Sputtering as a Line-of-Sight process - a computational case study

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9th International Workshop on Thin Films and New Ideas for SRF

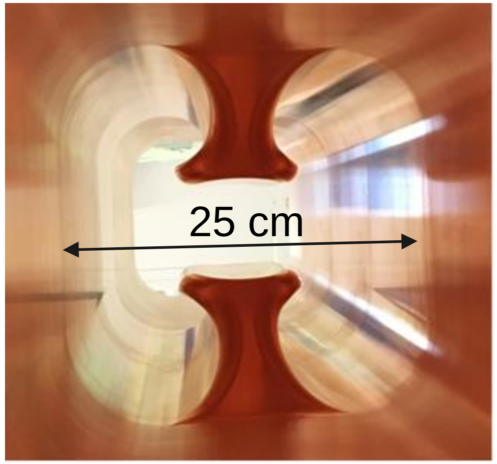
Outline

1. **The Wide-Open Waveguide Crab Cavity**
2. **Line-of-Sight based MC transport in *Molflow***
3. **Comparison with collisional MC**
4. **Rules for interpreting LoS-based MC**

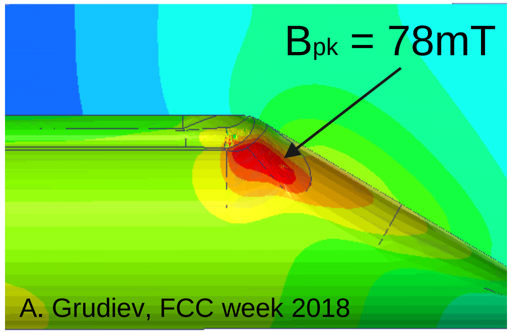
1 The Wide-Open Waveguide Crab Cavity

- **bunch tilting for head-on collisions**
- **key design features:**
  - stable operation at 4.5 K
  - competitive surface fields
  - optimized deflecting field quality
  - low shunt impedances
  - reduced HOM confinement
  - improved access for coating

K. Papke et al, Phys. Rev. Accel. Beams 22, 072001, 2019



$Q_0 = 4 \times 10^8$
P_{loss} = 67 W at 3MV



140 cm

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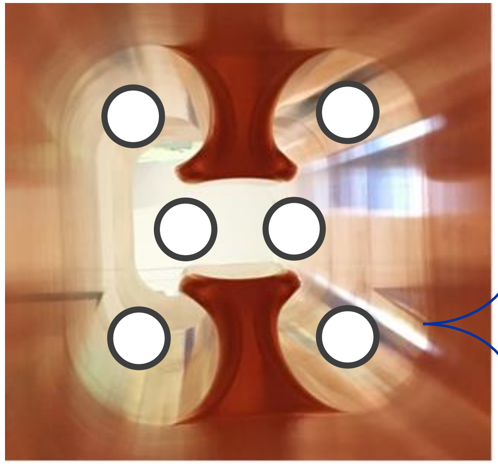
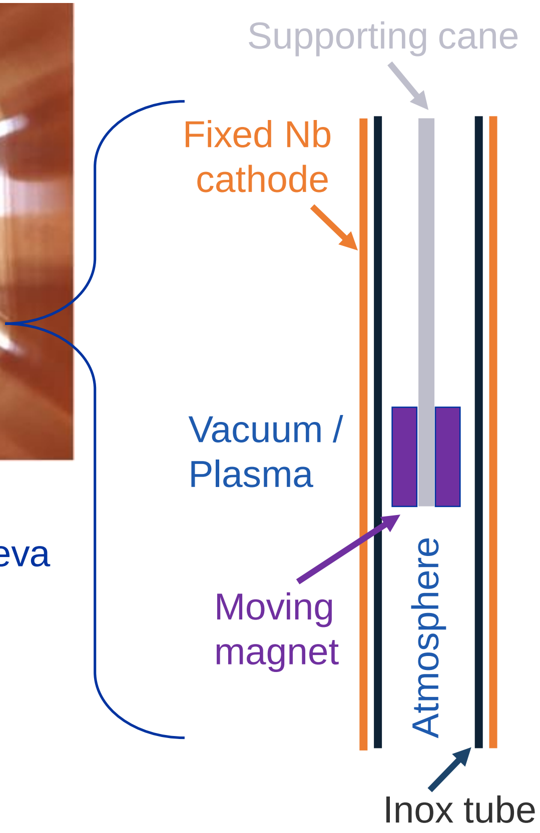


F. Avino et al, TTC,
5th February 2020 Geneva



→ Complex procedure requires **large number** of comparative simulations

2 What is Molflow?

- **Ray-tracing Monte Carlo simulation of an *ideal* gas in a bounded system**

M. Ady, R. Kersevan, 10th Int. Particle Accelerator Conf., Melbourne, Australia, 2019, doi:10.18429/JACoW-IPAC2019-TUPMP037

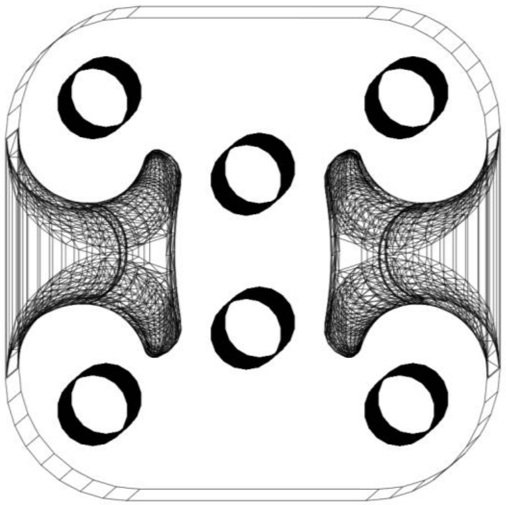
2 Basic external input

- **Ray-tracing Monte Carlo simulation of an *ideal* gas in a bounded system**

M. Ady, R. Kersevan, 10th Int. Particle Accelerator Conf., Melbourne, Australia, 2019, doi:10.18429/JACoW-IPAC2019-TUPMP037

NEED

- System geometry (.stl)
- Desorption maps



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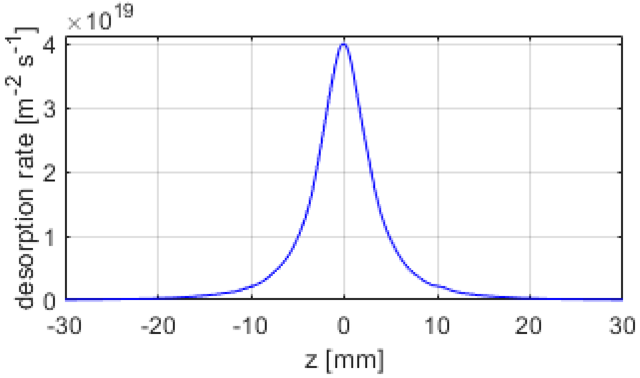
Fraunhofer IST: PIC-MC



A. Pflug, DSMC/PIC-MC Code Documentation, Fraunhofer IST, Braunschweig, Germany, https://simulation.ist.fraunhofer.de/doku.php?id=start

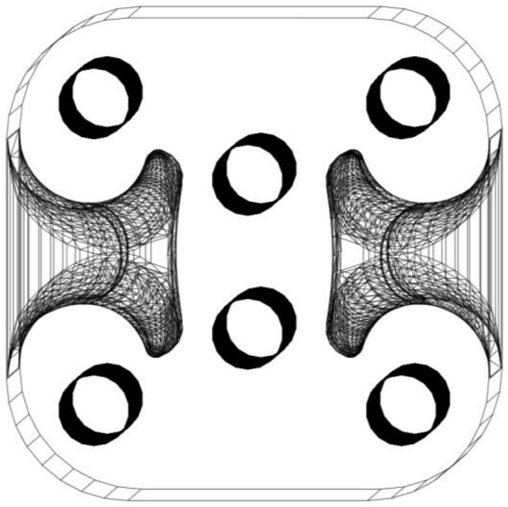
F. Avino et al, TTC, 5th February 2020 Geneva

