An Efficient Atomistic Method for Micro-Scale Film Growth from the Vapor Phase

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Computational physicist: Algorithms for classical process simulations

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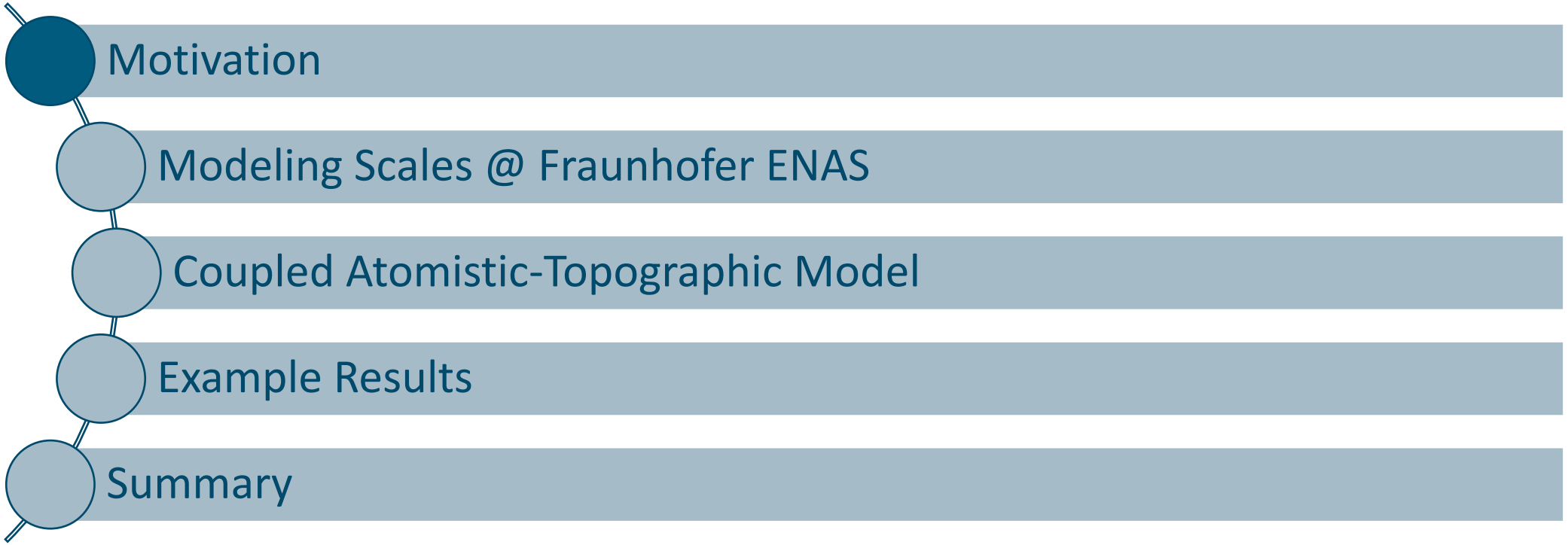
Outline



