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MFEM Workshop 2024 @ LLNL

Simulating atom probe tomography using MFEM

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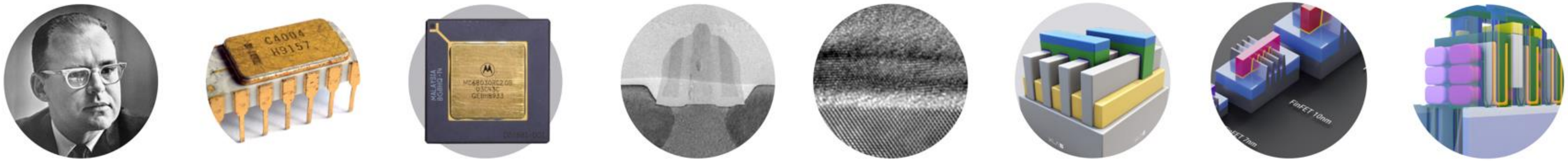
julian.luken@uantwerpen.be

Metrology of modern tech

Moore‘s Law	10000nm	1000nm	100nm	45nm	finFET 22nm	10nm	GAAFET 3nm



1965	1971	1984	2003	2007	2011	2016	2022

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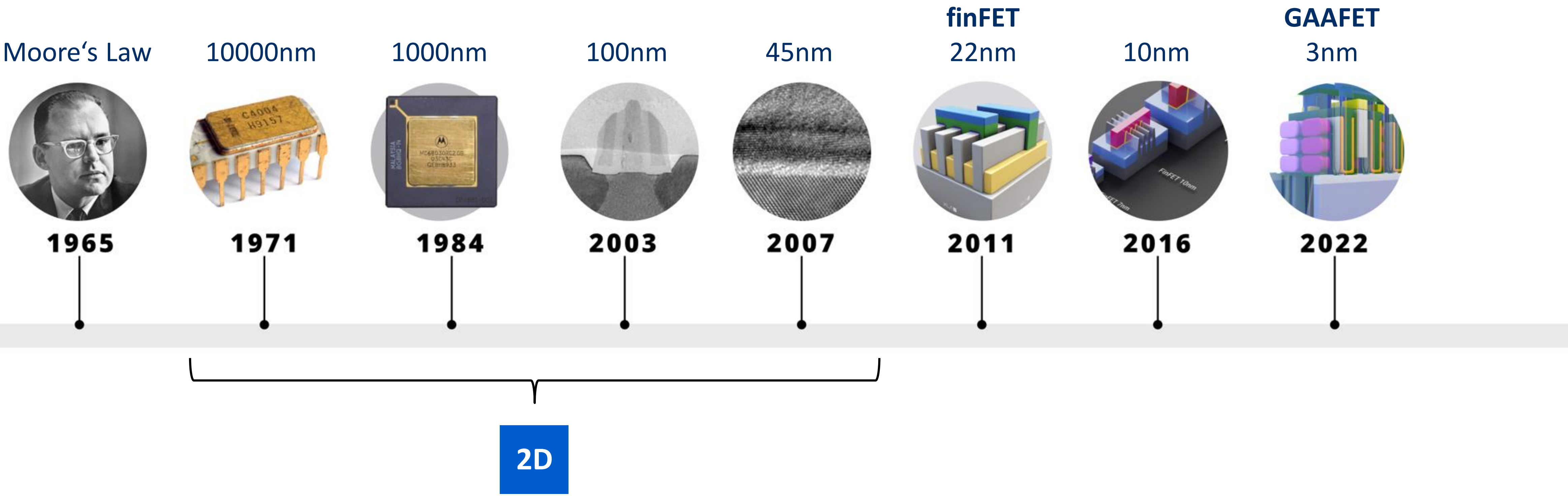
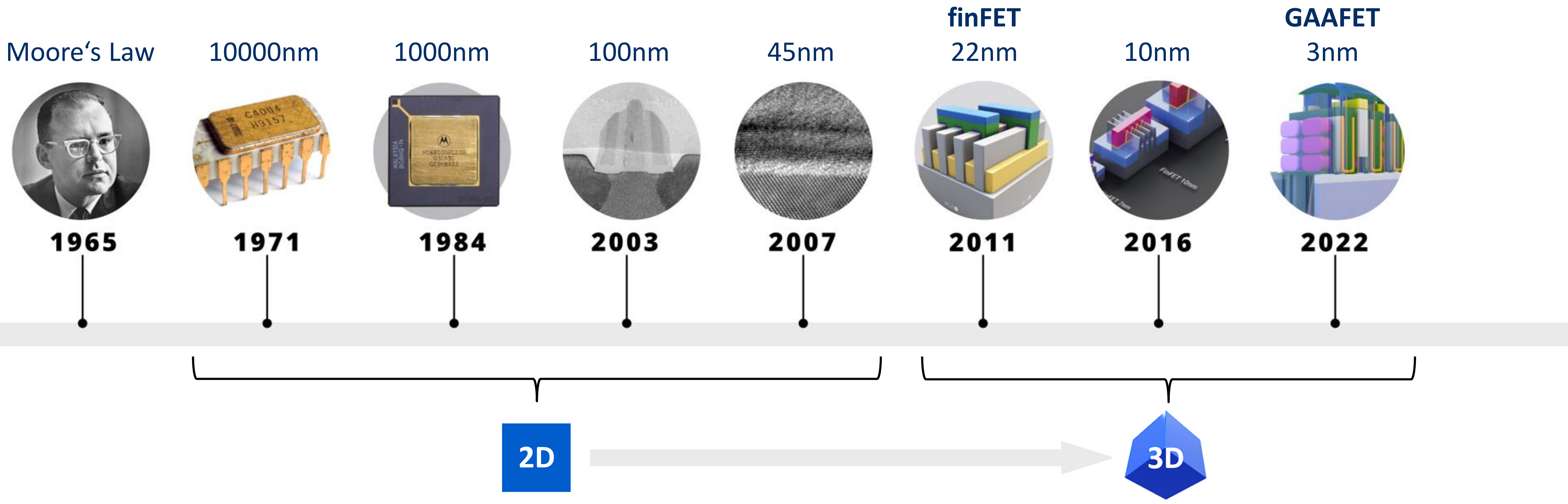
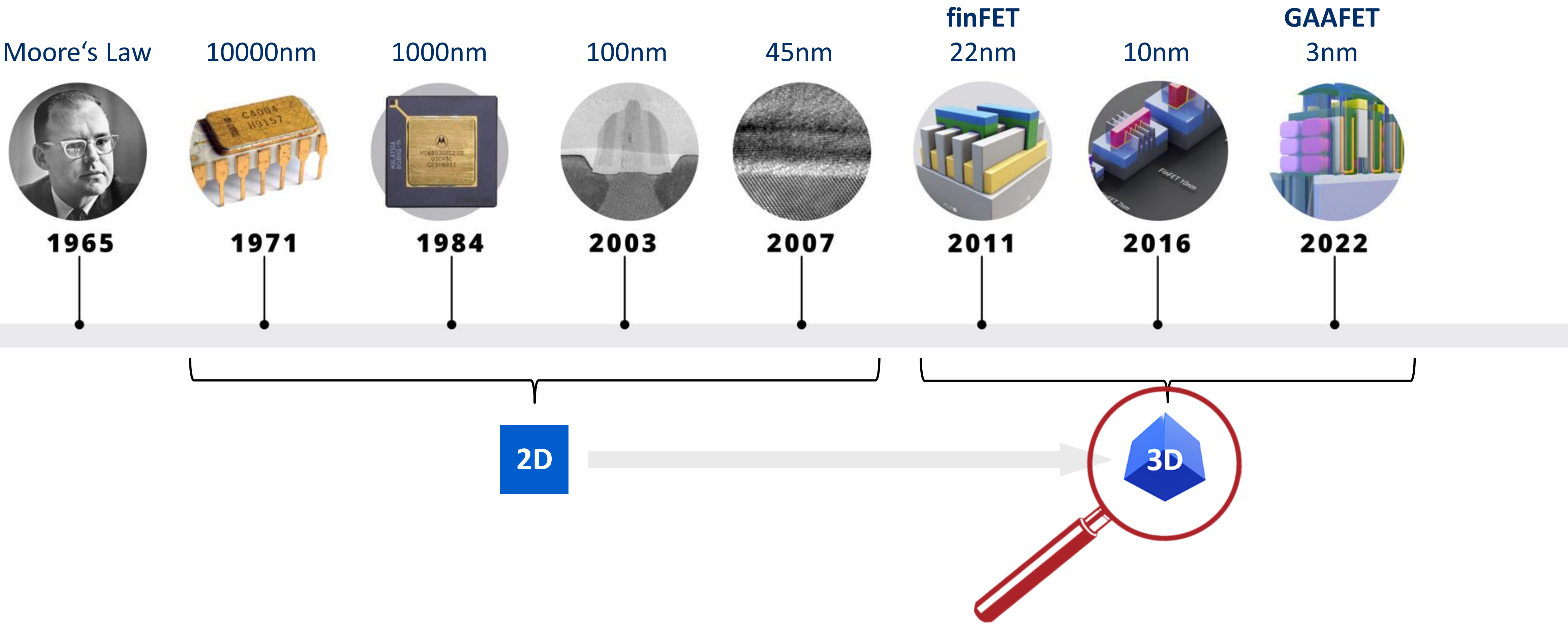
Metrology of modern tech