2 Well-designed settings

- **Ray-tracing Monte Carlo simulation of an *ideal* gas in a bounded system**

NEED

- System geometry (.stl)
- Desorption maps



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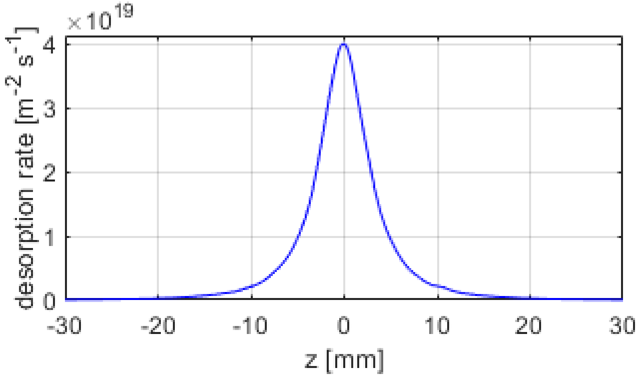
SET

- Boundary Conditions:
  - adsorb, reflect, emit, transmit
- Angular distributions:
  - (Power) cosine, specular, …
- Temperatures
- Particle mass, decay times, …

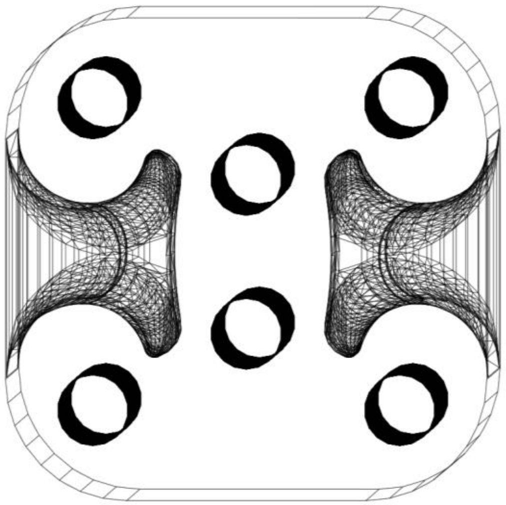


2 Versatile output

- **Ray-tracing Monte Carlo simulation of an *ideal* gas in a bounded system**

NEED

- System geometry (.stl)
- Desorption maps



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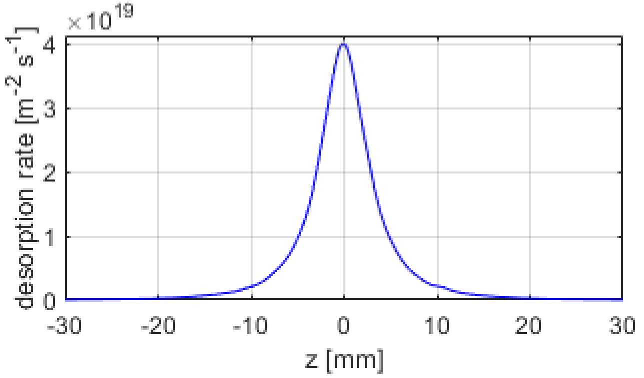
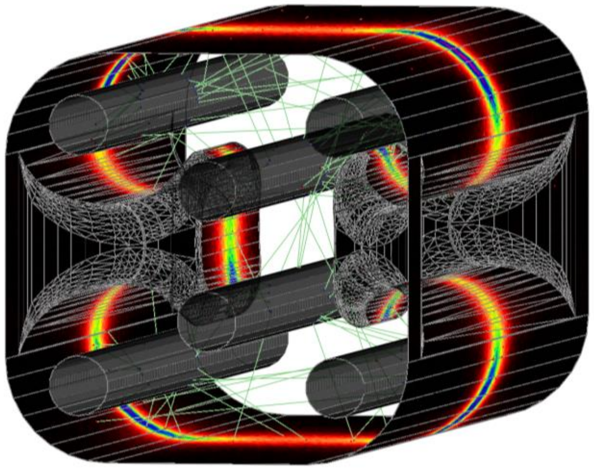


GET

- Leak / pumping check
- 3D texture maps
  - Pressure
  - **Impingement rates**



2 Clear limitations

- **Ray-tracing Monte Carlo simulation of an *ideal* gas in a bounded system**

NEED

- System geometry (.stl)
- Desorption maps

SET

- Boundary Conditions:
  - ➢ adsorb, reflect, emit, transmit
- Angular distributions:
  - ➢ (Power) cosine, specular, …
- Temperatures
- Particle mass, decay times, …

GET

- Leak / pumping check
- 3D texture maps
  - ➢ Pressure
  - ➢ **Impingement rates**

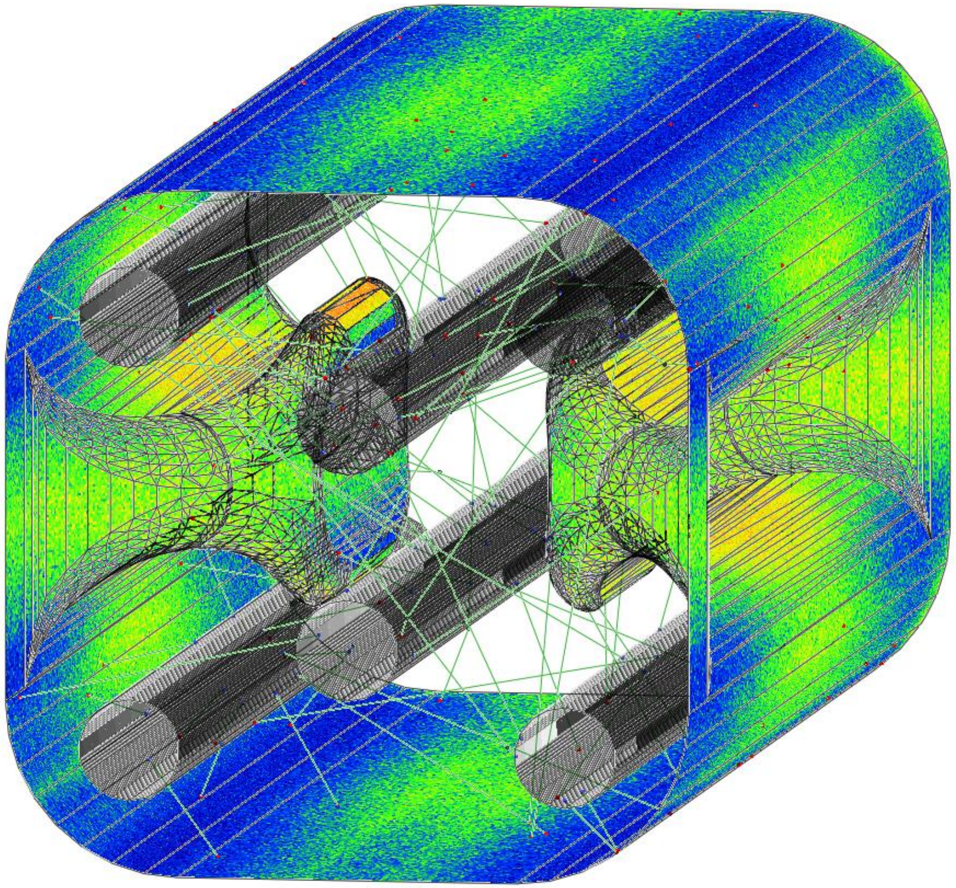
! single species, no volume collisions, no fields !