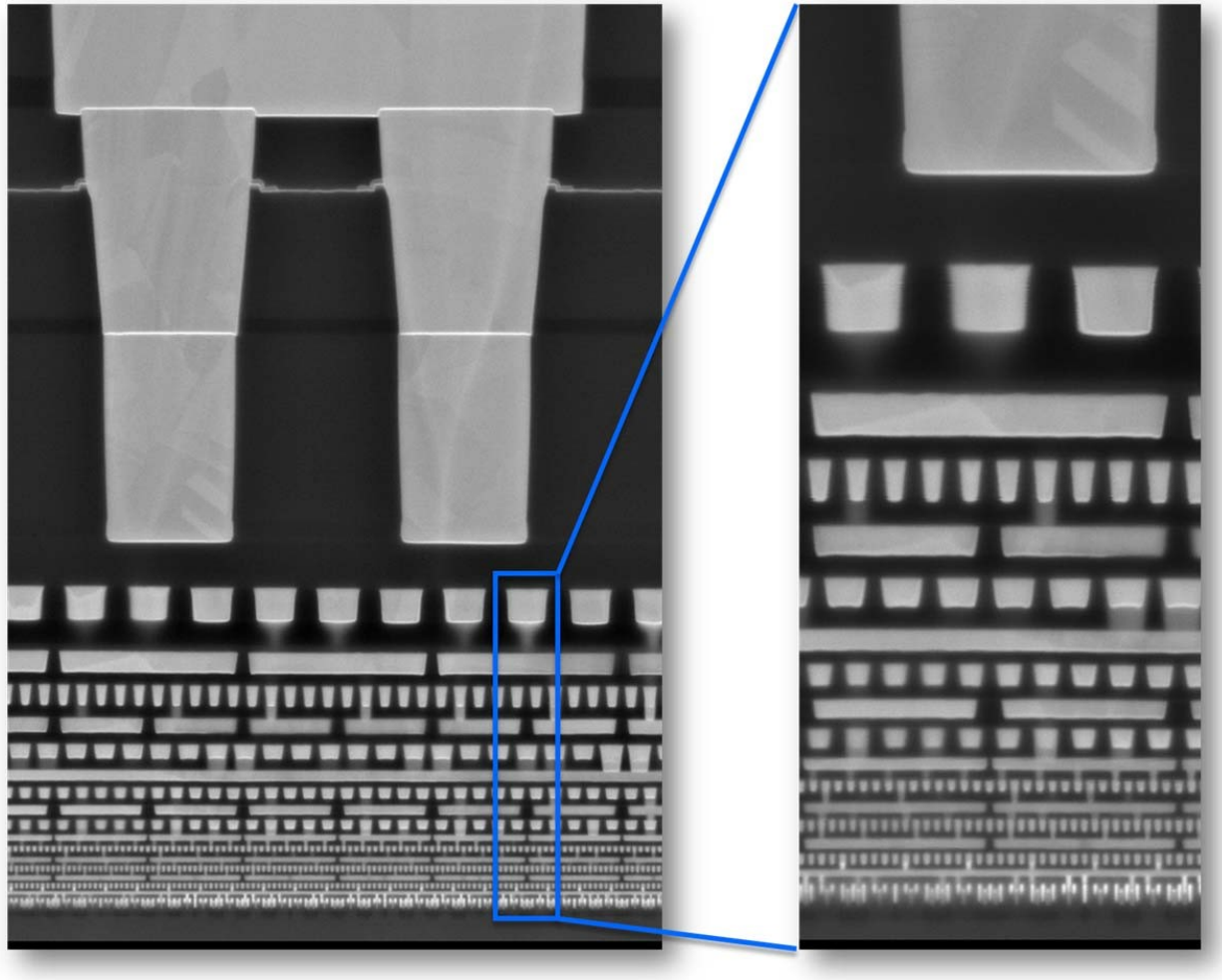
Motivation

Atomistic Thin Film Growth

- Semiconductor applications
  - Traditional devices → already at nm scale
  - Emergence of neuromorphic devices, quantum devices, and wearables
- Continuum theories don’t hold anymore

Goal

- Process optimization with respect to growing films
- Atomistically resolved film morphology, topography, composition
- Processes: PVD, CVD, ALD, ALE



Cross-section of Intel4 BEOL structure
[Intel, 2022, 10.1109/VLSITechnologyandCir46769.2022.9830194]

Simulation of Processes, Materials, and Devices for Micro- and Nanoelectronics

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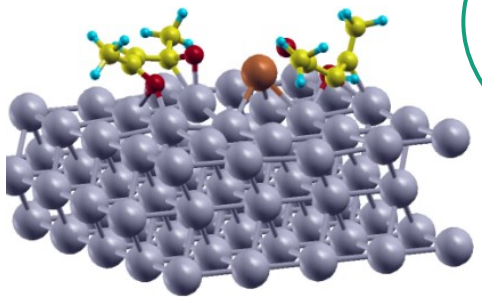
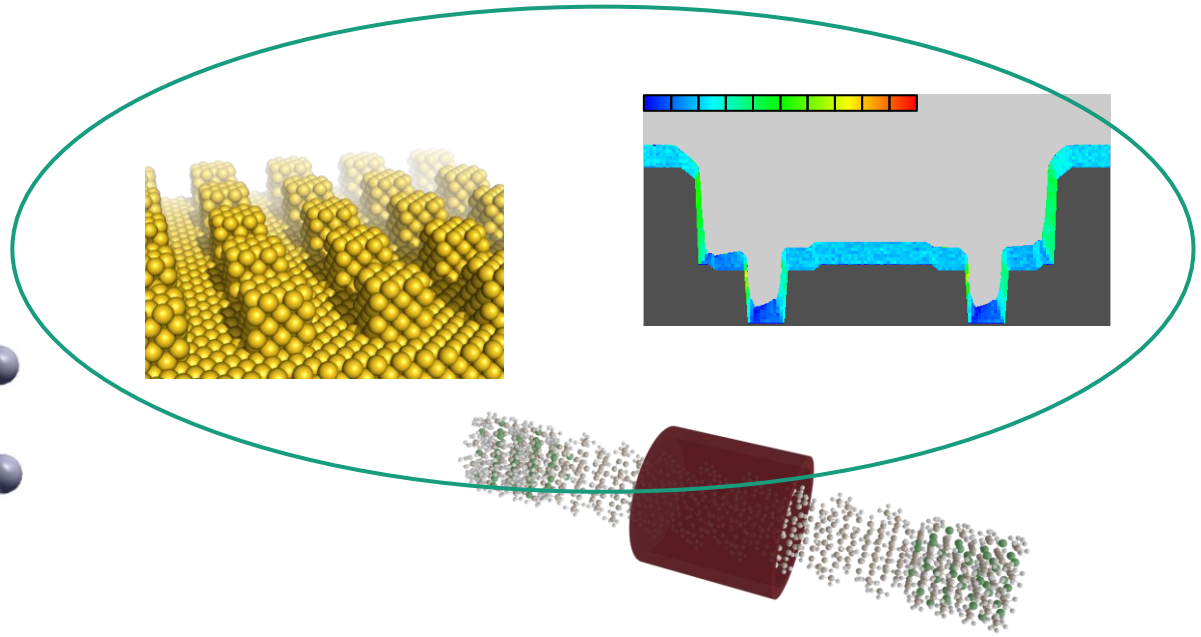
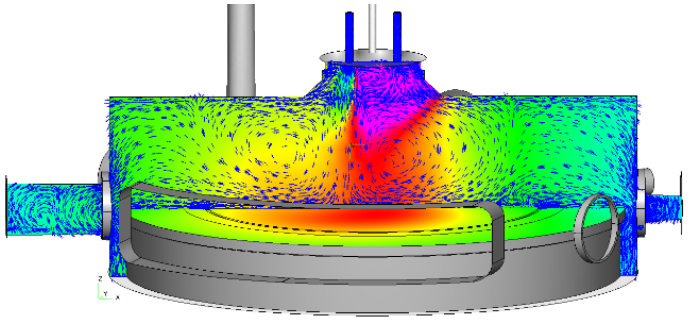