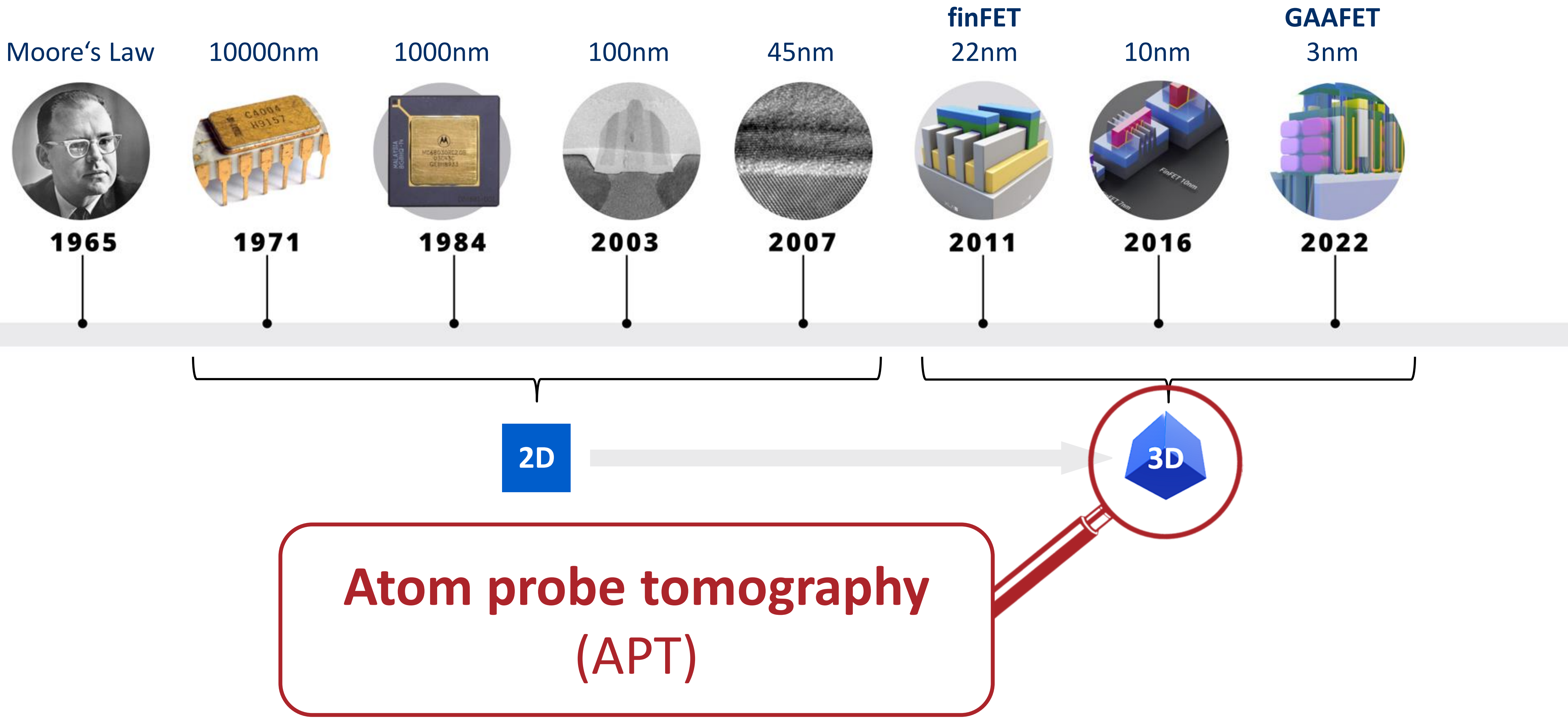
Metrology of modern tech



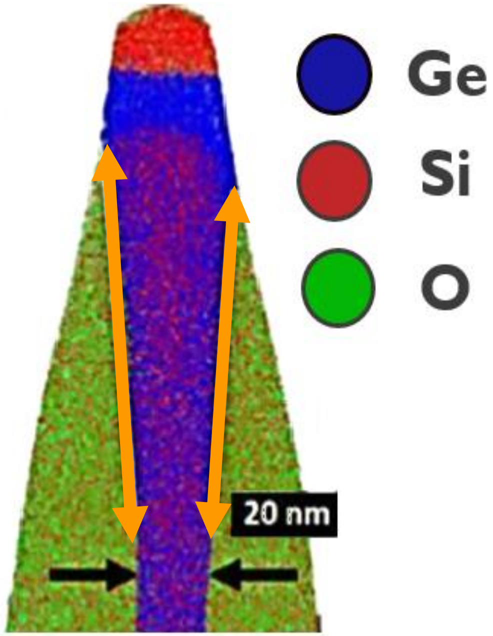
Metrology of modern tech



Metrology of modern tech

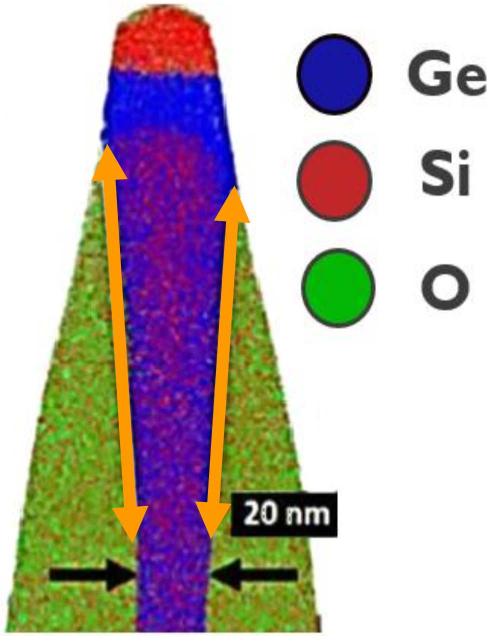


Problem statement



APT

Problem statement



APT

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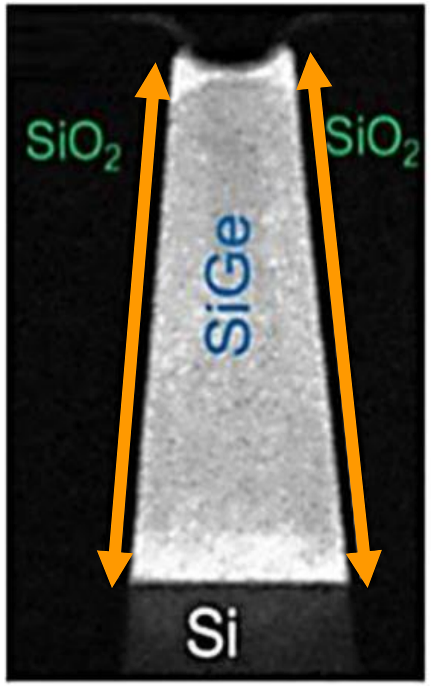
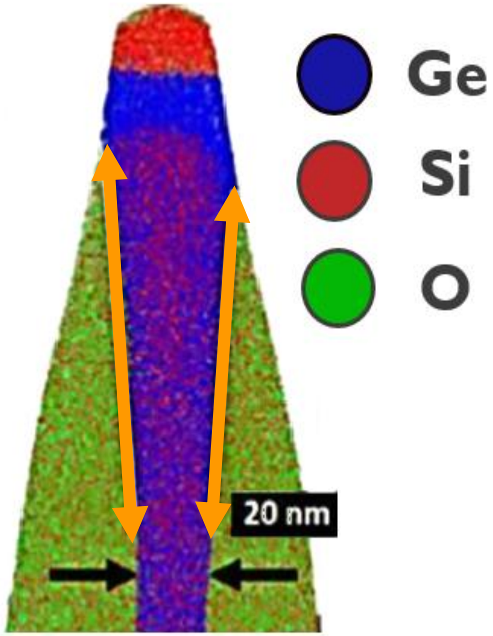


TEM

Problem statement



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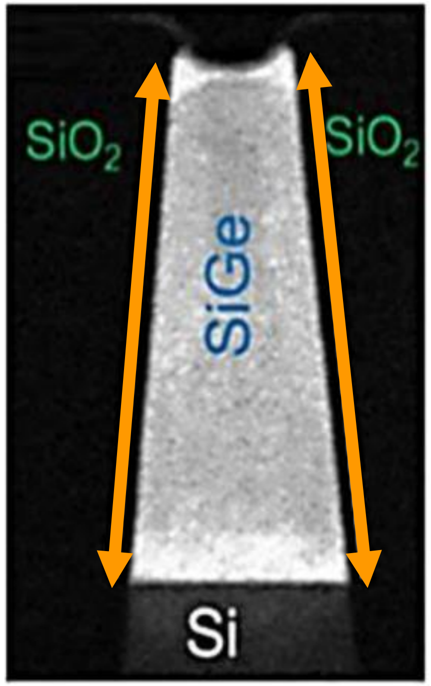
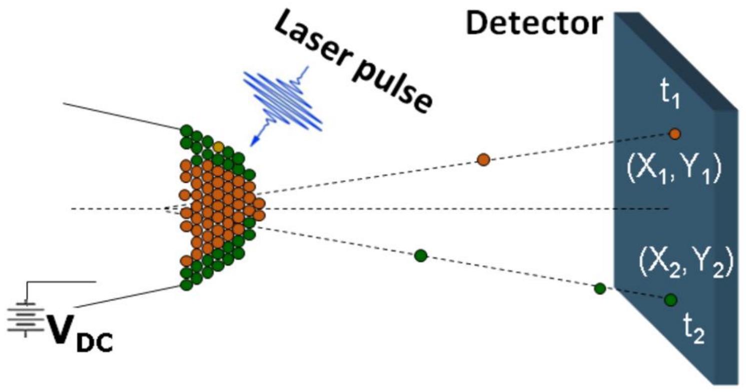


APT

TEM

But why?



