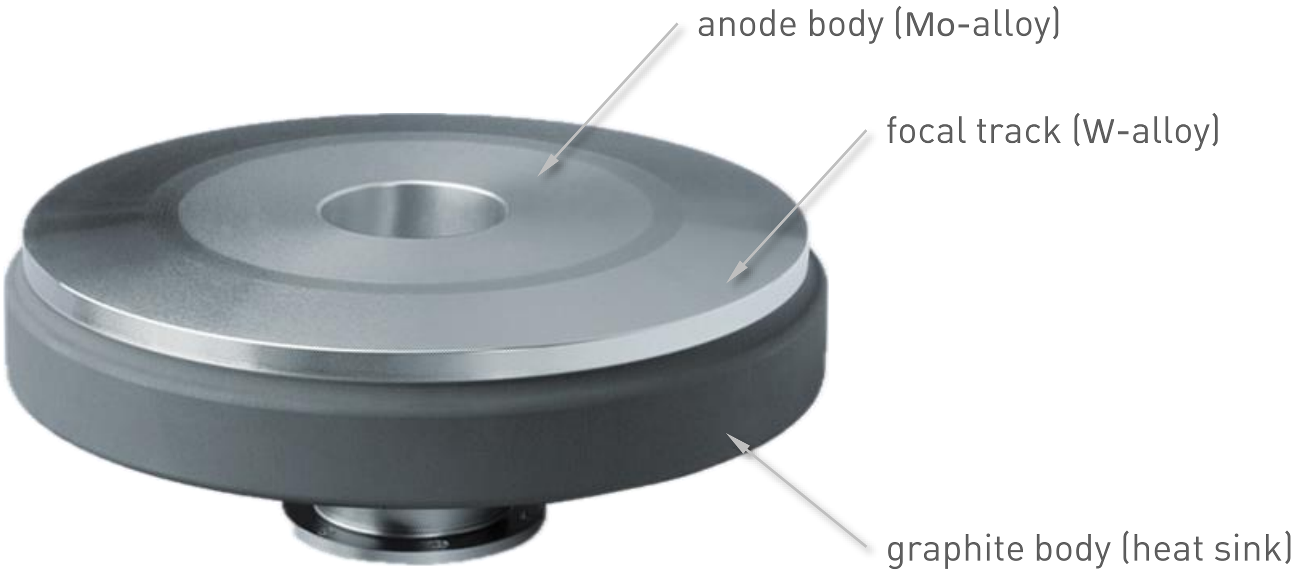


Ref: reproduced from [Poludniowski et al., 2022]

Monte Carlo model implementation

- using COMSOL Multiphysics 6.1
  - no ready-made interface for coupled electron-photon transport
  - COMSOL “Particle Tracing Module” allowing custom implementation
- main features:
  - particle types:
    - electrons
    - photons
    - excited target atoms (energy transfer to medium)
  - particle state variables:
    - particle energy *E* (Note: “massless” formulation)
    - quantities for sampling and statistics
  - interaction model:
    - using *Velocity Reinitialization* and *Secondary Emission* features
    - interaction data (cross sections etc.) for Mo, W, Re from EPICS-database (IAEA)
    - random sampling methods [Salvat, 2019] implemented in extensive function library (native/external C++)
  - domain accumulators: energy deposition (absorbed dose)
  - boundary accumulators: fluence and energy fluence