2 Efficiency and consistency

- **1-3 khits /s on desktop PC**
- **MC noise levels below (≈ 15%) need ≈ 10 min per sputtering source for 1mm textures**

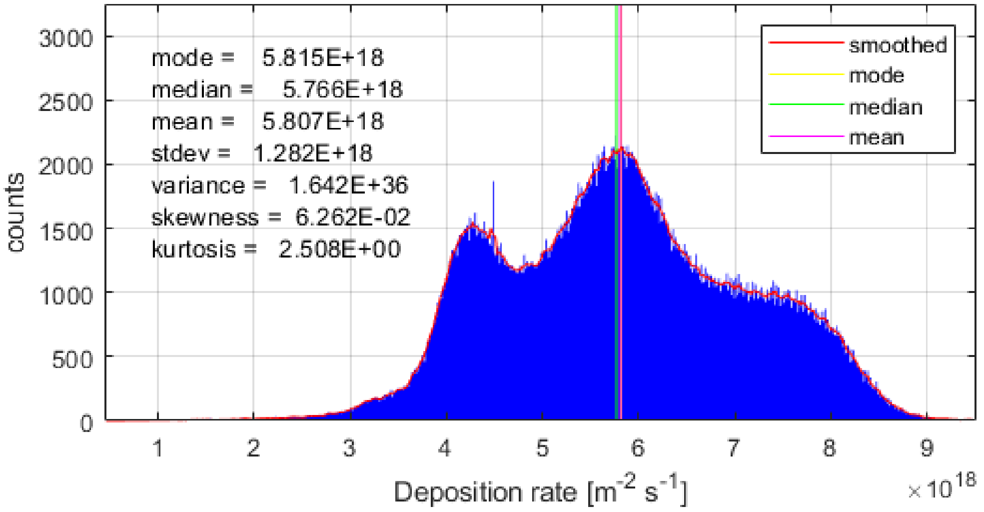
→ full set of cathodes with 25 mm magnet spacing: <u>10 - 20 h</u>

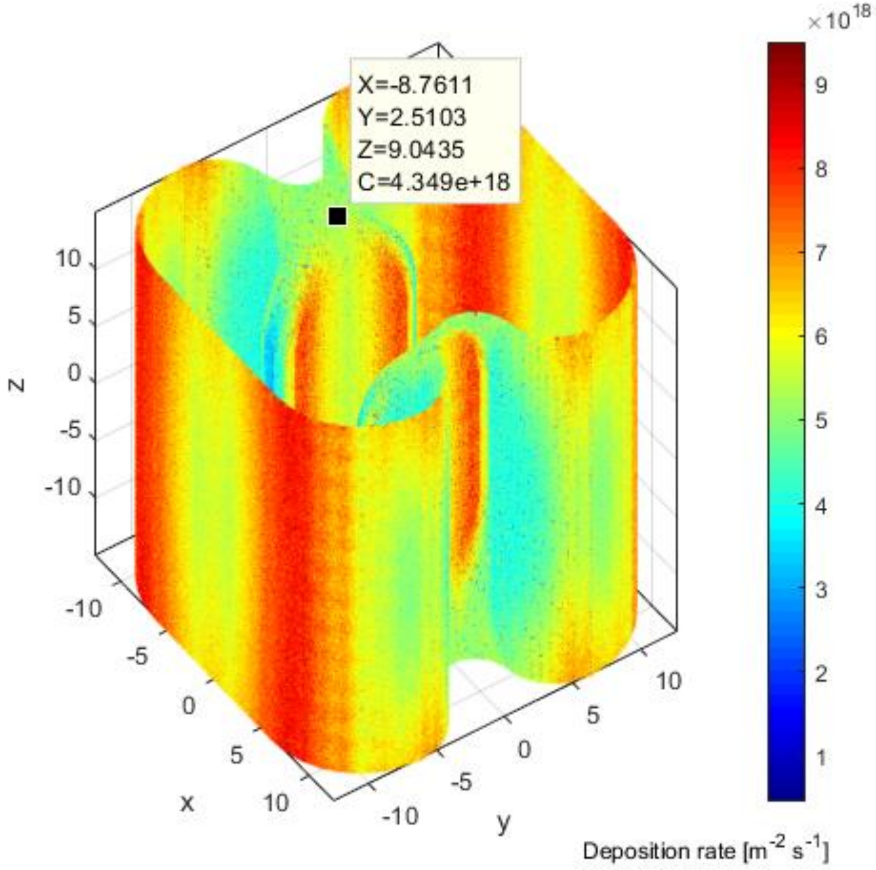
- **intrinsic conservation of total flux with < 2 % resolution input errors**



2 Raw data from textures: a first look

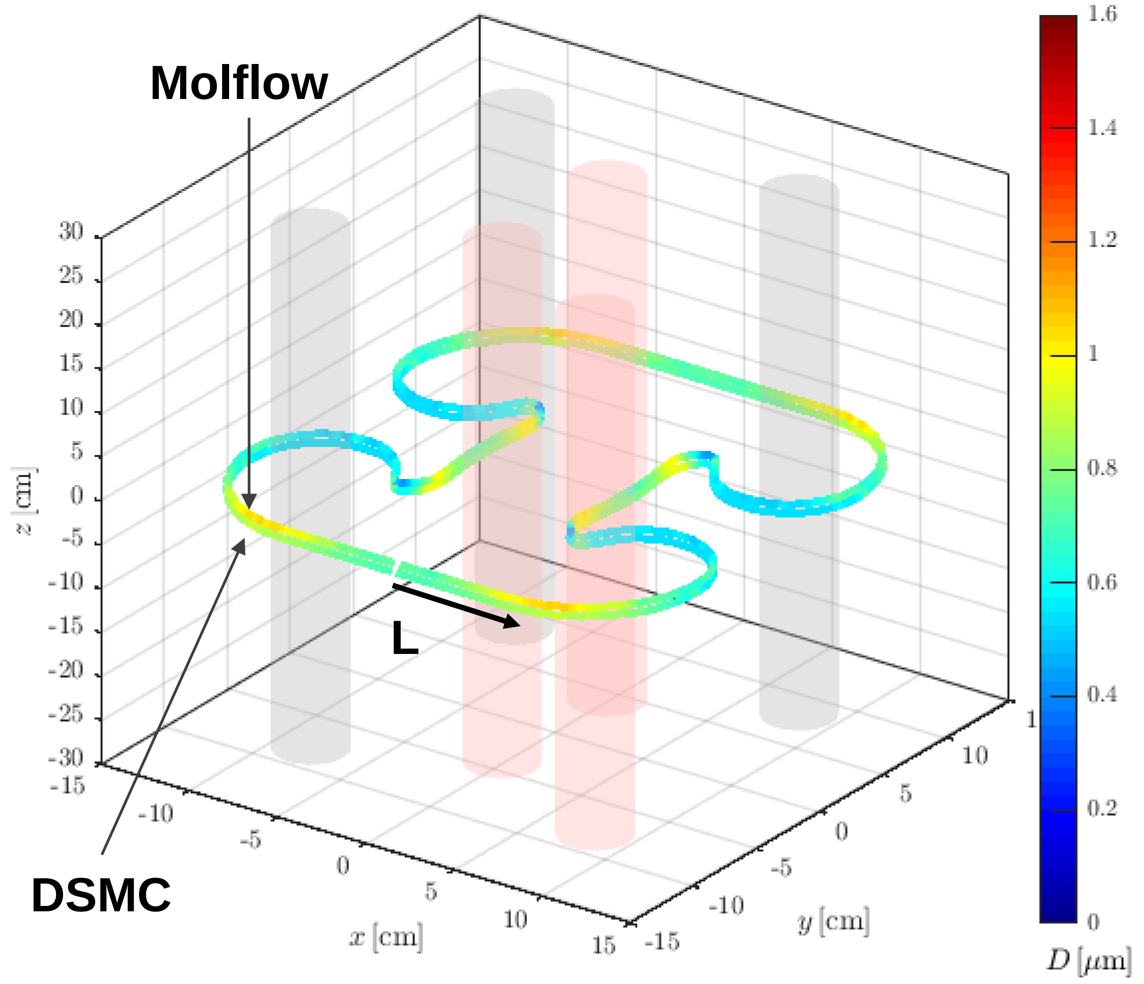
- **check for remaining MC outliers**
- **compare basic deposition maps**
- **post-processing needed for 1D profiles**