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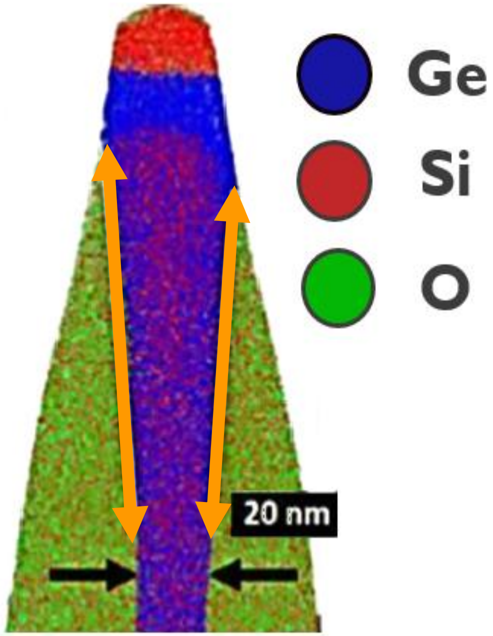

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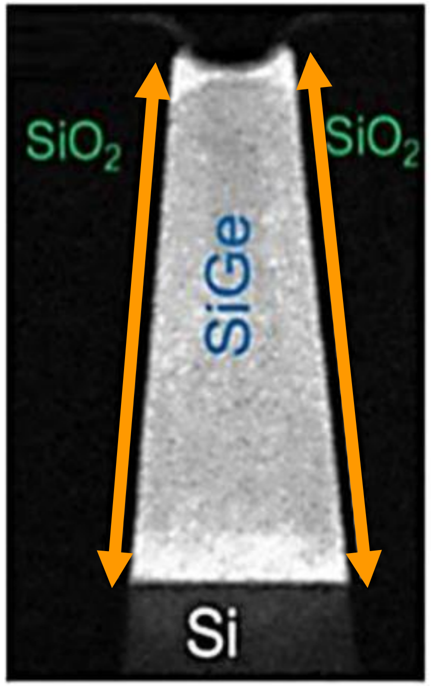

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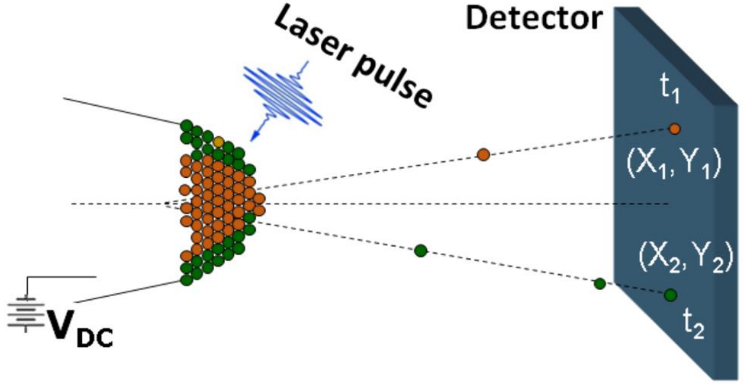

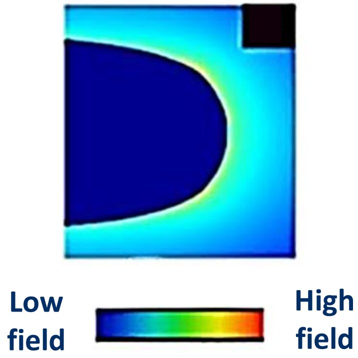

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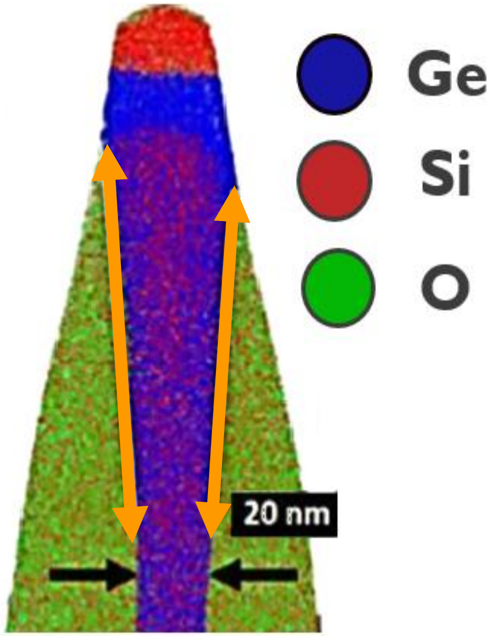

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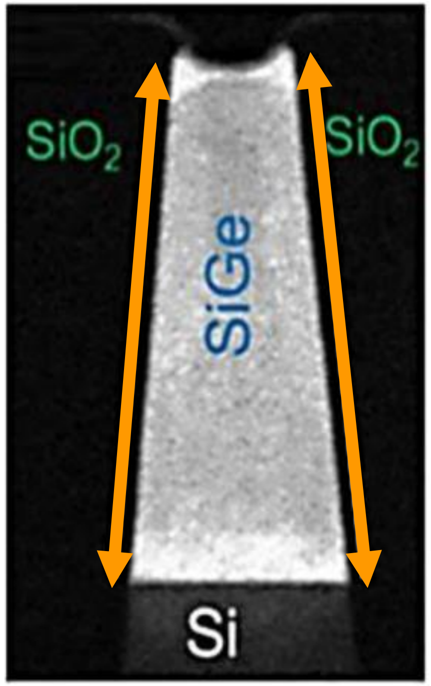

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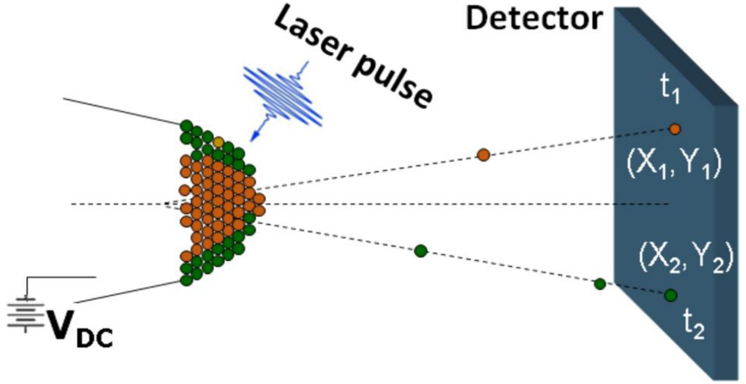
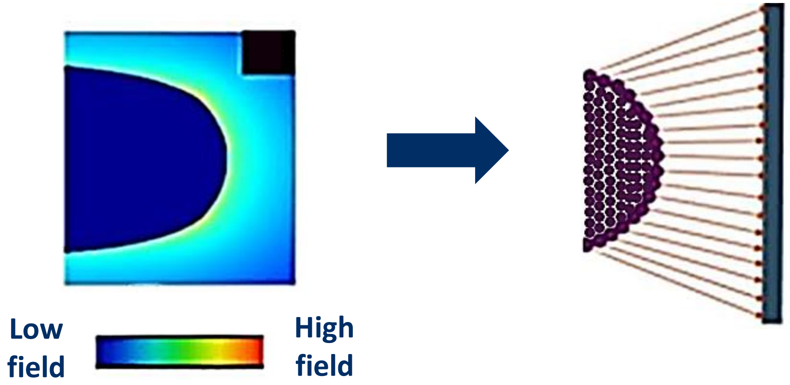
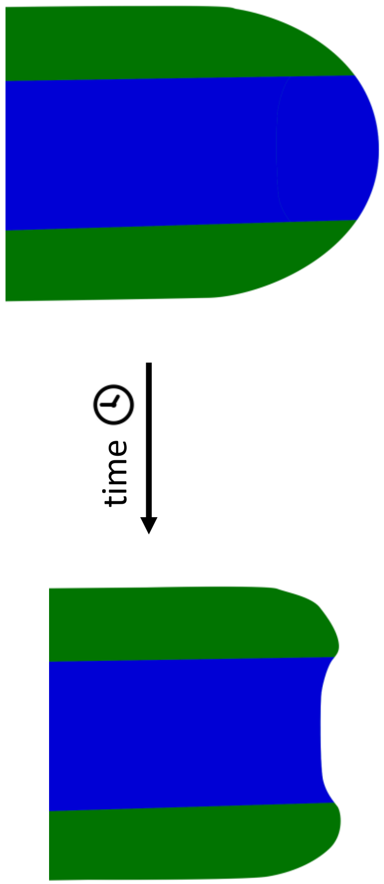