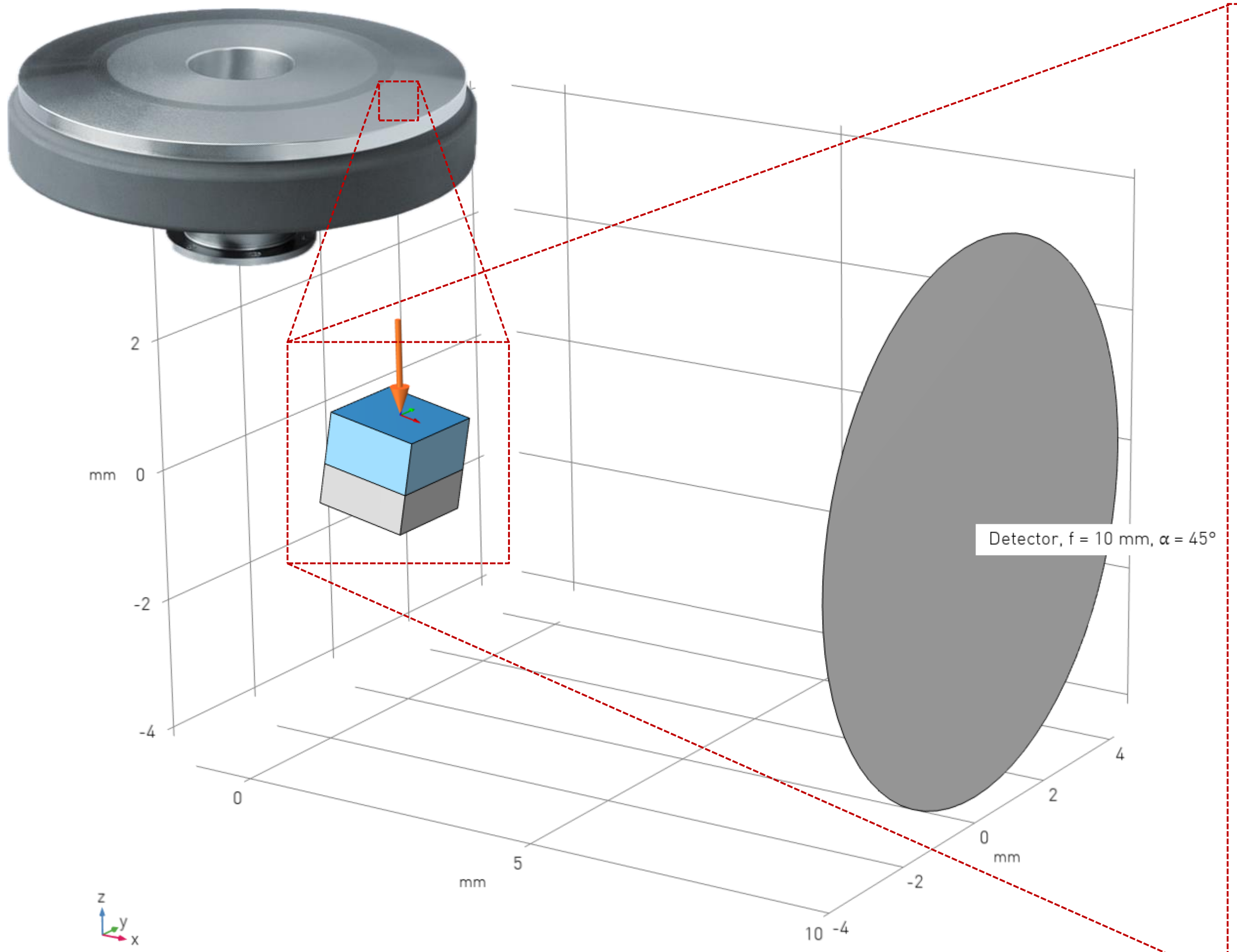
Typical rotating X-ray anode with graphite body