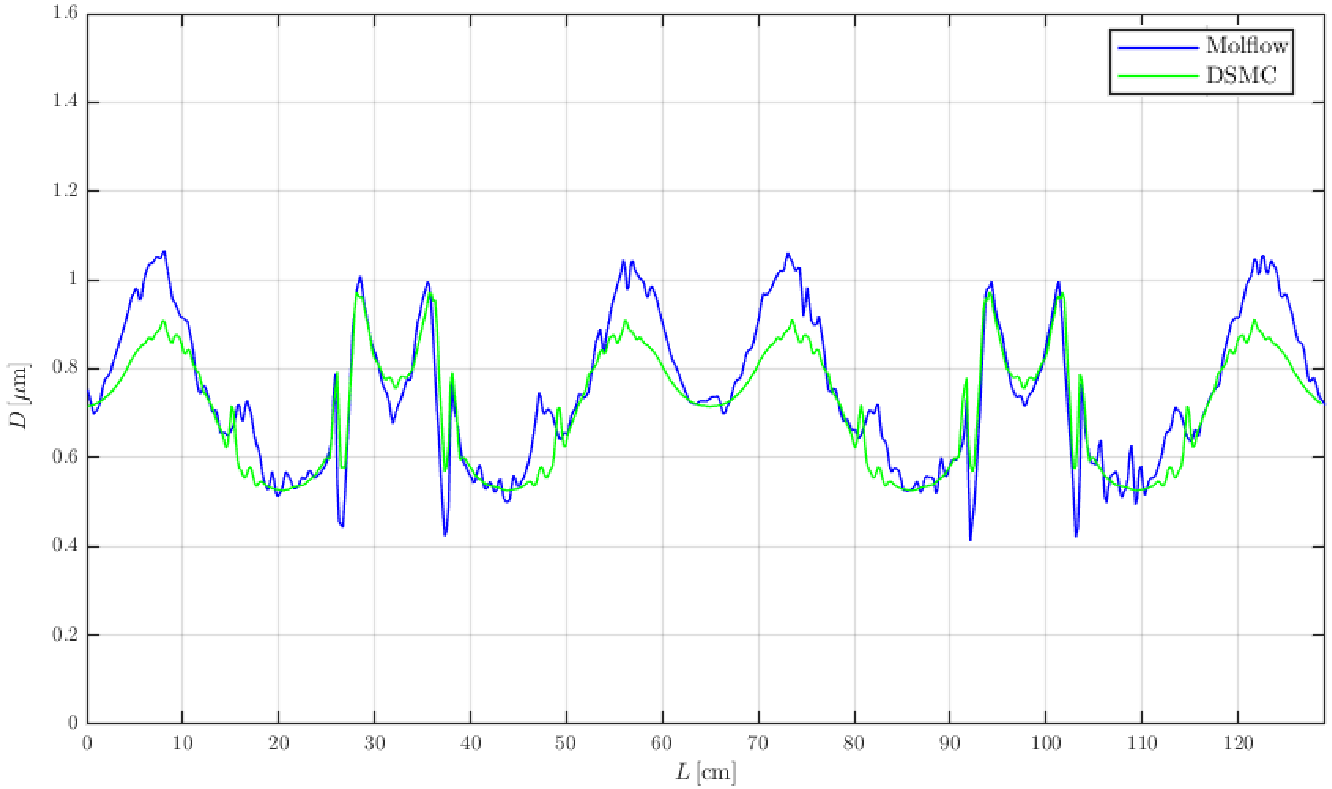
3 Defining cross-sectional profiles

- **Select one or more z ± dz**
- **Linear, regular, smooth and yield preserving coordinate L**
- **Display as flux, growth rate, film thickness or normalized**
- **Comparison with collisional DSMC results from *Fraunhofer IST Braunschweig***