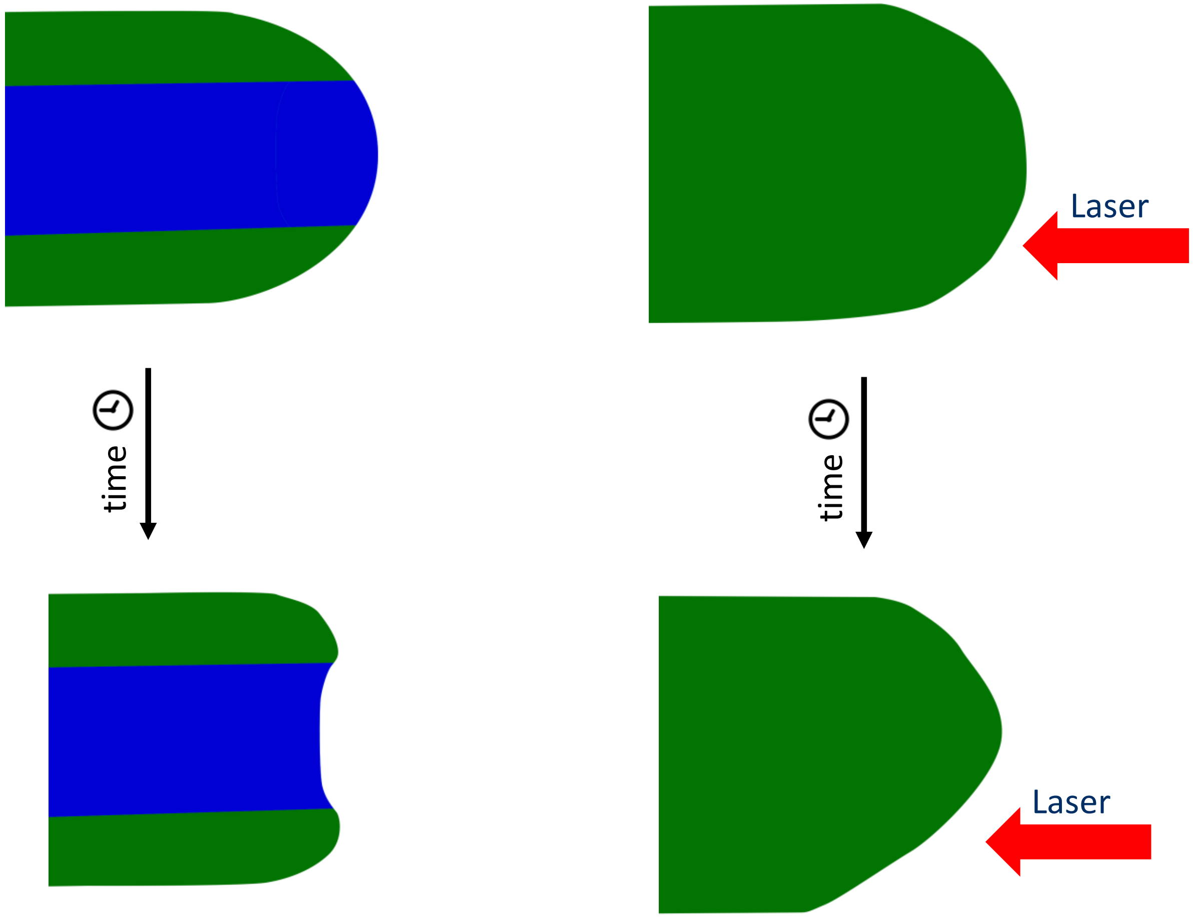
Complex reality of APT

Material effects



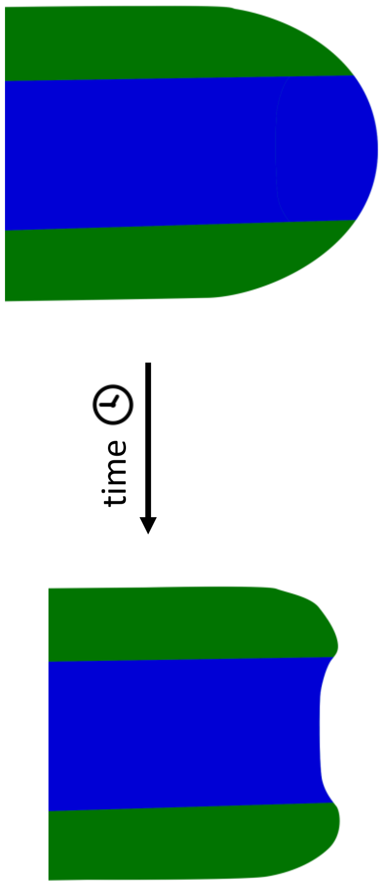
Complex reality of APT

Material effects Laser effects

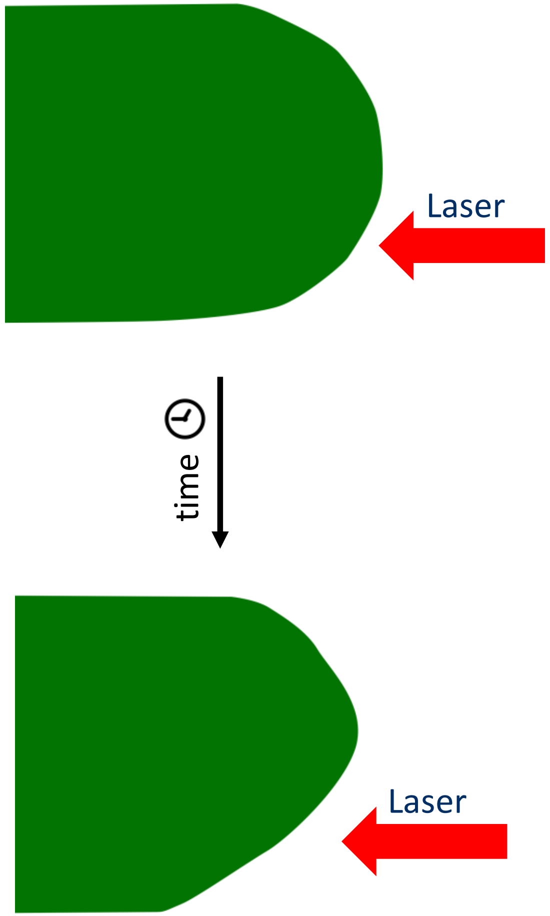


Complex reality of APT

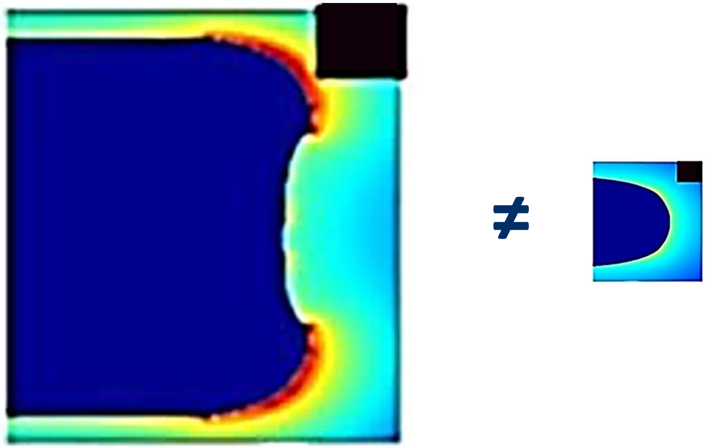
Material effects



Laser effects



Shape affects electric field



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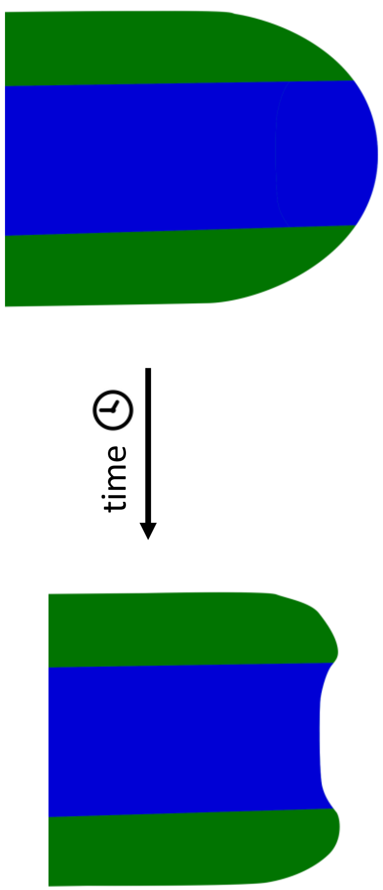
Complex reality of APT

Material effects



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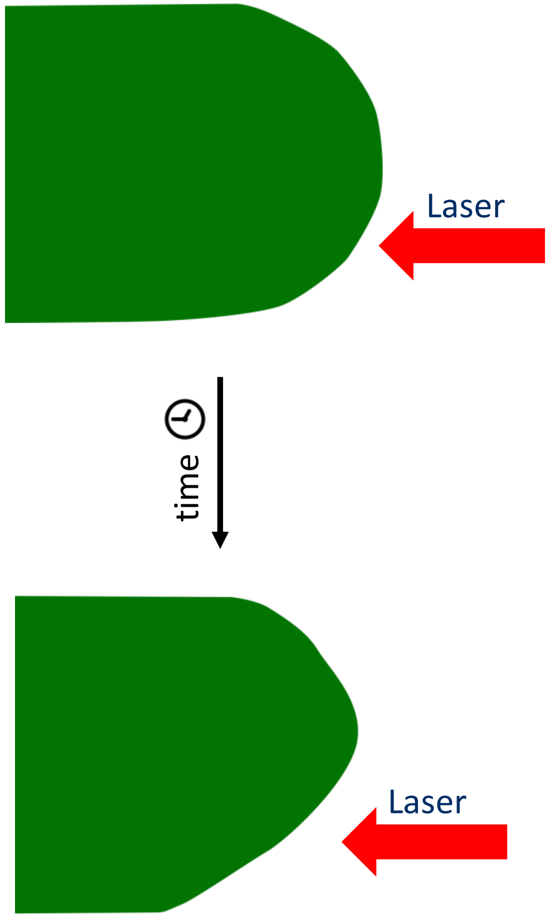

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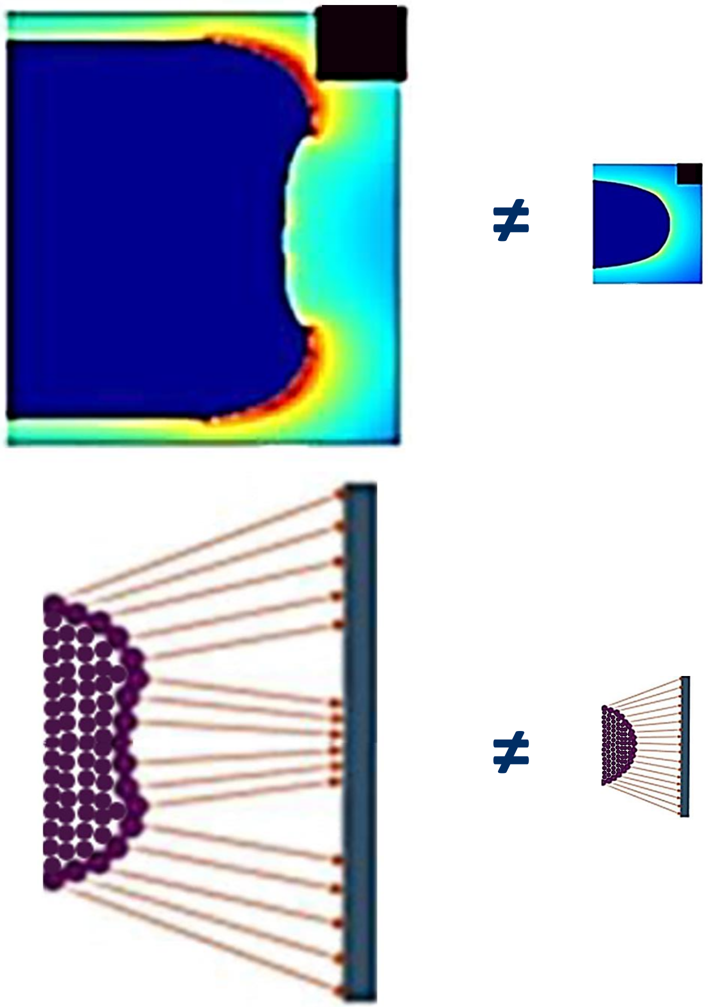
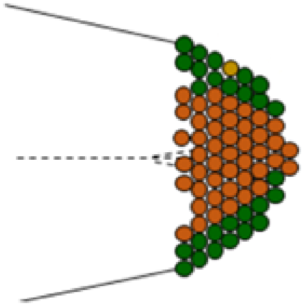


Research aim

What?

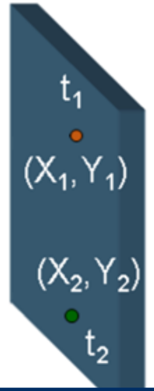
Develop an **accurate** reconstruction model

How?