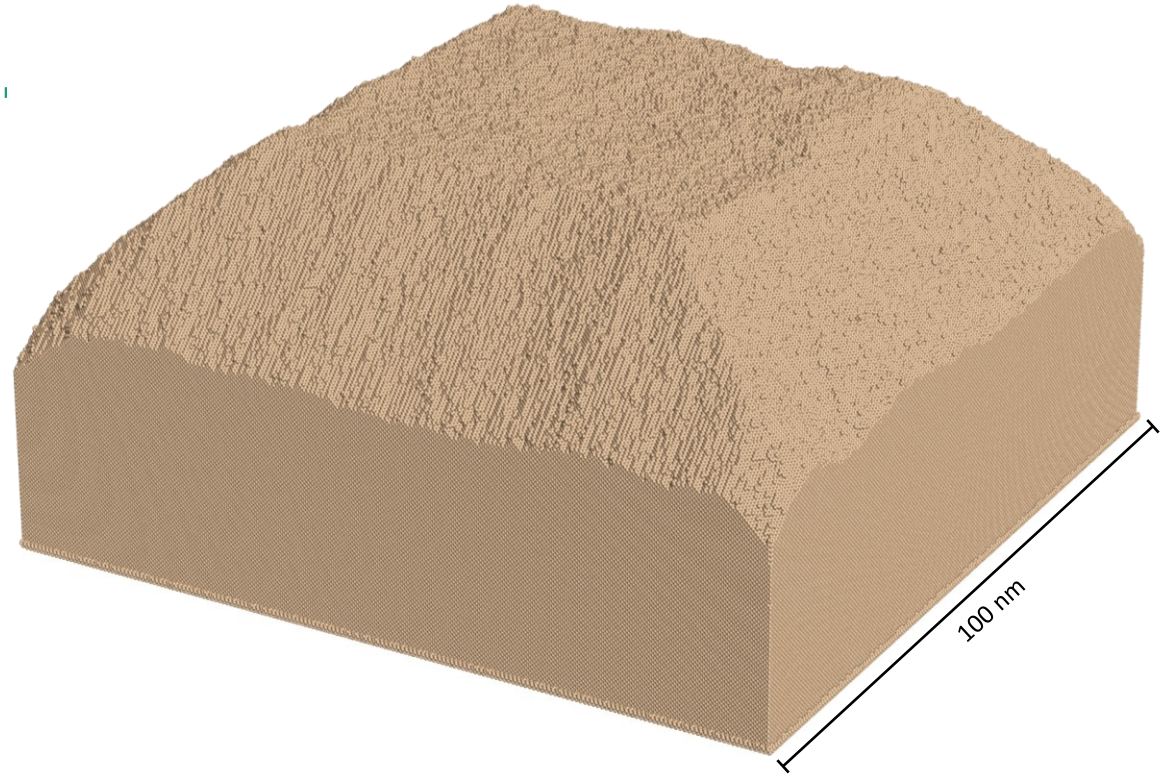


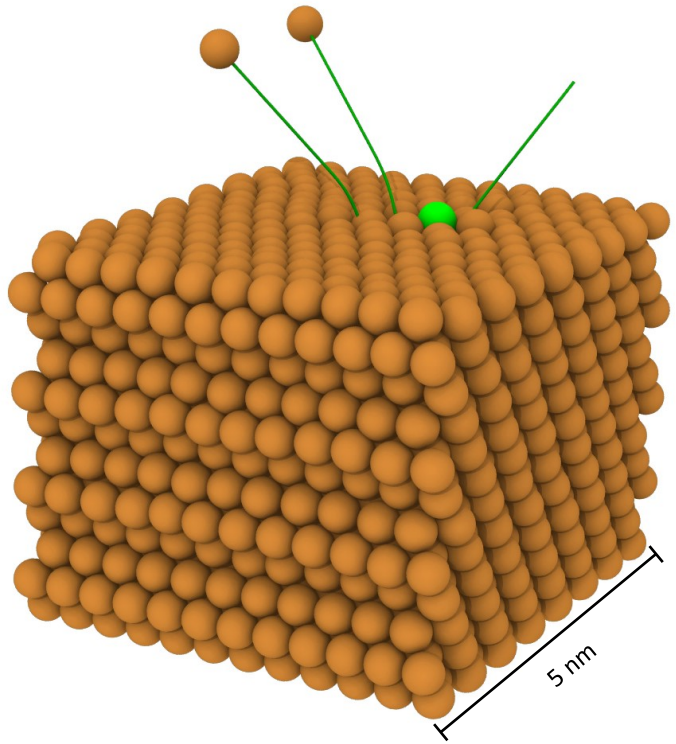
Nano (nm)
- Atoms and molecules
- Surface processes