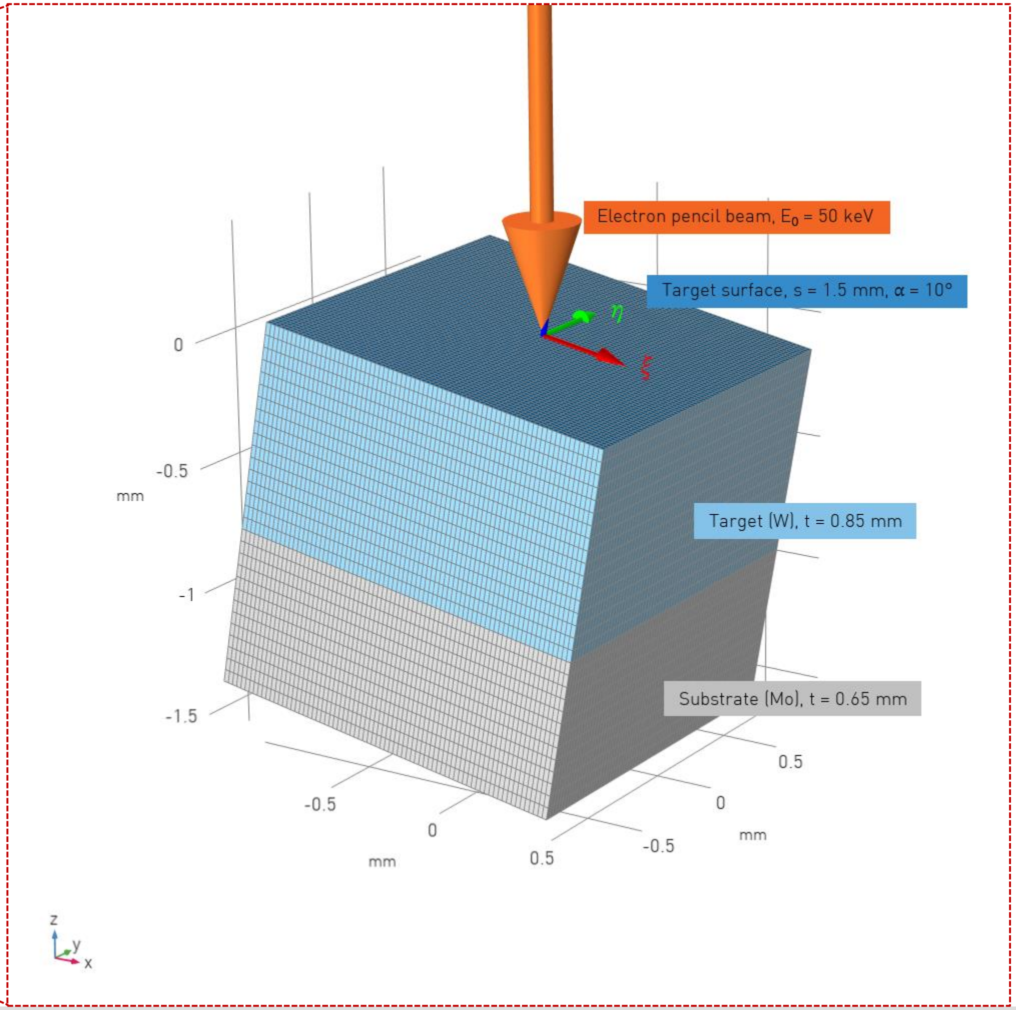
Ref: PLANSEE

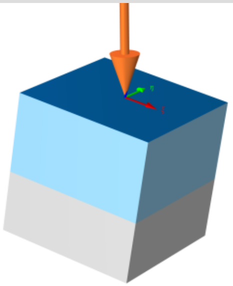
System

Geometry with target and detector



Computational domain with accumulator grid

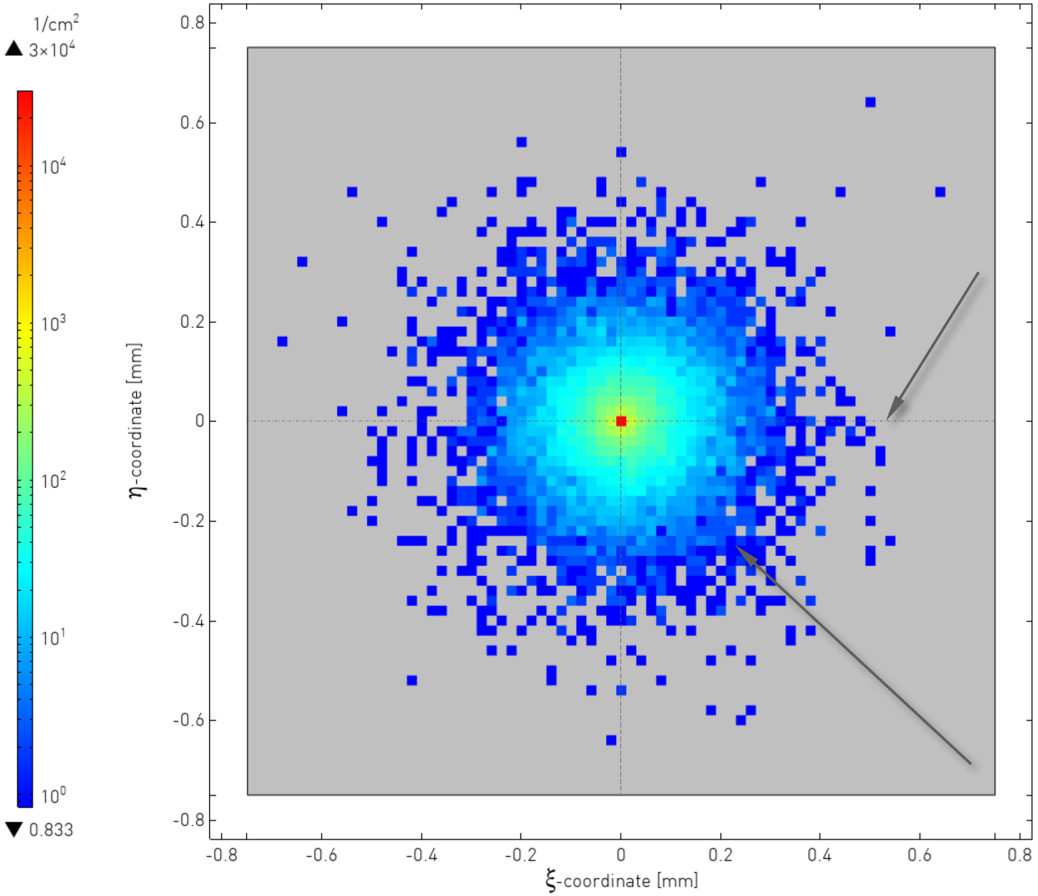




Results for pencil electron beam