Step 1
FORWARD OPERATOR

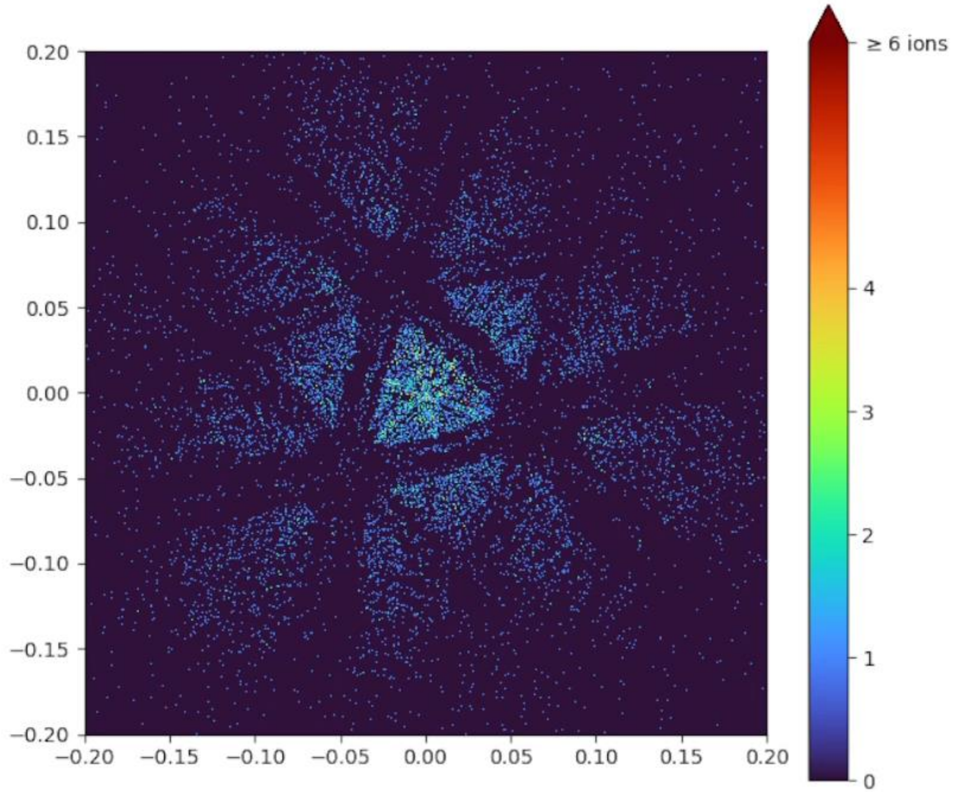
Step 2
RECONSTRUCTION OPERATOR

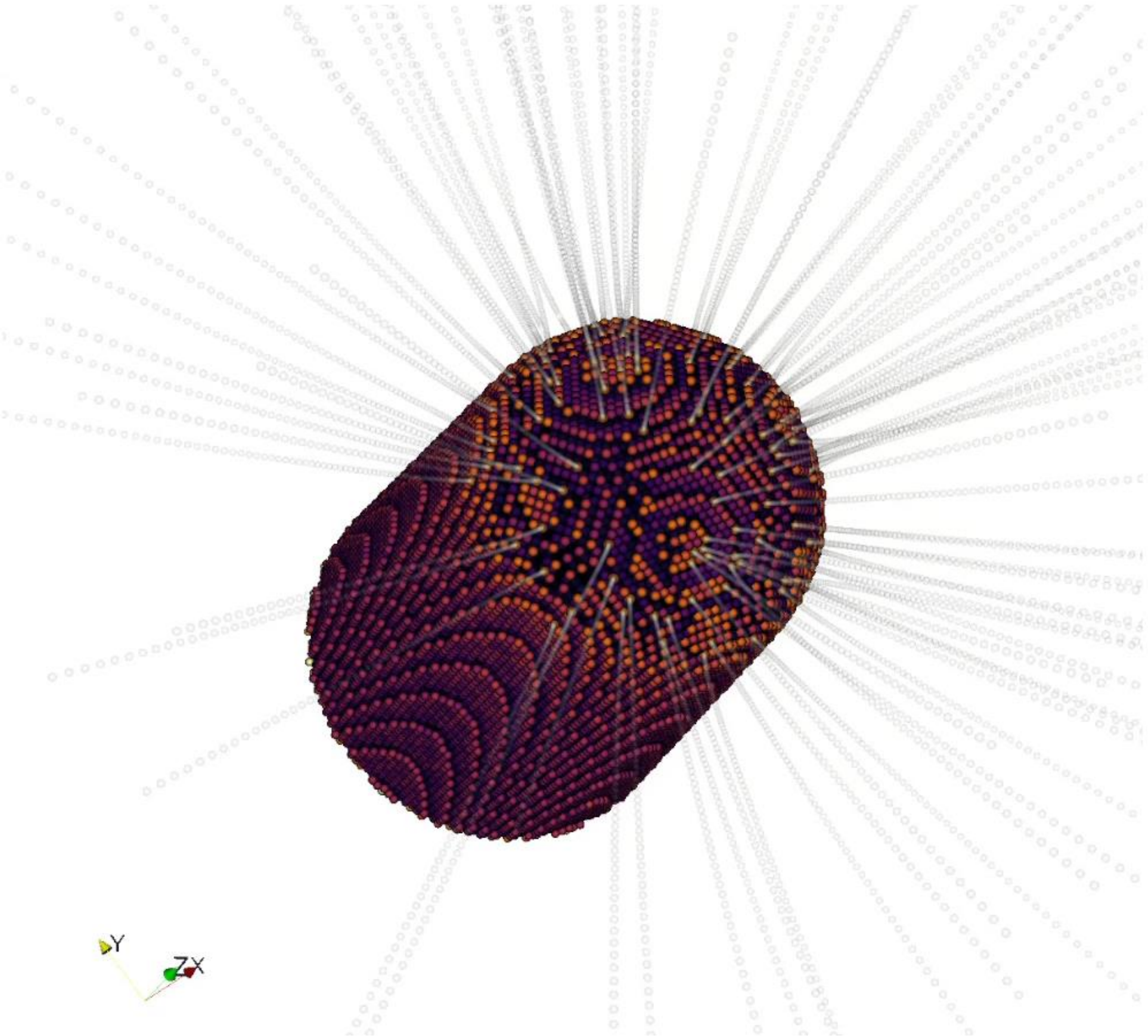


Specimen

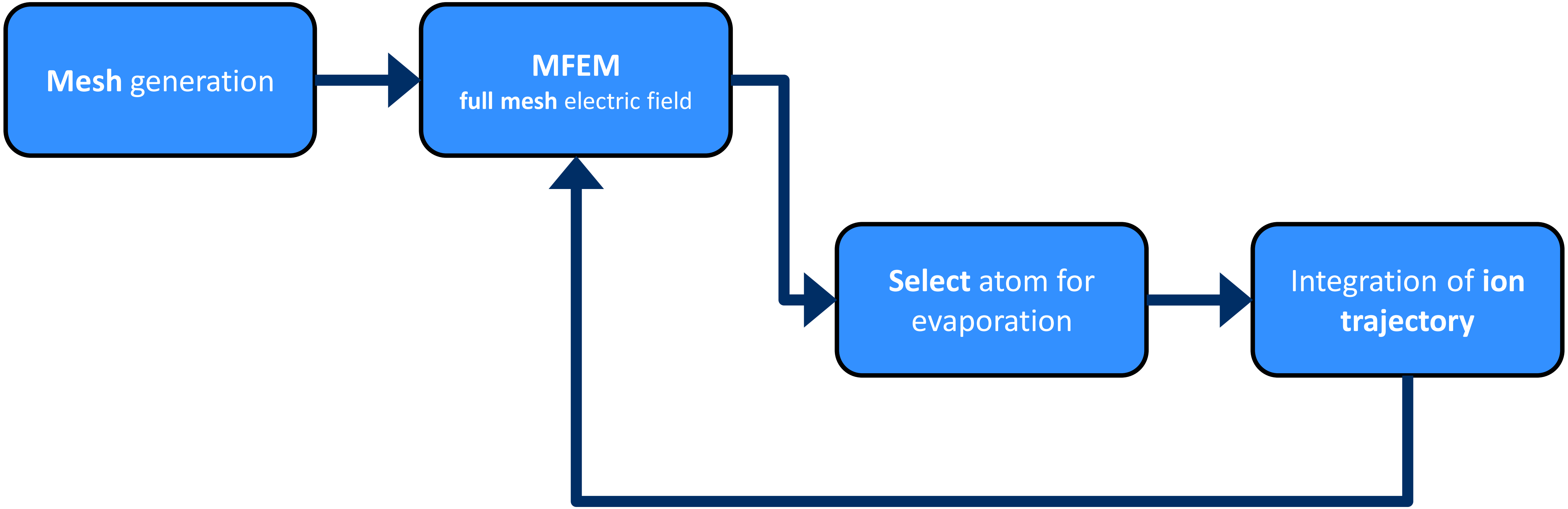
Ions on detector

Forward operator: Atom probe simulation based on FEM





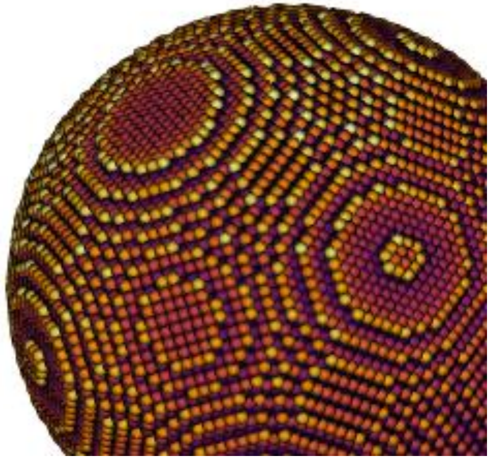
Forward operator: Atom probe simulation based on FEM