Intermediate (nm - µm)
- Small features
- Evolving topographies

Macro (mm - m)
- Equipments
- Wafer

Pure classical methods: Kinetic Monte Carlo and Molecular Dynamics





Kinetic Monte Carlo (KMC)

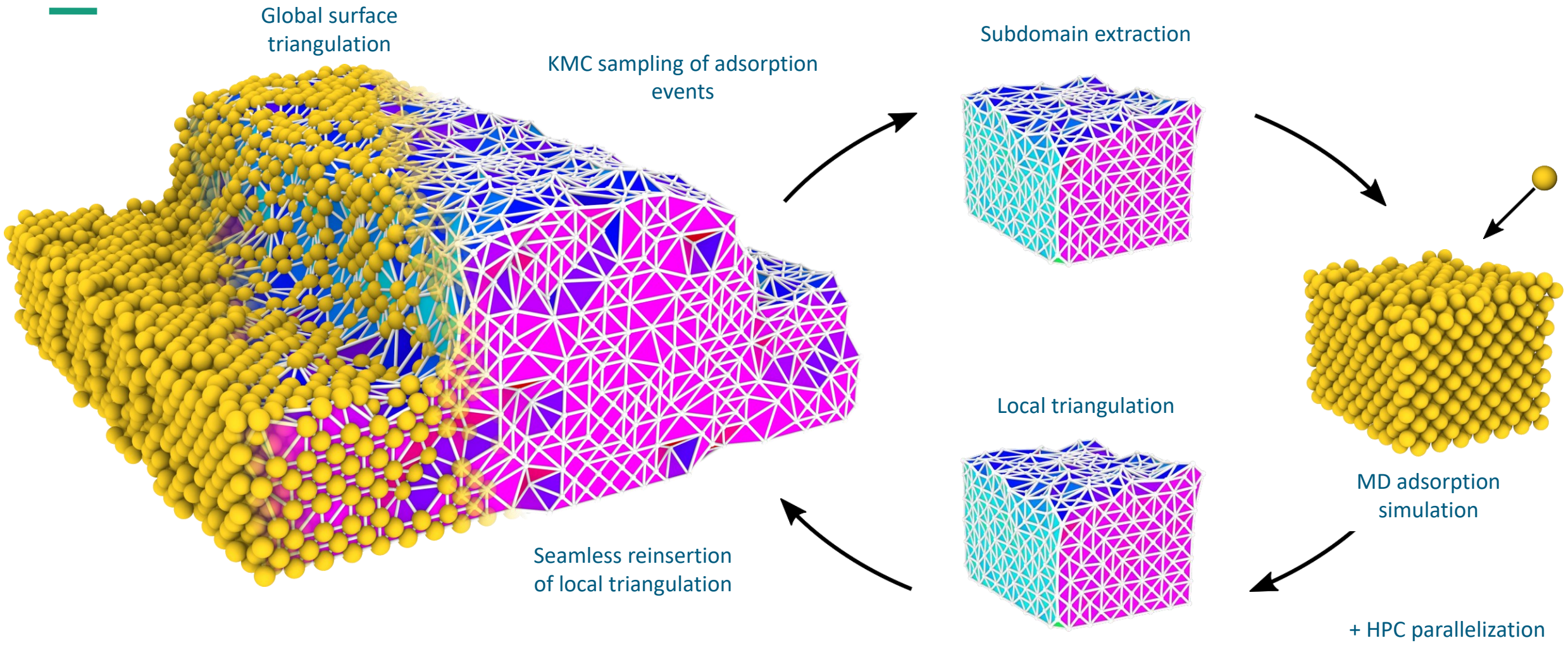
- Transition event sampling
  e.g. single-atom adsorption, diffusion, desorption
- Typically lattice-based, sequential, rigid events

Molecular Dynamics (MD)

- Newtonian motion of atoms in force fields;
  empirical, reactive, MLIP
- Limited to microseconds, or 10^8 atoms