3 Good overall agreement with DSMC

- **For same total *sputtering* flux, qualitative trends agree**

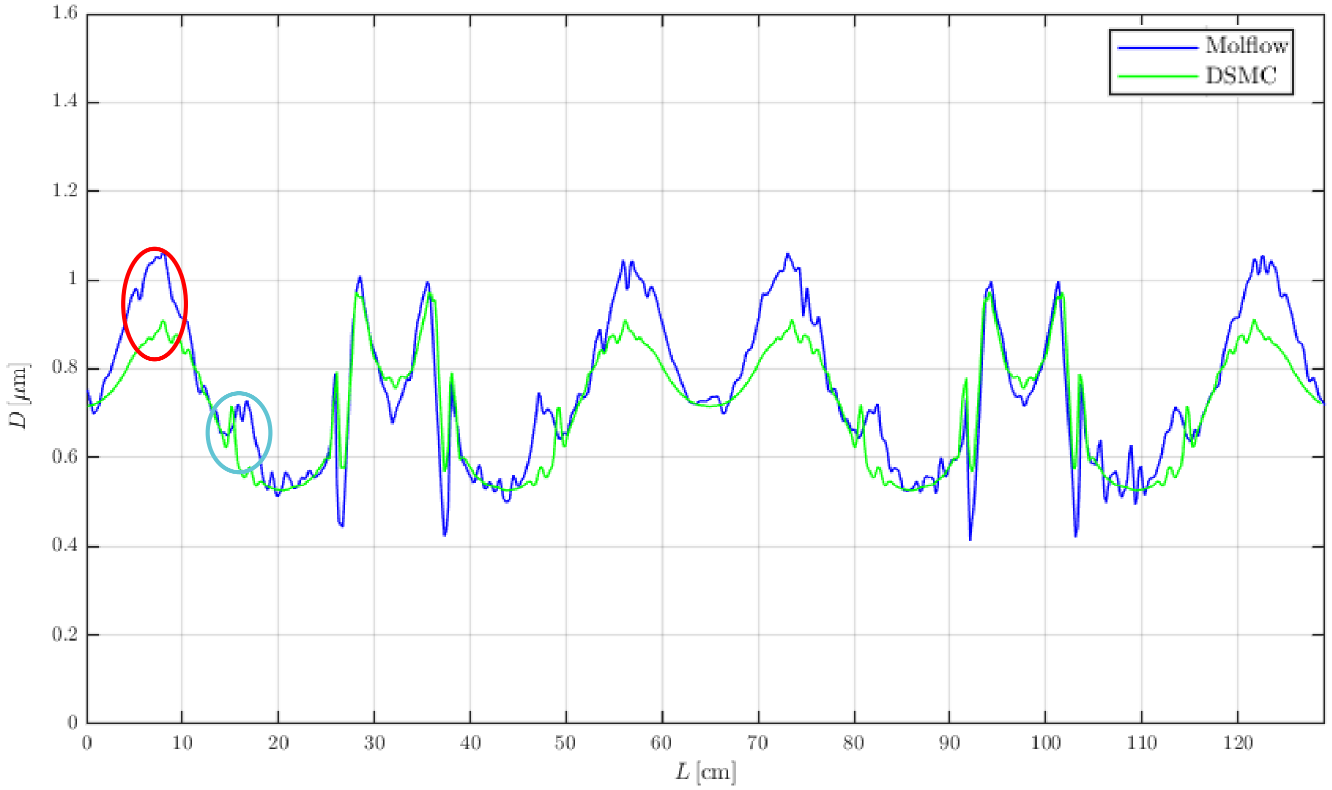


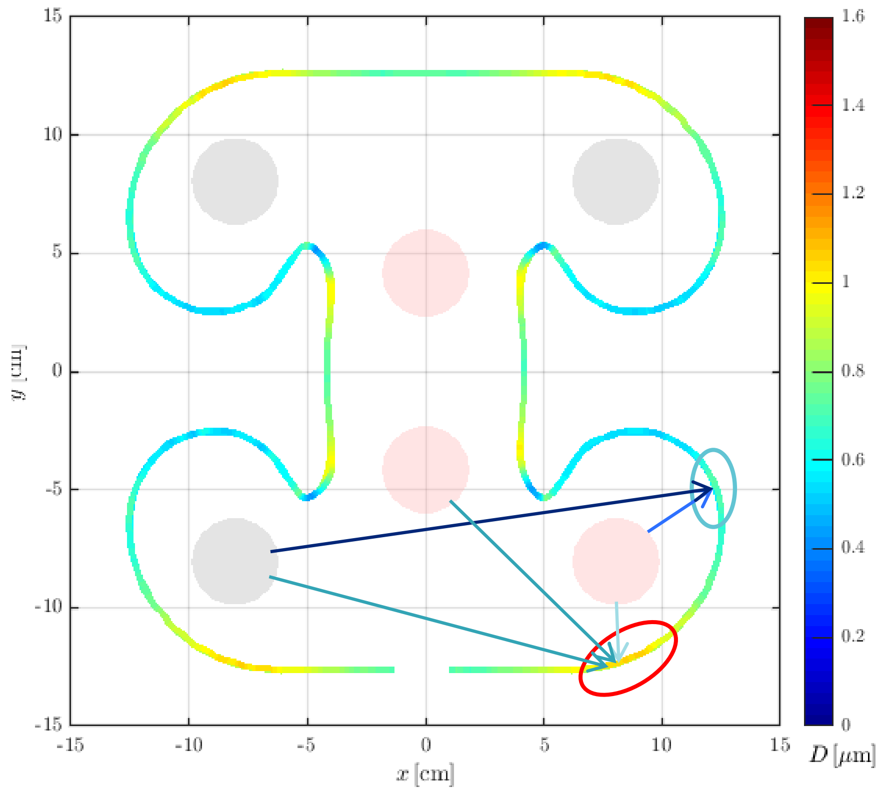
→ *deposition* flux 5% higher

→ Local discrepancies

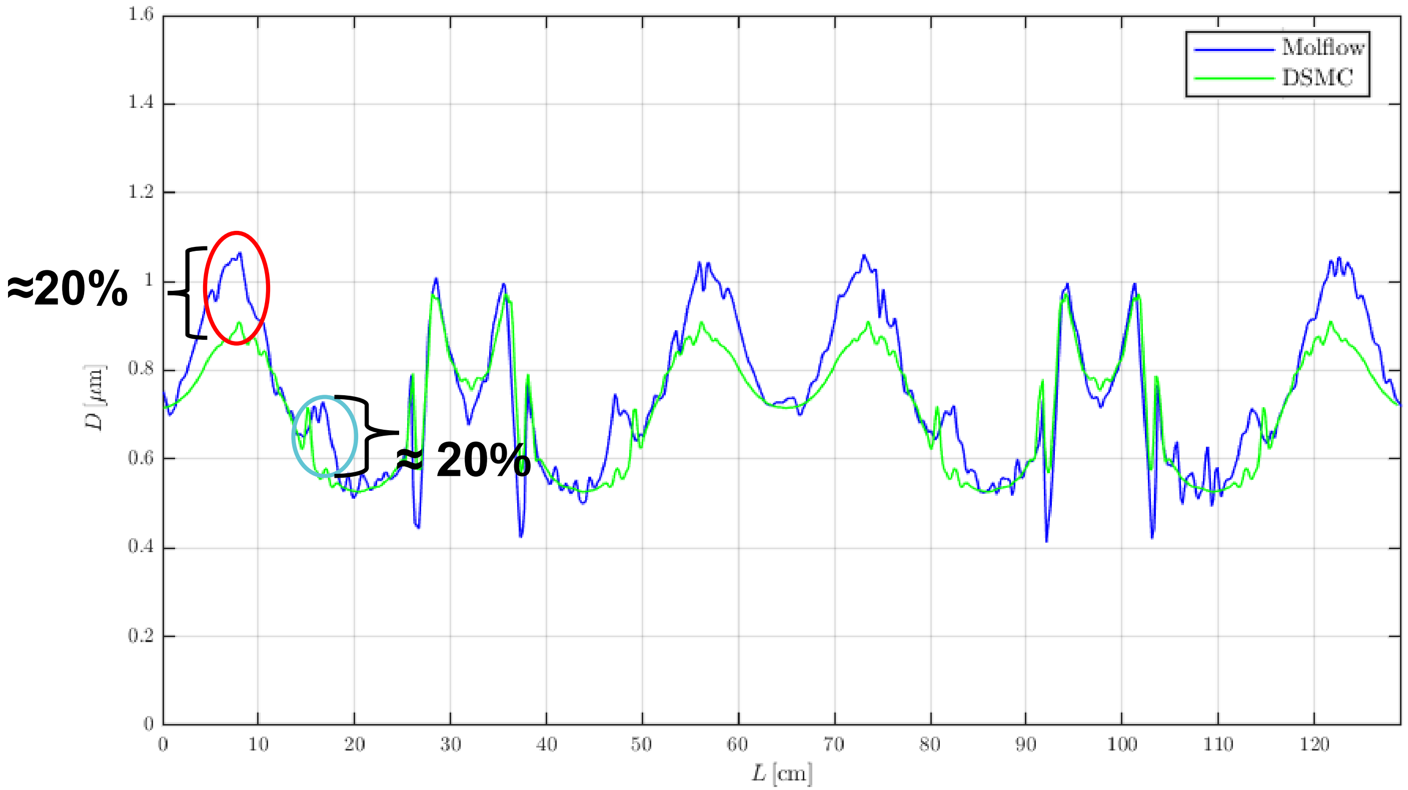
3 Accounting for local features

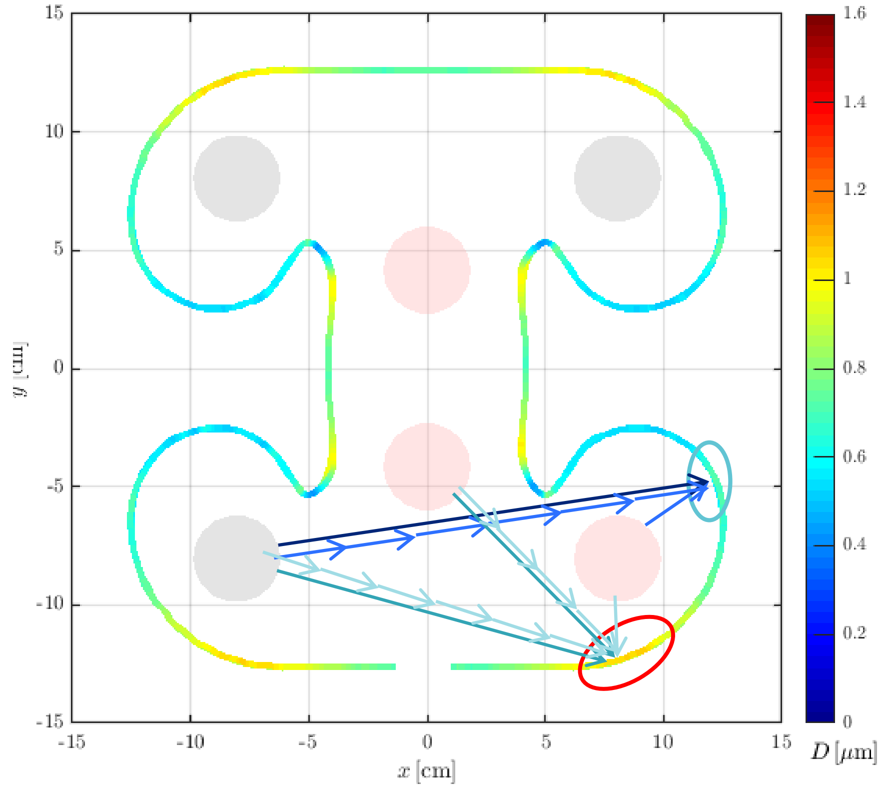
- **Localization in cross-section: where multiple cathodes contribute**





3 The impact of secondary lines-of-sight





→ **Discrepancies as roughly expected from 1/R dependence of flux**

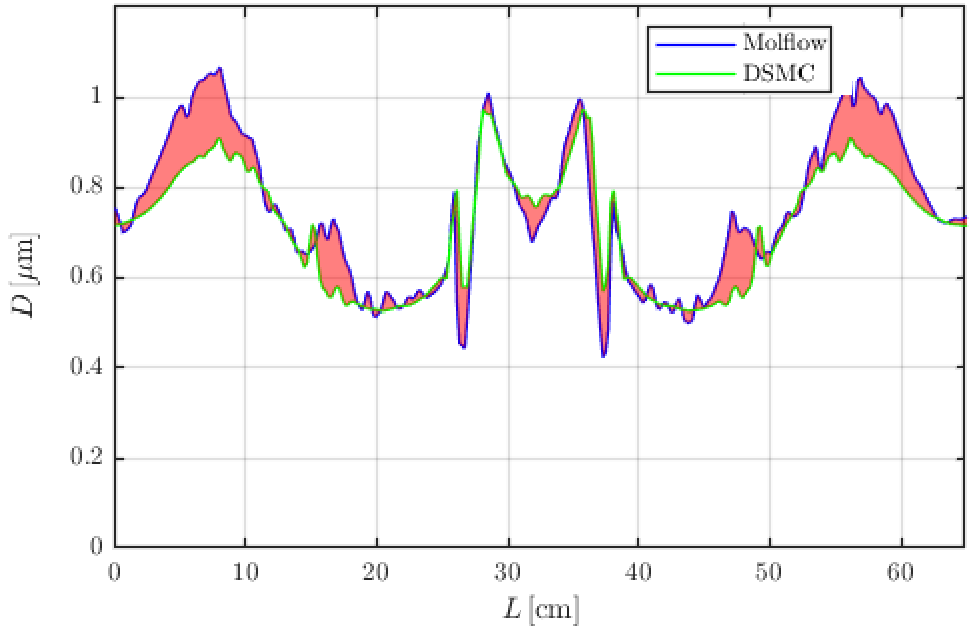
→ **Volume collisions redistribute flux: mean-free-path ≈ 6cm**