Mesh generation

Atom vertices

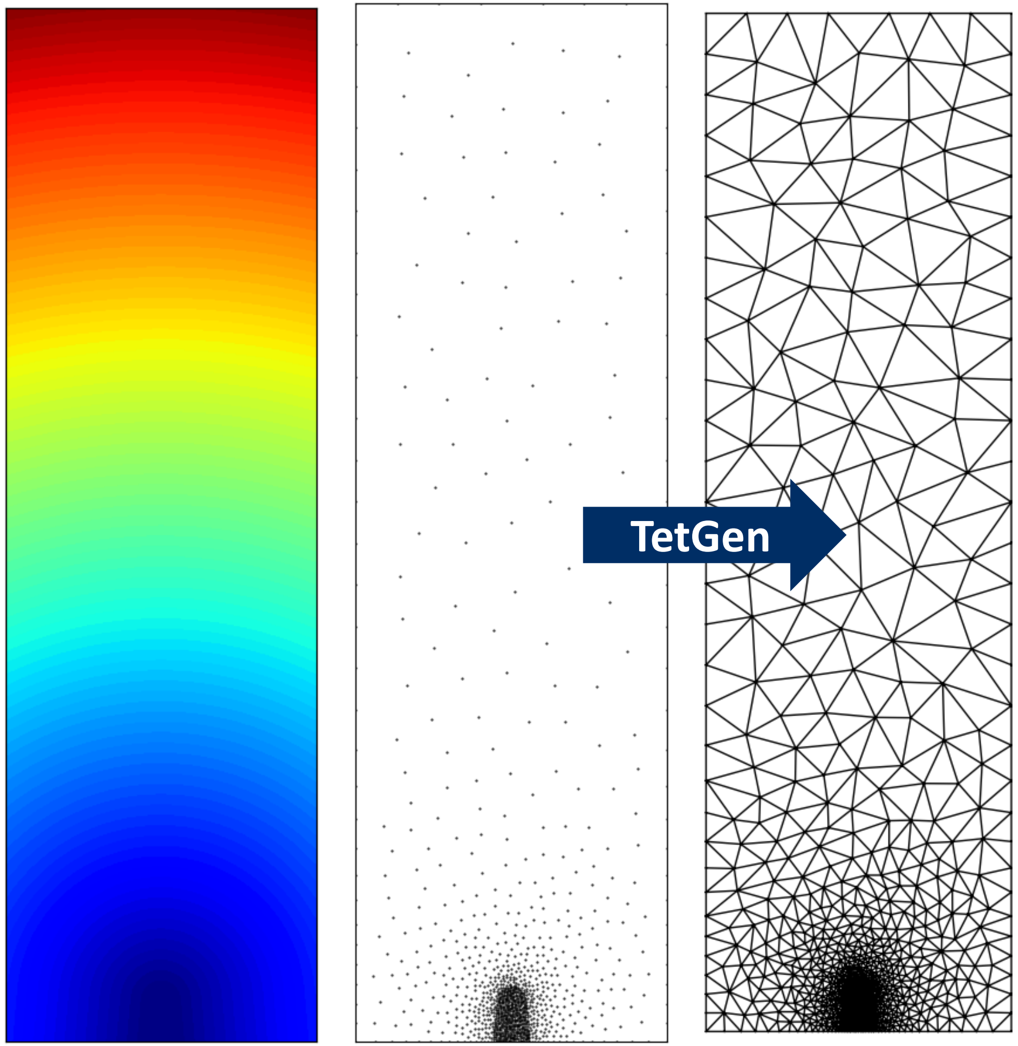
- Specimen size: 10s of nm
- Each atom locus in the specimen is represented by one mesh vertex
- This way we can capture the geometric protrusion of single atoms due to “terraces”



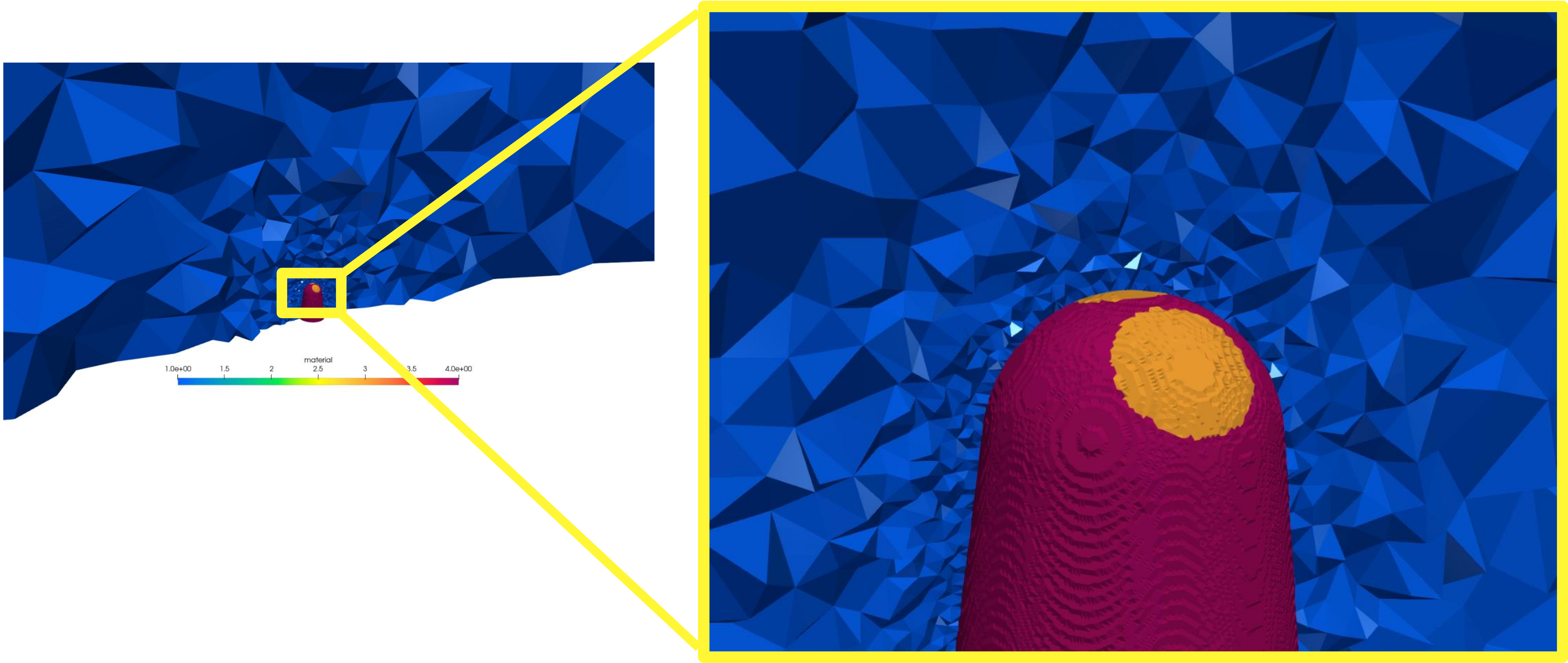
Vacuum vertices

- Vaccum chamber size: ~10cm
- Continuous resolution vertex placement method: “Tree-based variable density Poisson Disk Sampling”

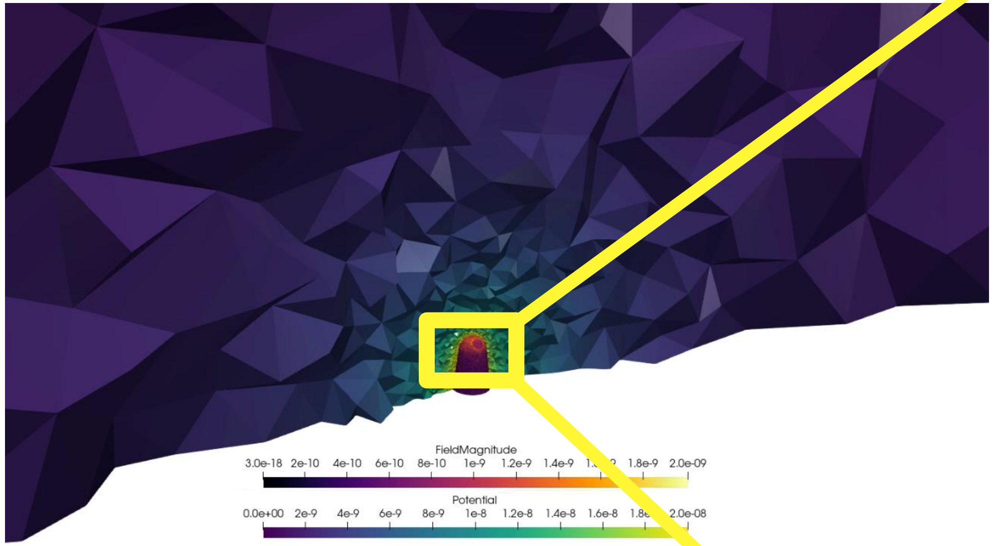
	Relative volume	% of vertices
Vacuum	> 99%	**2%**
Atoms	< 1%	98%