Our method: Coupled KMC+MD through surface triangulations

KMC for event sampling, MD for adsorption simulation



Requirements for Coupling Method

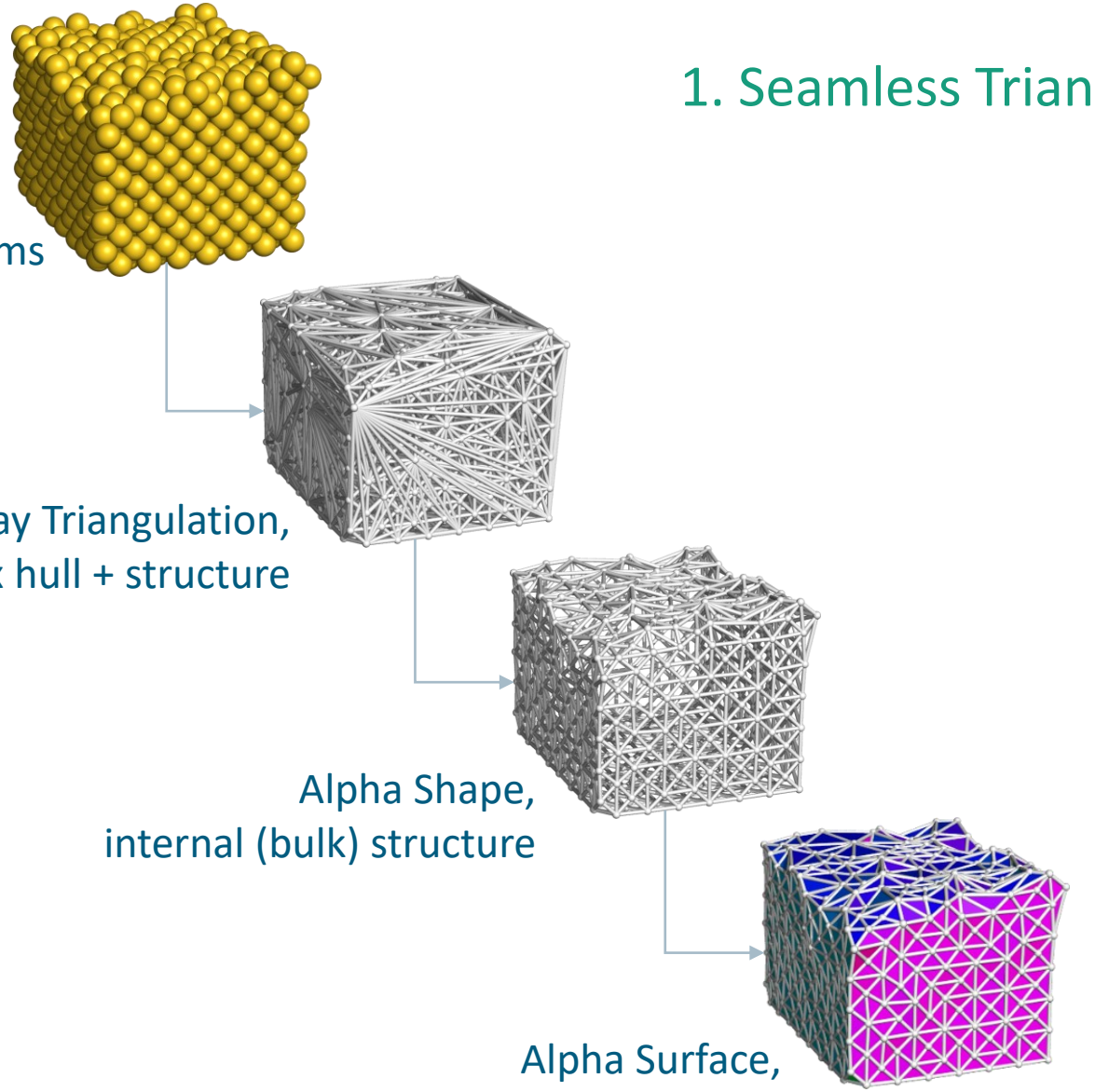
1. Seamless Triangulation

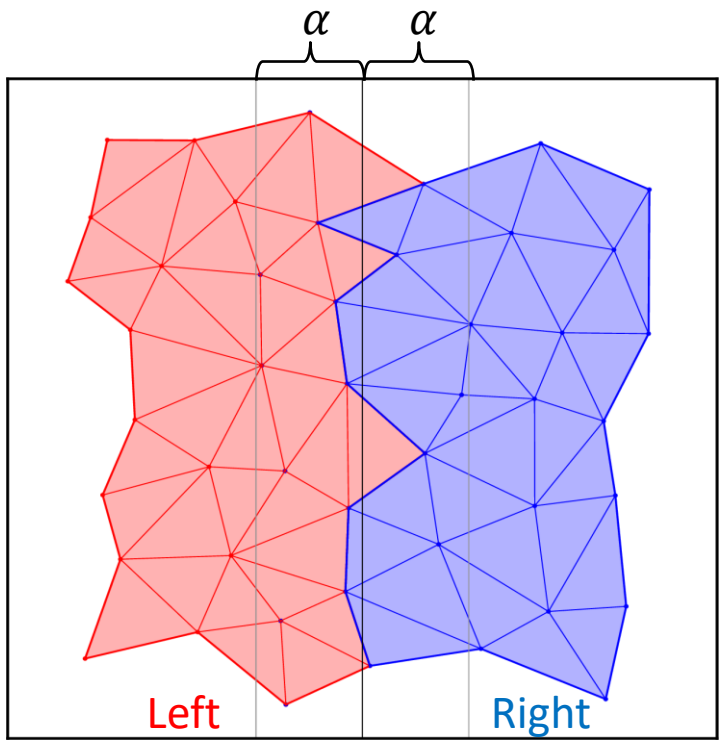
- Concave hull
- Internal triangulation
- Update-able on closed, convex subdomains

2. Fast KMC

- Arbitrary event indices
- Floating-point event rates
- Large number of dependent (thus eventually invalidated) events in MD range
- Target: 1 µs per event, for 10^8 indexed events