3 Differences due to back-scattering

- Small angle collisions → smoothing, shadows effectively broaden
- Large angle collisions → back-scattering, non-LoS deposition

→ increase total deposition onto cathodes: 19% → 24%

→ difference in profiles: -4.7 % at z=0



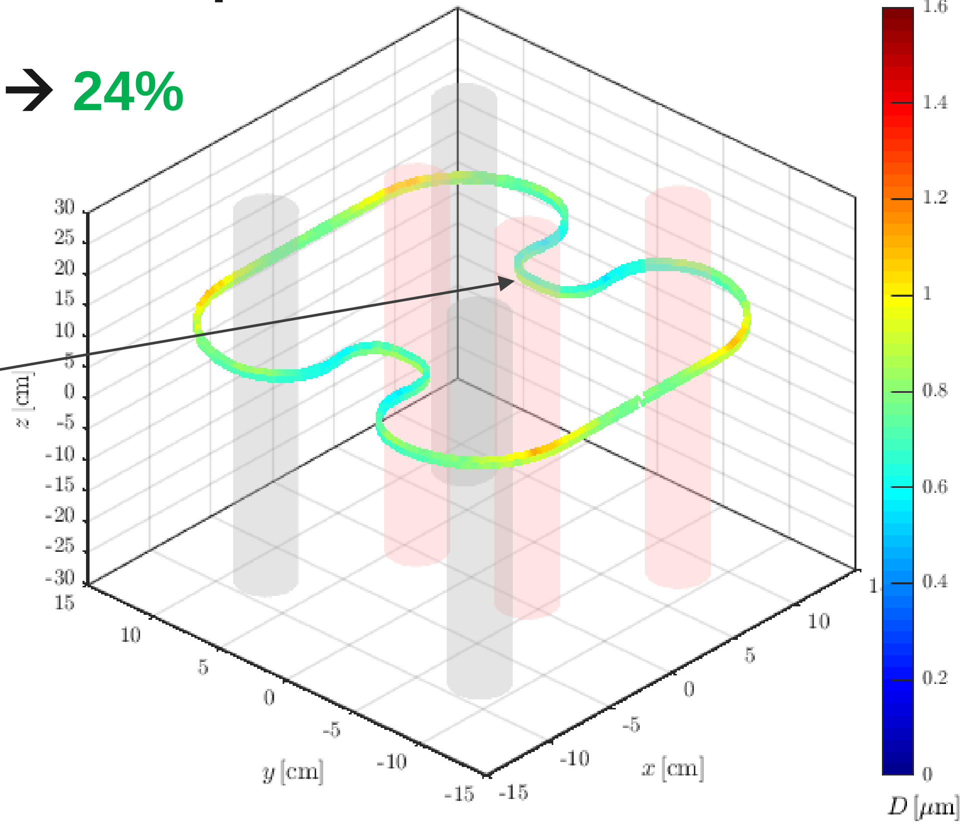
3 Local deposition through collisions

- **Small angle collisions → smoothing, shadows effectively broaden**
- **Large angle collisions → back-scattering, non-LoS deposition**

→ increase total deposition onto cathodes: 19% → 24%

→ difference in profiles: -4.4 % at z=12

→ local scattering onto tapers



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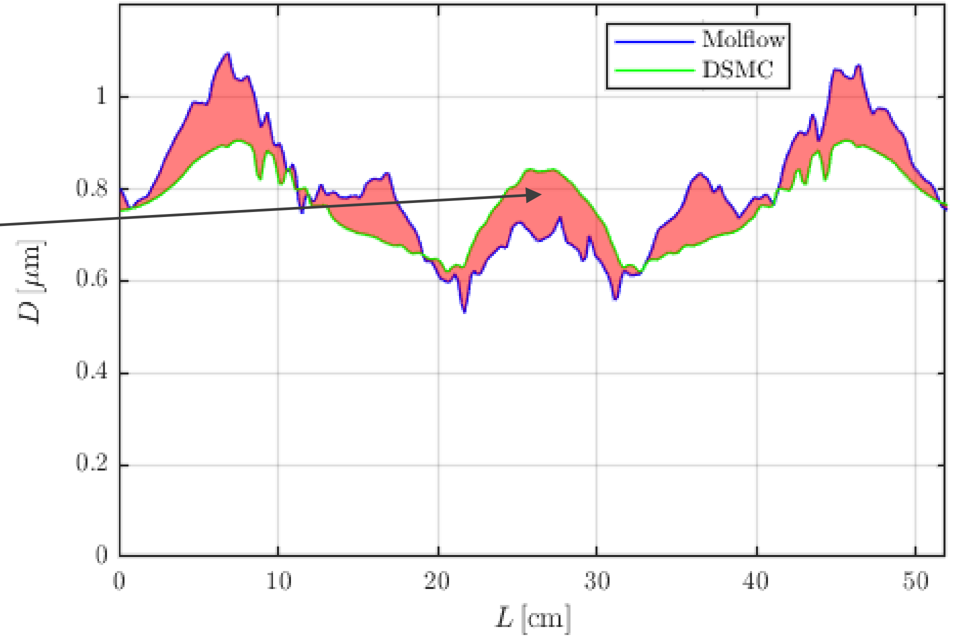
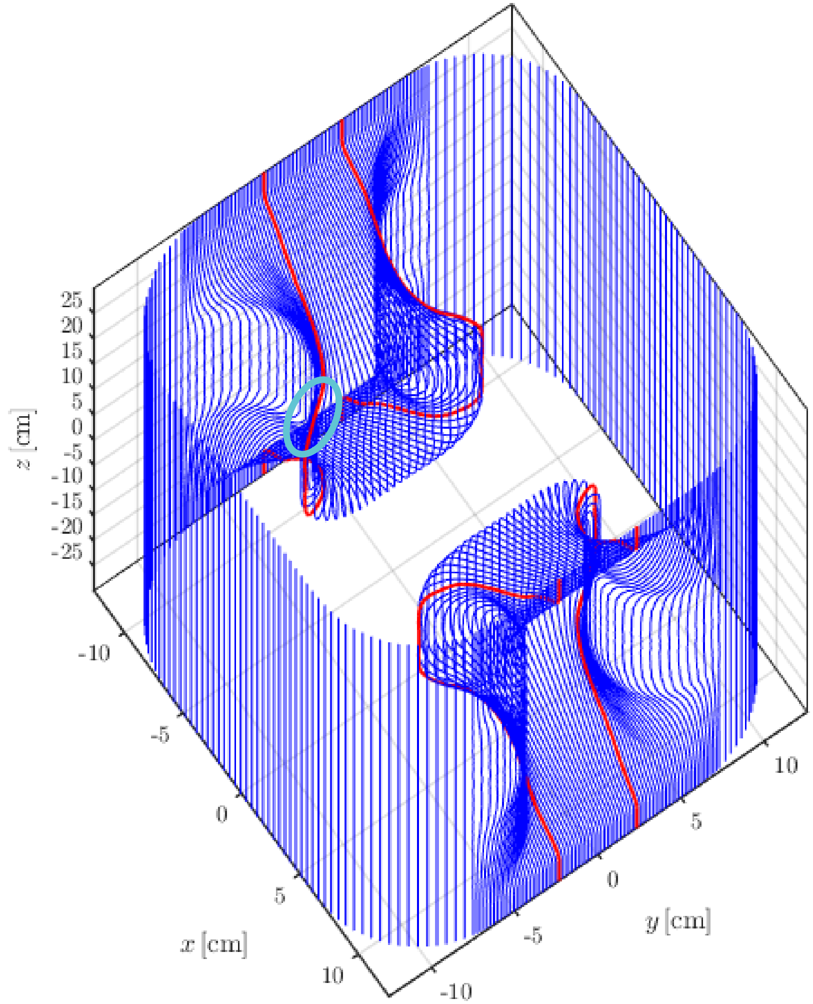