Mesh generation: Variable density Poisson disk sampling



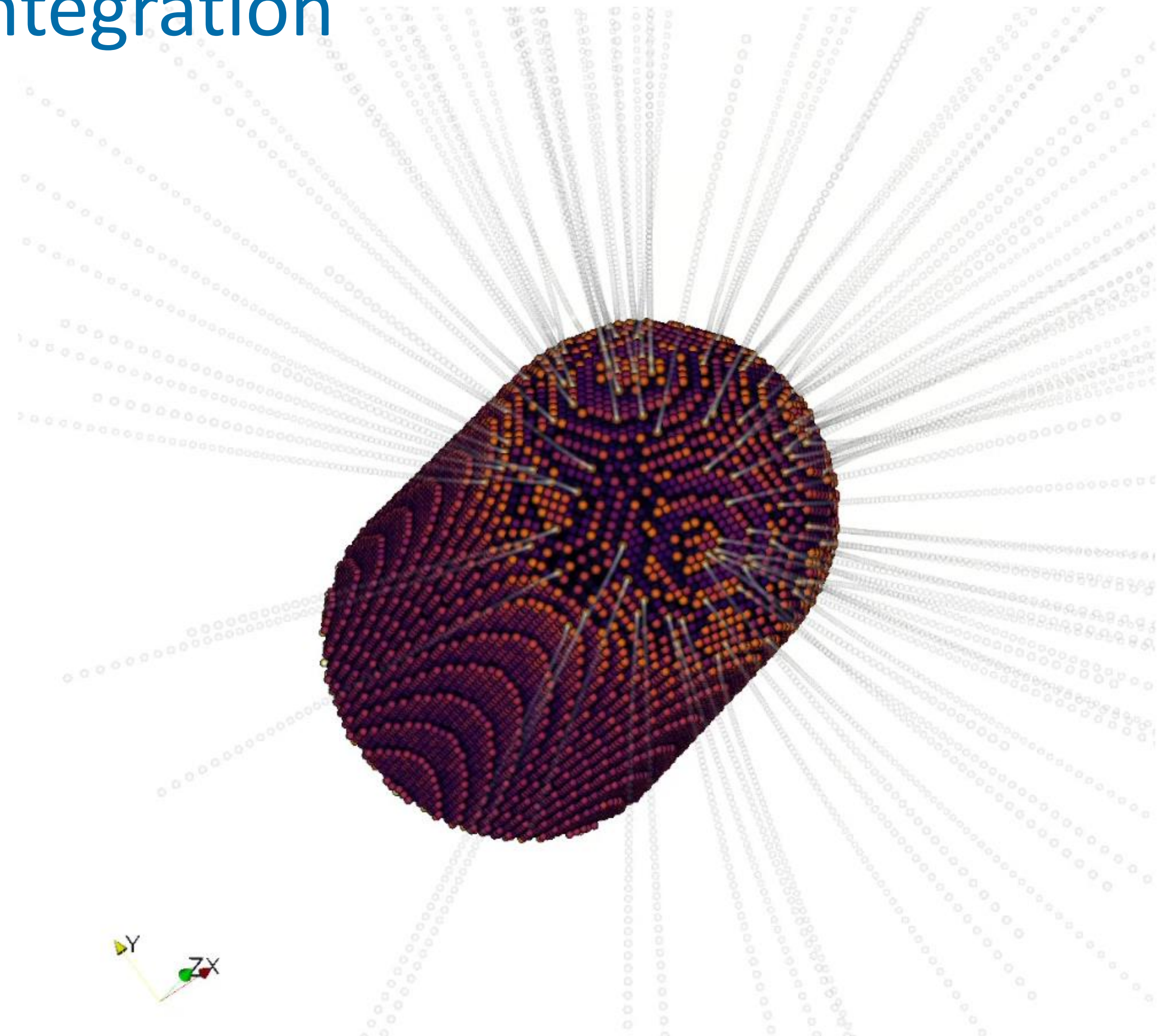
MFEM: Electric field calculation



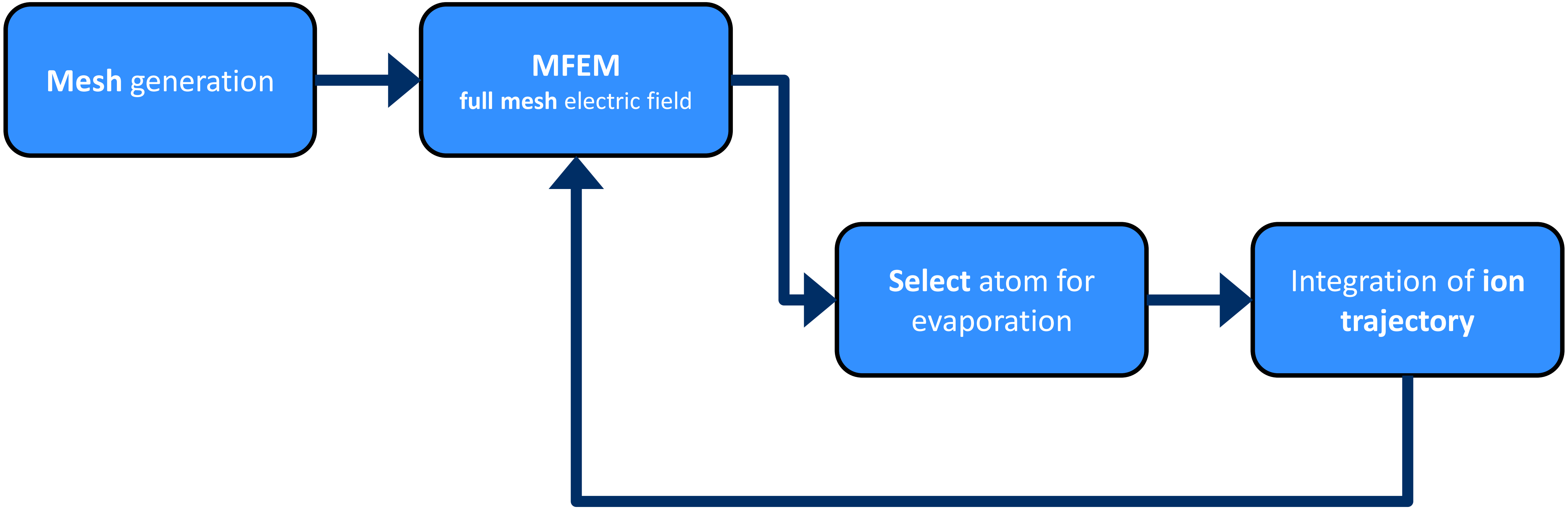
- Potential
  H1 FESpace + **DiffusionIntegrator** + PCG
- Field [= -grad(Potential)]
  H1 FESpace + **DerivativeIntegrator** + PCG
  (Want to know field **at vertex locations**)

Selection and trajectory integration

- Forward Euler
- **Variable** time steps



Forward operator: Atom probe simulation based on FEM



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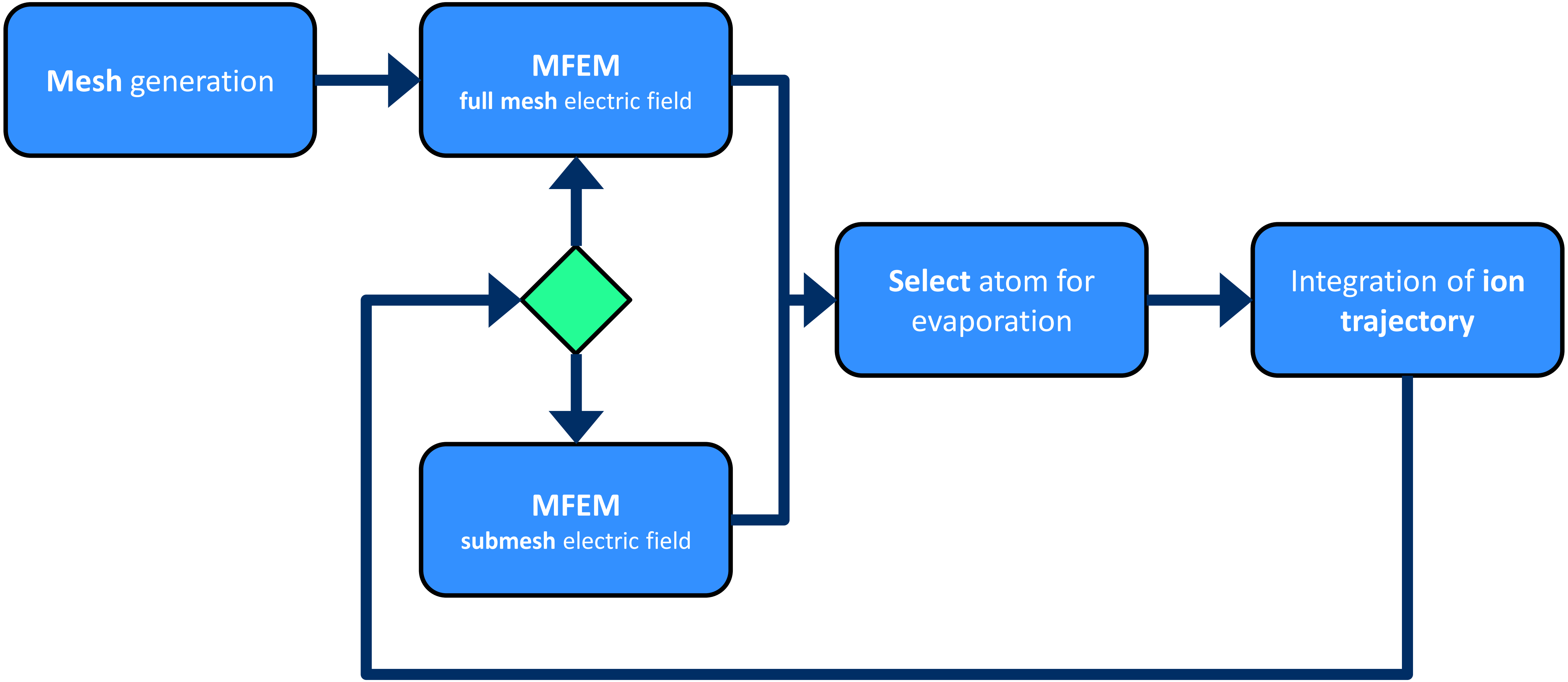
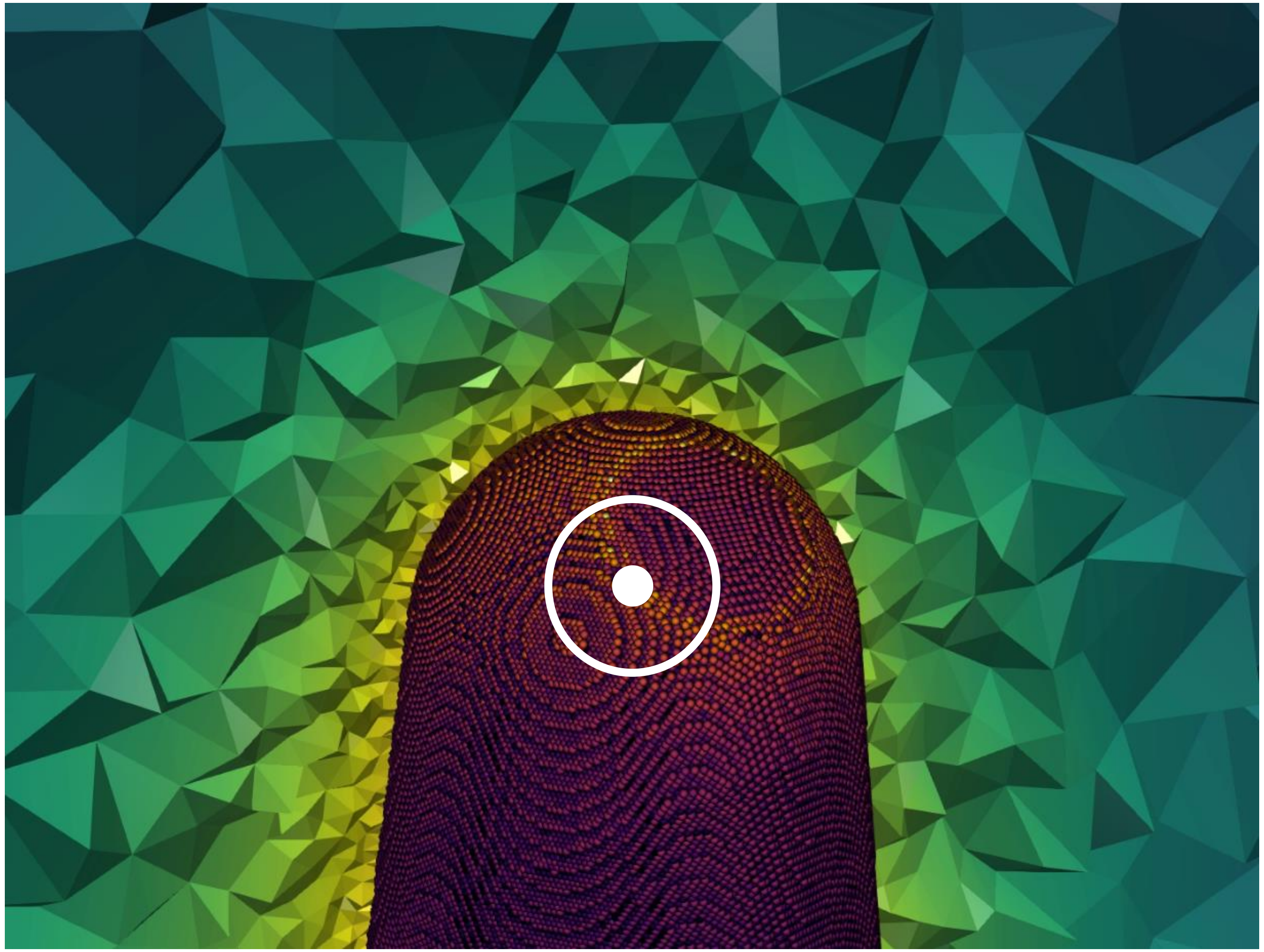
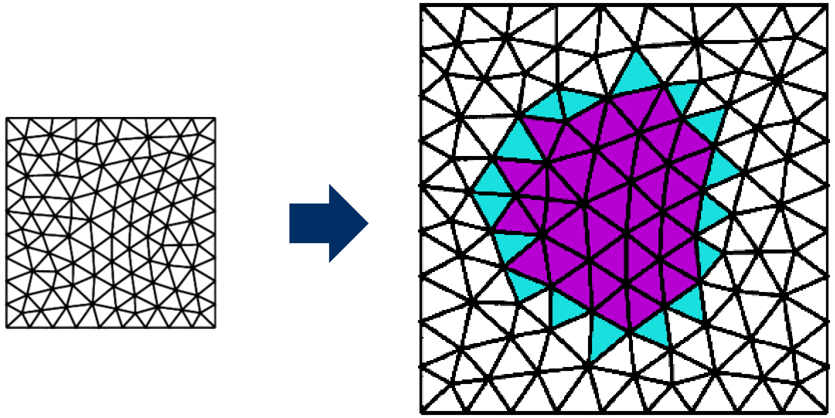
Forward operator: Atom probe simulation based on FEM