1. Seamless Triangulation



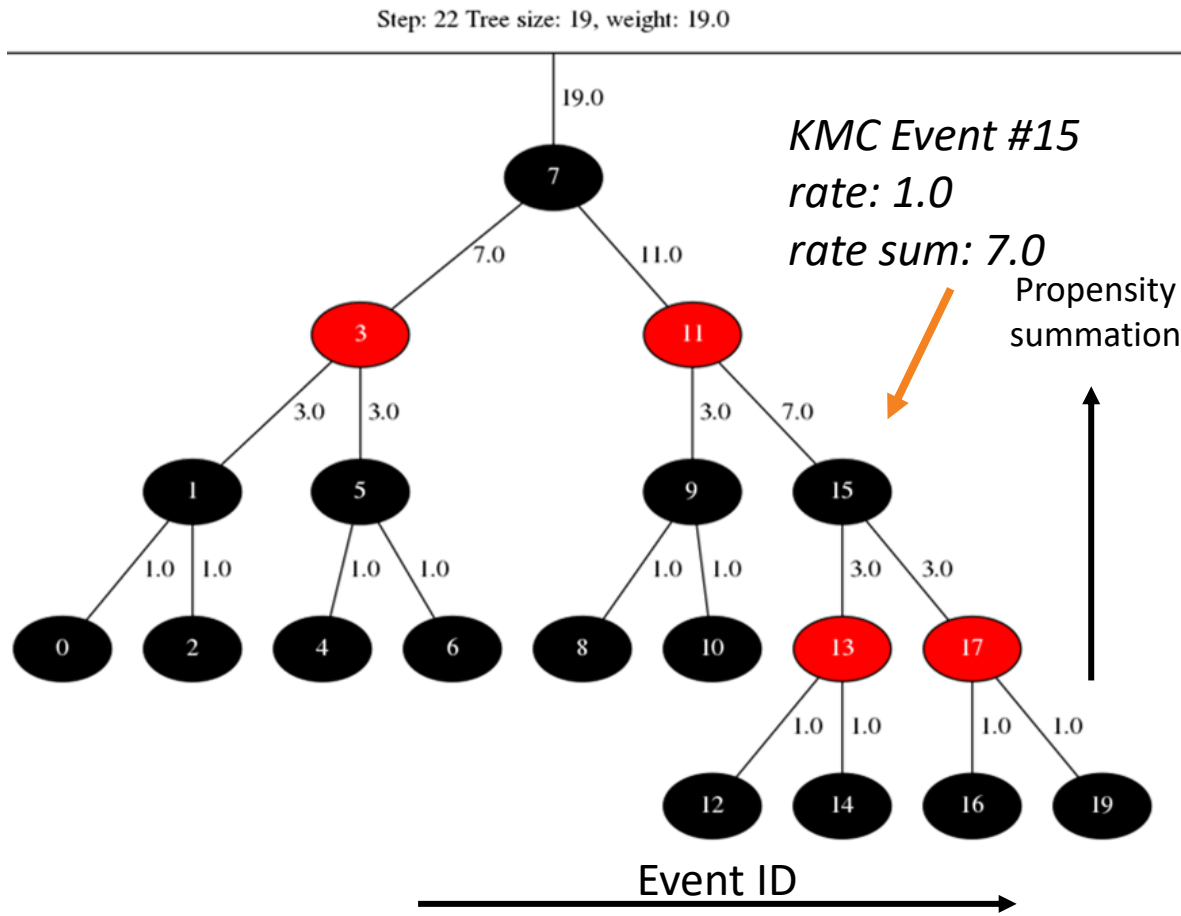


Seamless, stitchless, unique triangulation through 2α overlap and attribution criterion

Result: Trivially parallelizable bulk/surface triangulation

Integrated indexing-summation datastructure

- Common datastructure (red black tree) with dual representation (ID and Rate)
- Arbitrary event rates and indices
- Support for bulk insertion/deletion of neighboring events
- **Direct Method KMC**
  → No log-calculation overhead for dependent events



Of course, There's no free lunch. Ask me about the drawbacks during Q&A or the coffee break