3 Dedicated axial profiles

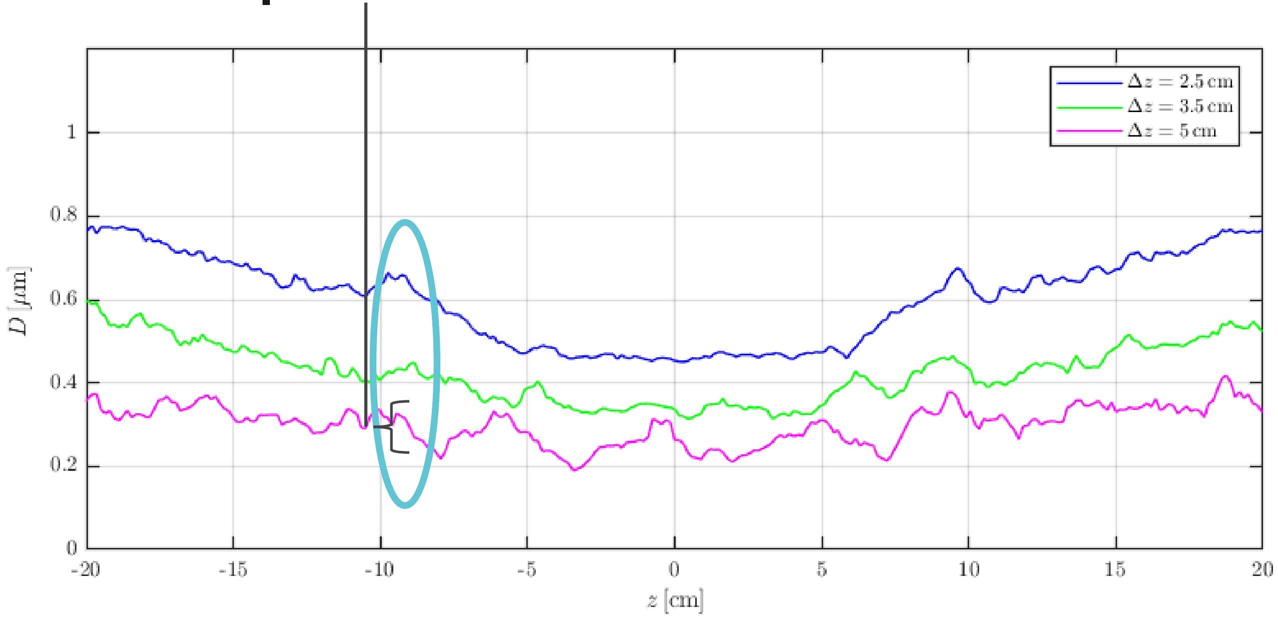
- Profiles along cavity length, but not along z
- follow relevant regions (e.g. RF hotspot)

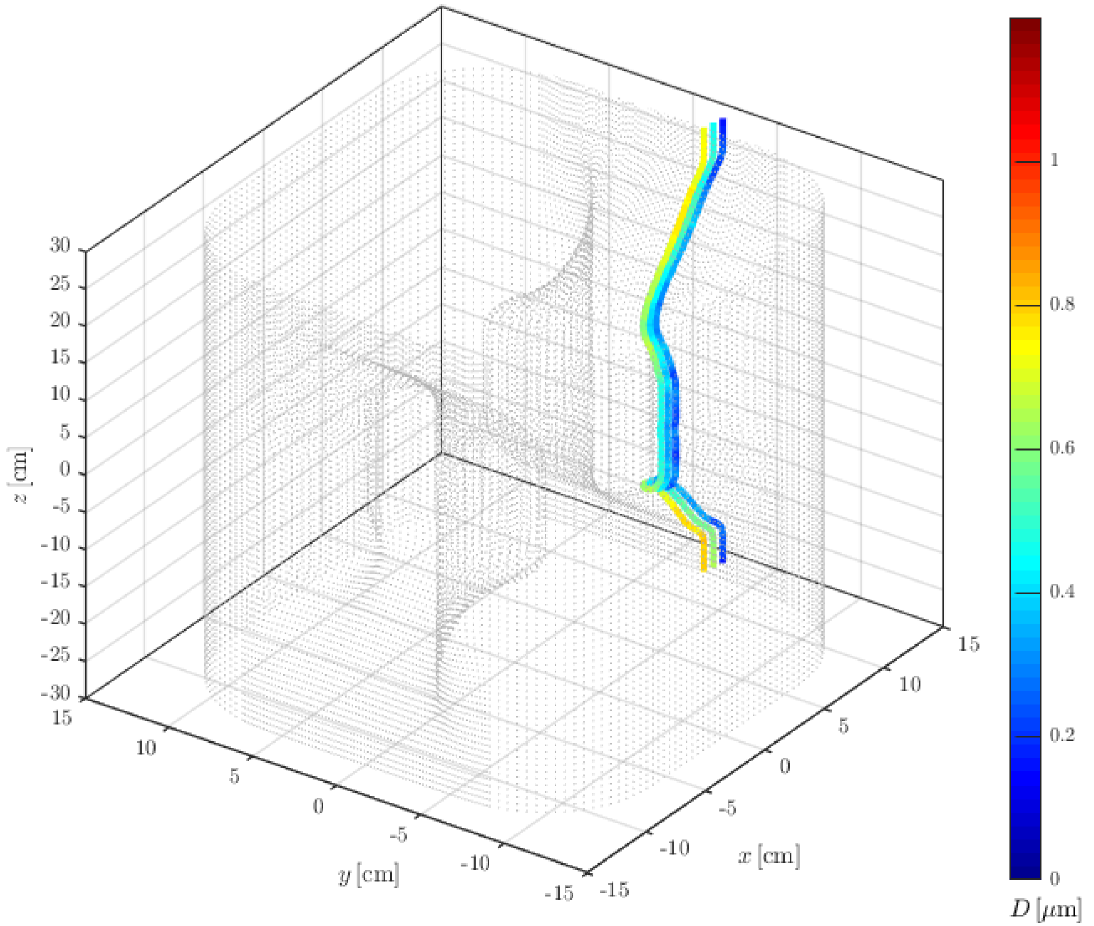


3 Worst-case assessment for magnet step sizes

central hotspot line:

- **overall reduction towards cavity center**
- **For increasing step size Δz:**
  - **→ Reduced total deposition proportionately**
  - **→ Up to ≈ 40% local variations**