Total target photon fluence and energy fluence per incident electron

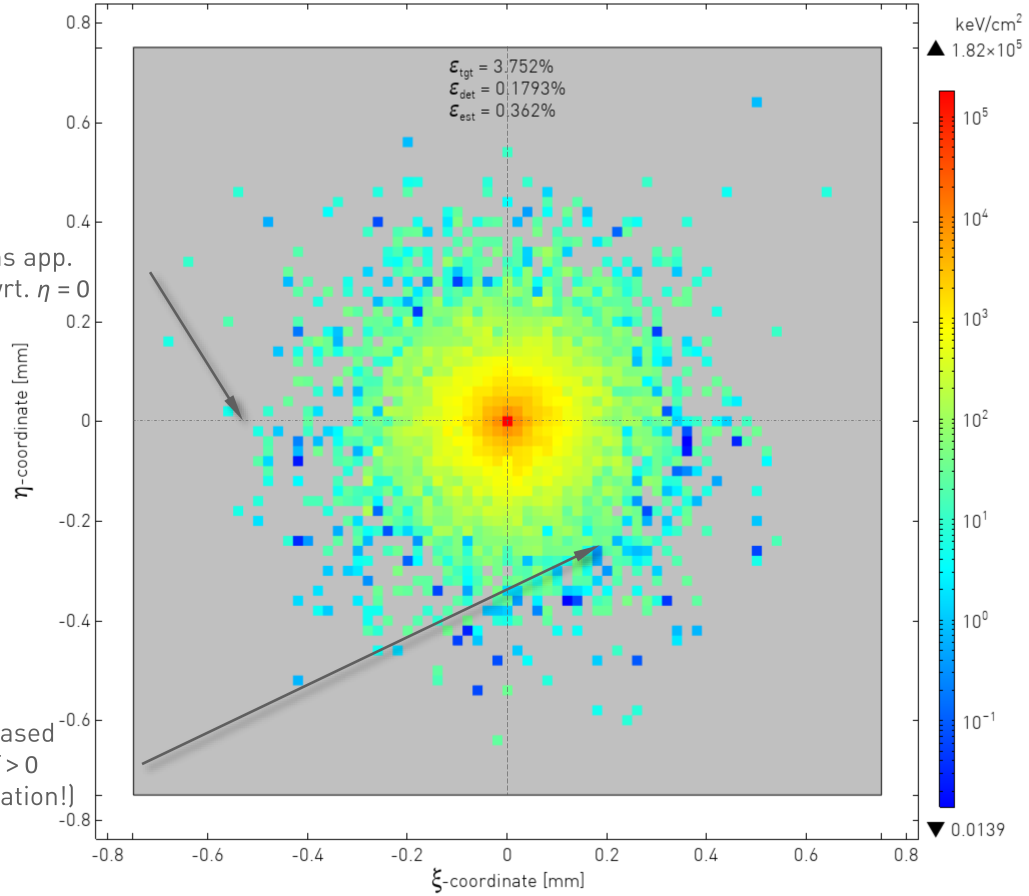
Fluence $\bar{\Phi}_\gamma$



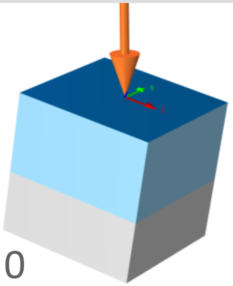
Energy fluence $\bar{\Psi}_\gamma$

distributions app. symmetric wrt. $\eta = 0$

(slightly) biased towards $\xi > 0$ (target inclination!)