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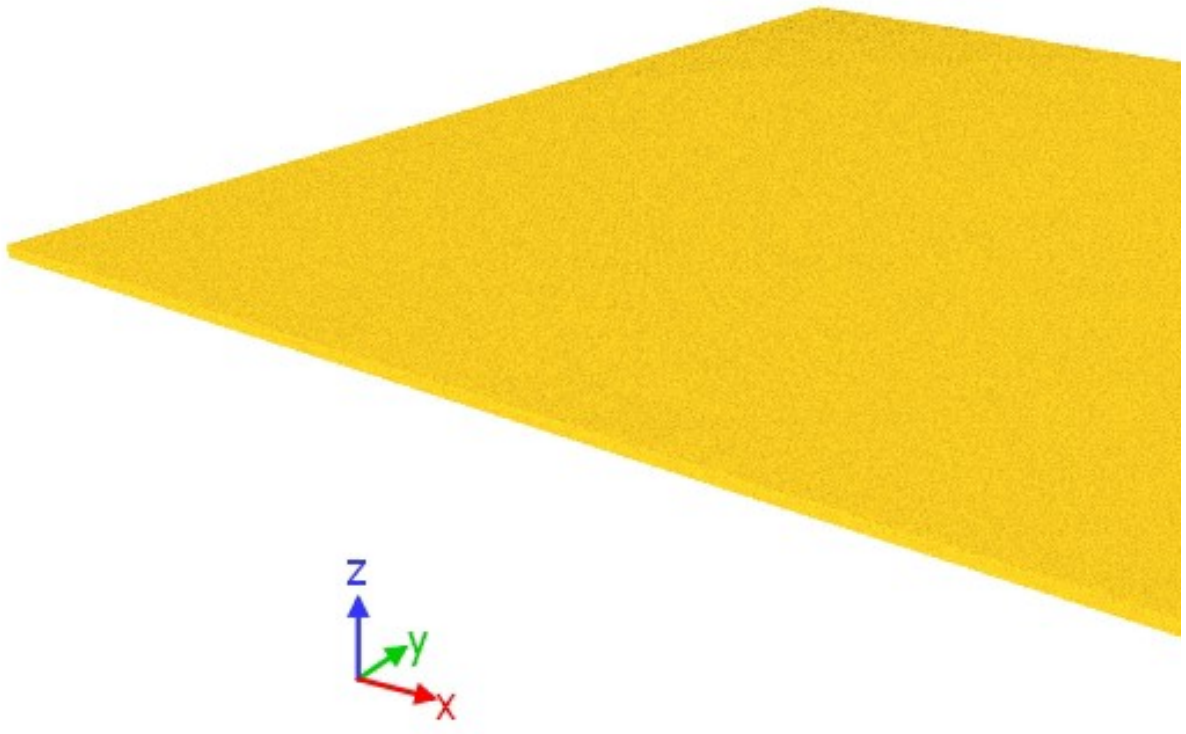
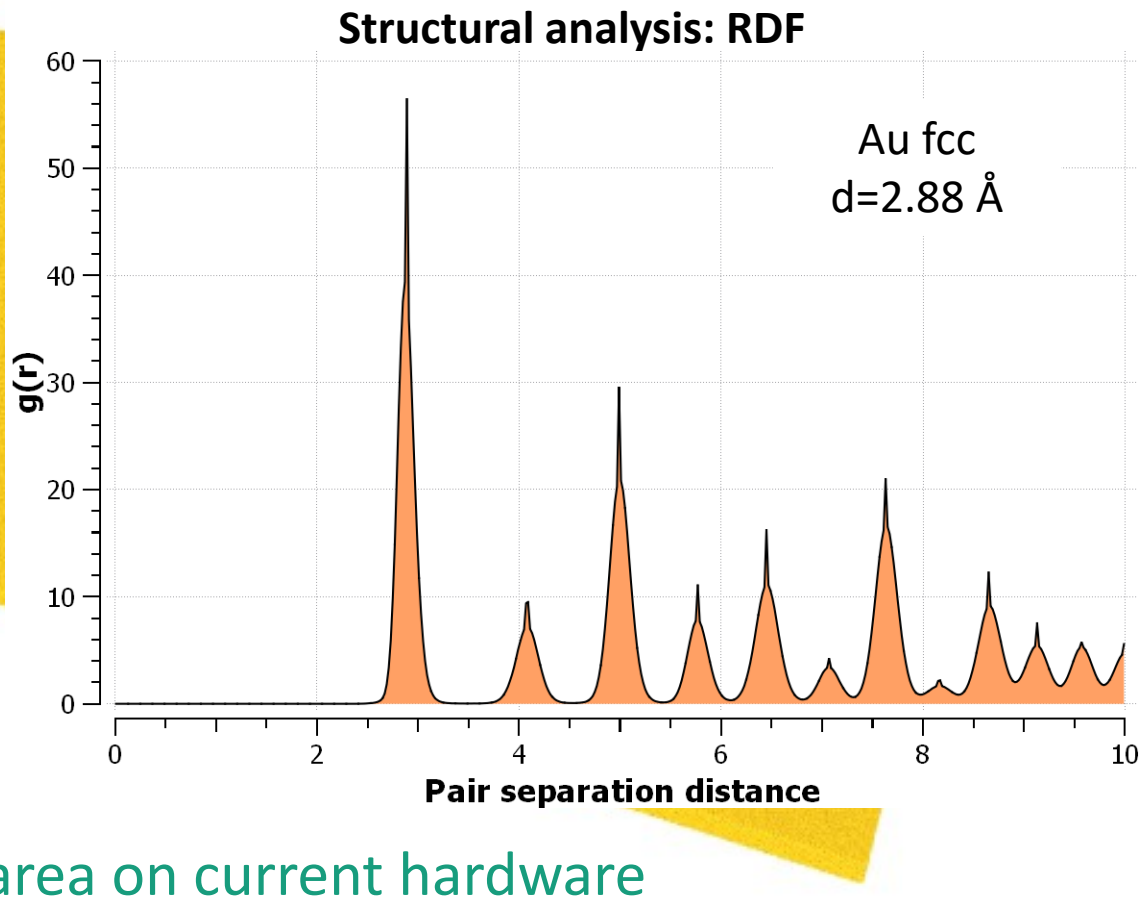
Demonstration: 300x200nm, 10nm Gold PVD