Submesh iterations



- Evaporation **changes** the electric field
- This change only occurs **close** to the evaporation site

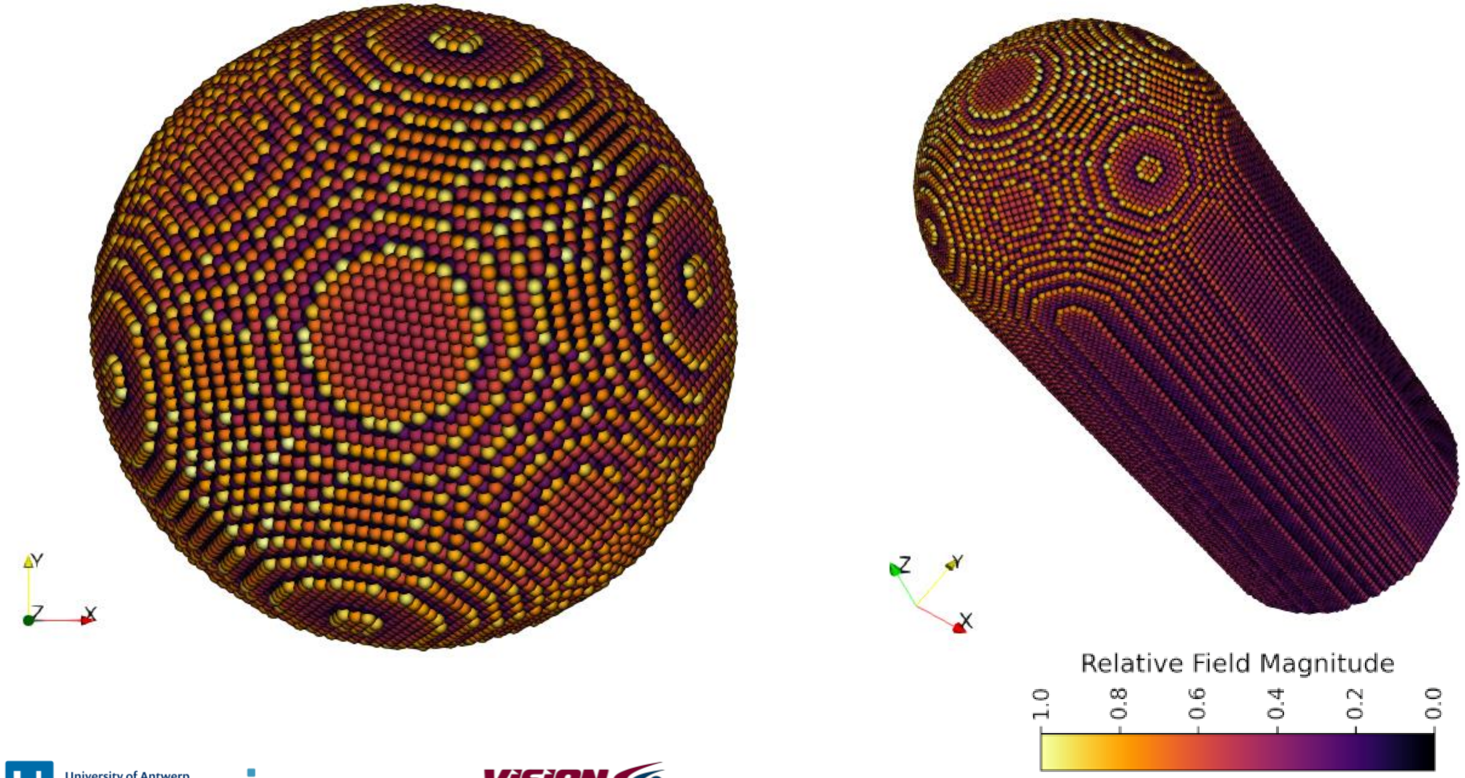


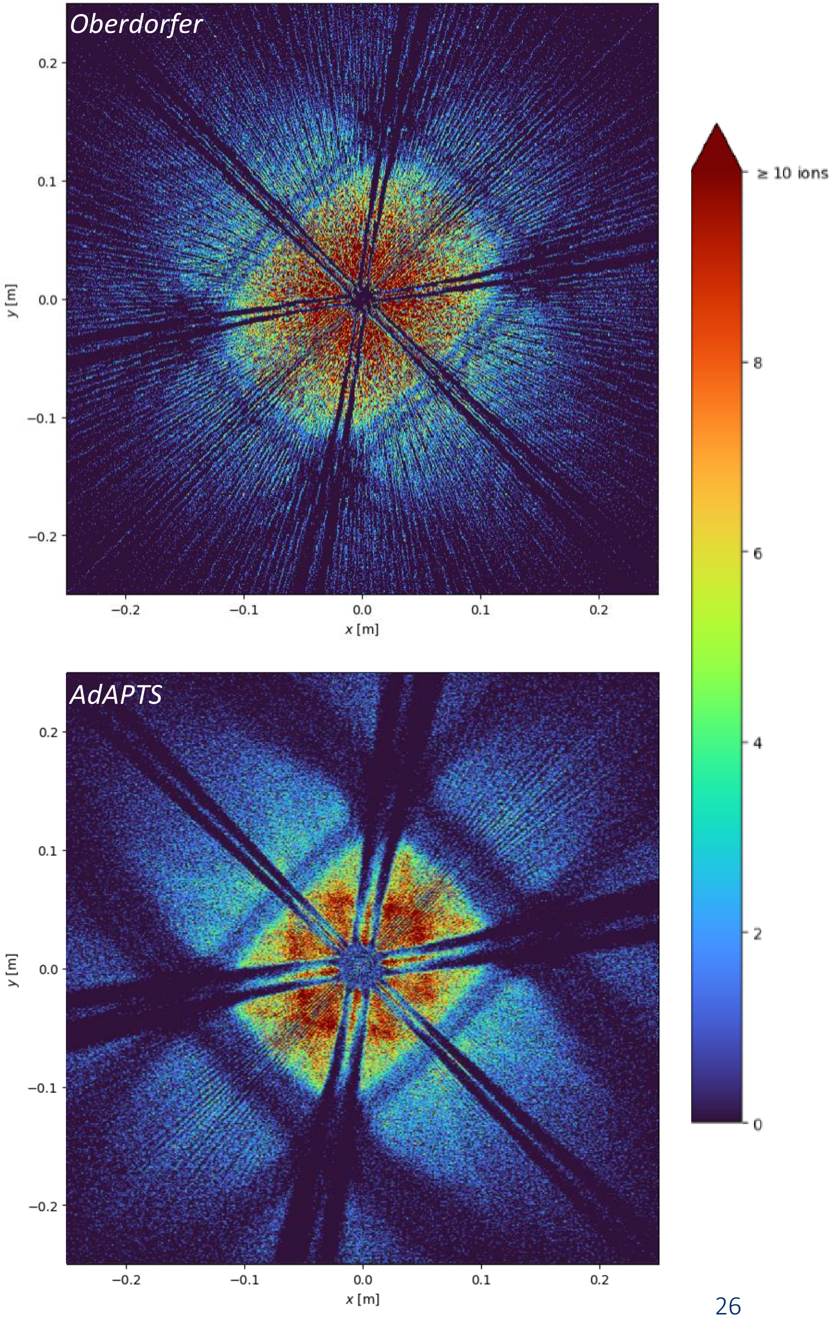
Comparison to Oberdorfer *et al.*

Tool	Time
Oberdorfer	6h 18min
AdAPTS (ours)	1h 20min

Almost

5x as fast





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Thank you for your attention

More questions? **julian.luken@uantwerpen.be**

References

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