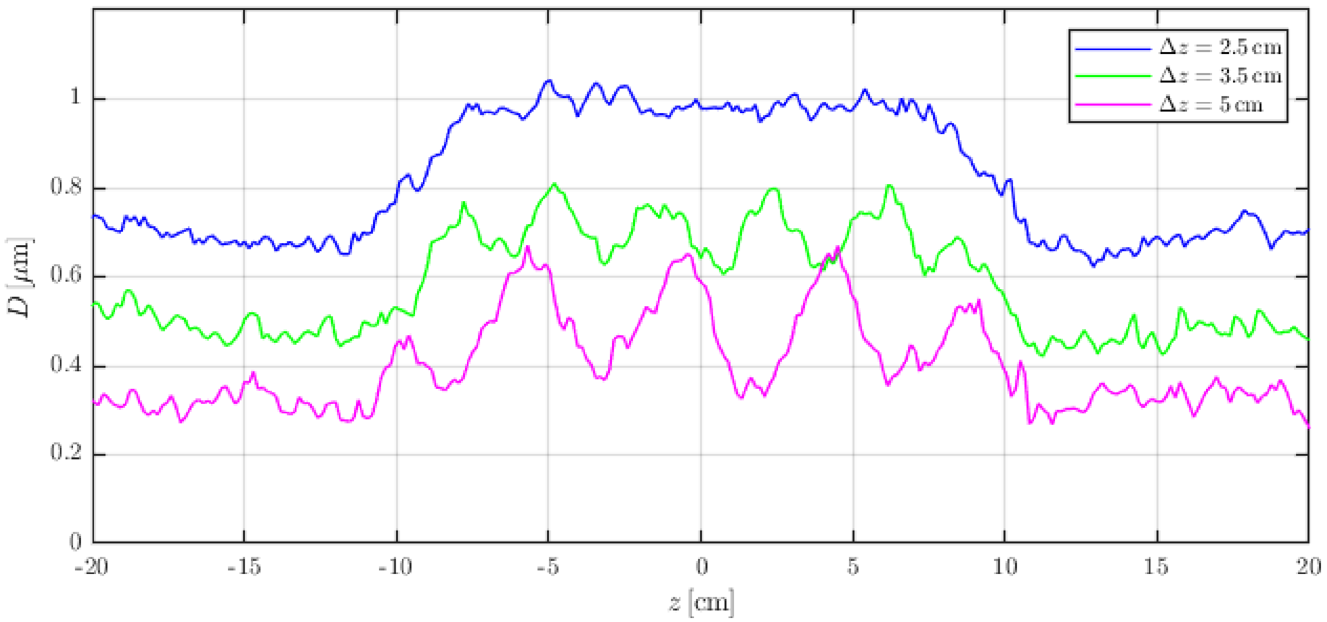


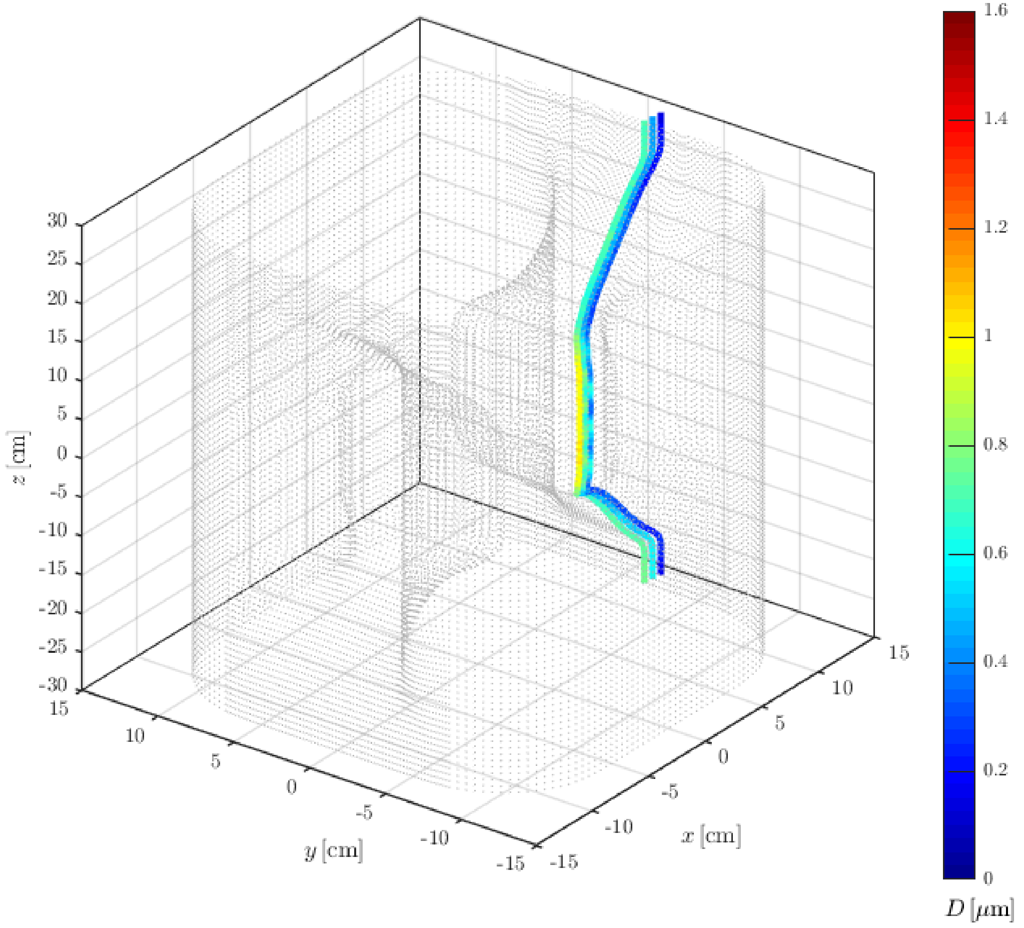


3 Worst-case assessment for magnet step sizes

Line above hot spot

- Strong rise towards cavity center
- Local variation persists and grows





4 Rules for interpreting LoS-based MC

- **Overall agreement with collisional code within ≈ 25%**
- **More subtle than it seems: geometry vs mean-free-paths**

→ Consider secondary sputtering sources when assessing maxima

→ Their 3D distribution / orientations matter

→ Beware large gas volumes about surface normal

→ Often "worst-case" near local and global minima

→ Highly efficient tool during early design, development ongoing

Thank you for your attention !

Questions ?

home.cern

Comparing experimental data

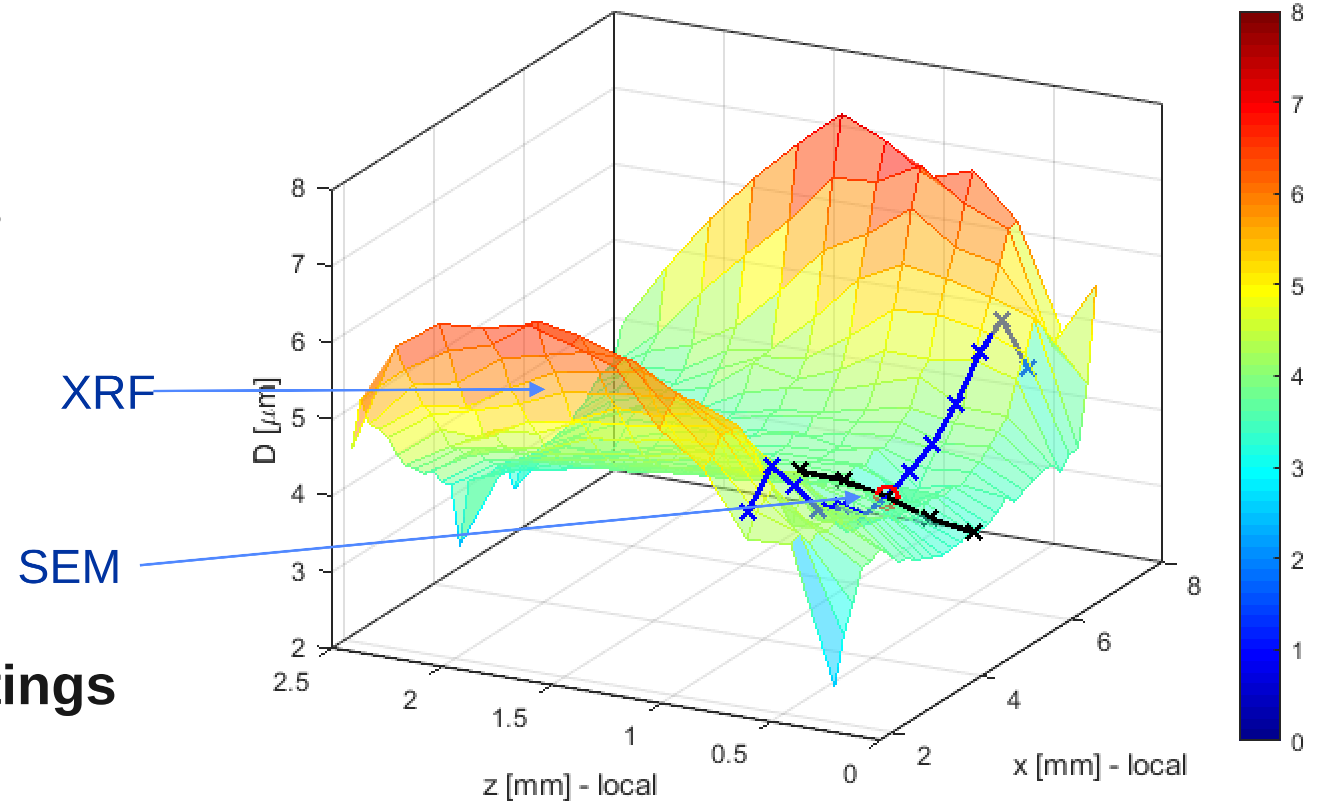
SEM positions as “sights of interest” marked on sample edge

→ project to measurement position

on sample central profile

XRF-data needs view-angle corrections

→ begin cross-comparing both



→ Excellent agreement for HiPIMS coatings