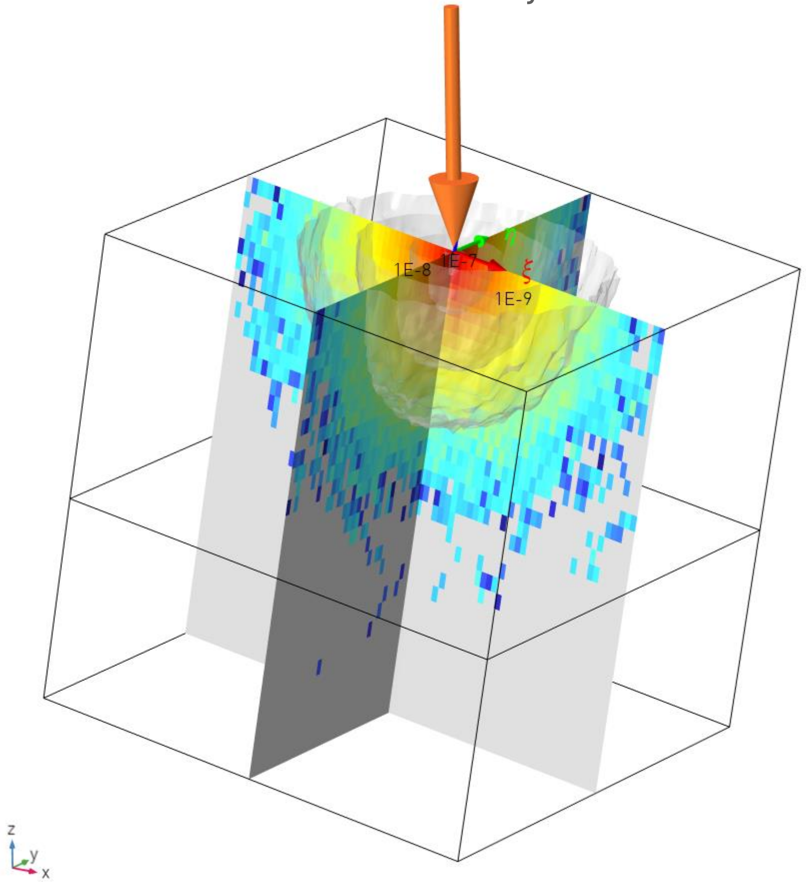
sample size: $N_e = 3 \cdot 10^5$



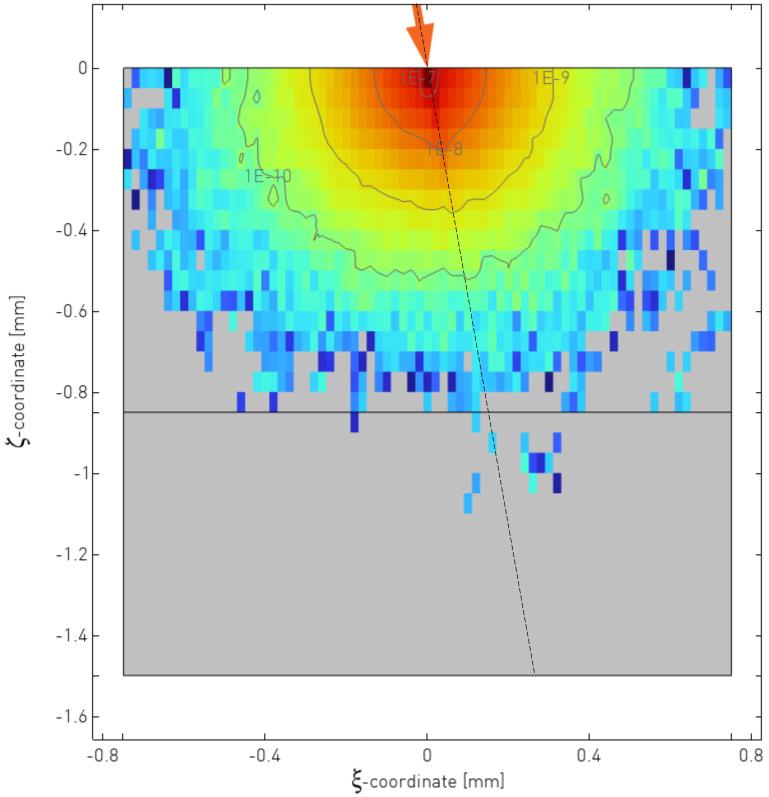
Results for pencil electron beam

Absorbed dose per incident electron $\bar{D}$

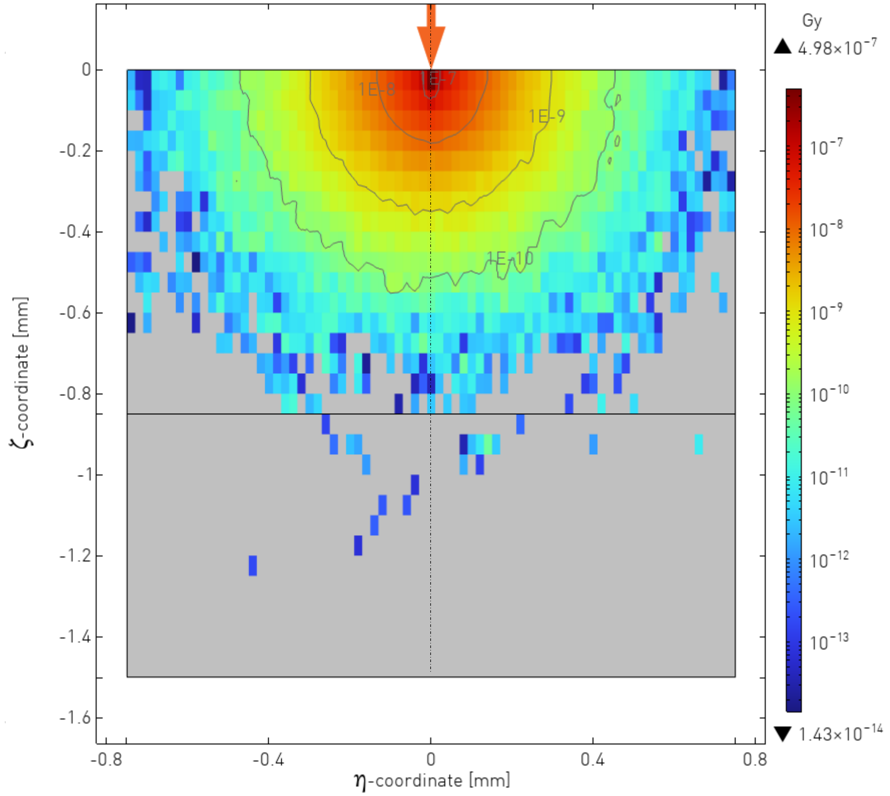
Solid body



Focal spot section $\eta = 0$



Focal spot section $\xi = 0$



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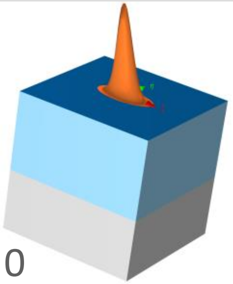
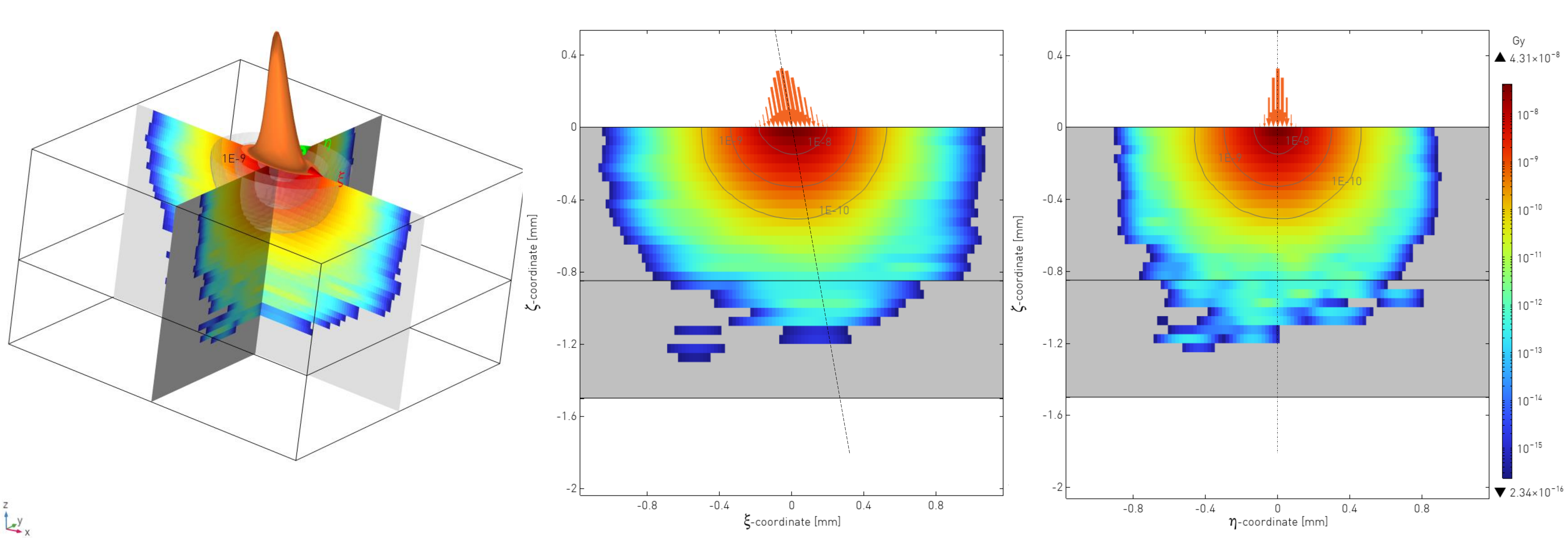


Results for GAUSSIAN electron beam

Absorbed dose per incident electron $\bar{D}$



transformation from electron pencil beam to arbitrary finite beam using convolution theorem (beam shape as kernel)

Summary

- implementation of Monte Carlo model in COMSOL Multiphysics
- radiation transport in solid X-ray targets
- focus on bremsstrahlung emission (continuous spectrum)
- state-of-the art sampling methods
- convolution of pencil electron beam results to arbitrary finite e-beam

Outlook

- model enhancement
  - performance improvements, increase sample size
  - radiative transitions and characteristic X-ray production
- model application
  - assessment of main parameters: tube voltage, target angle, thickness
  - better understanding of heat source distribution for use in nonlinear cyclic thermo-mechanical FEA

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...thanking you for your attention and
looking forward to your questions