41 million atoms, 33 million MD adsorption simulations, EAM force field

~60 hours runtime on 480 now-10-year-old CPU cores



Animation



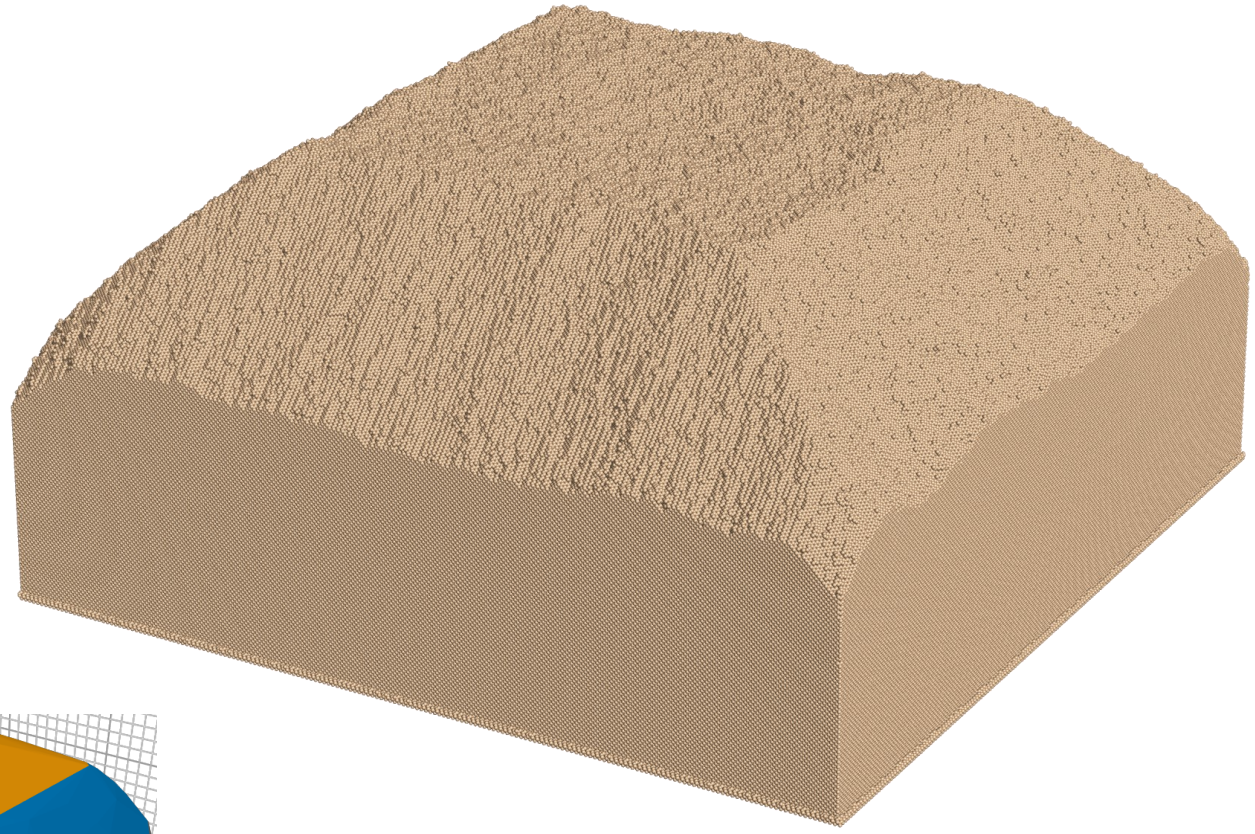
→ Linear scaling up to 1,6 µm x 1,6 µm active area on current hardware

Application example: SiGe:B faceting

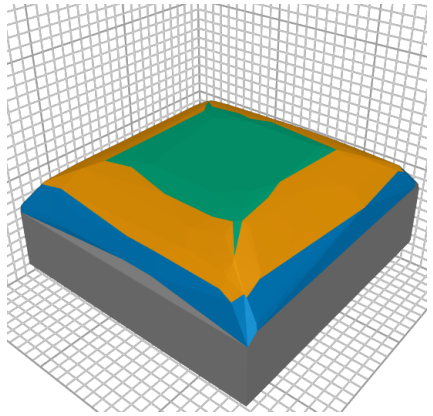
Goal: Optimization of faceting during growth

- SiGe:B epitaxy
- Includes surface diffusion of molecules from the surrounding topography

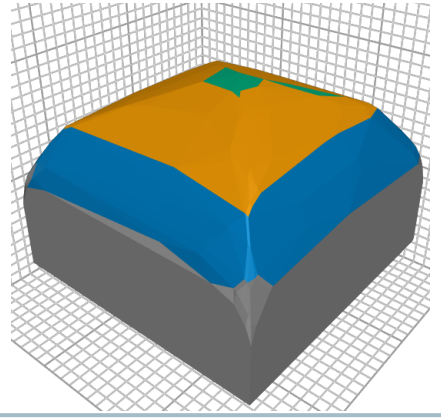
➔ Surrounding topography has to be modeled



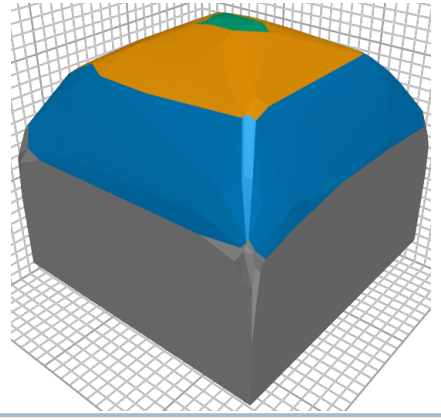
20 s



60 s

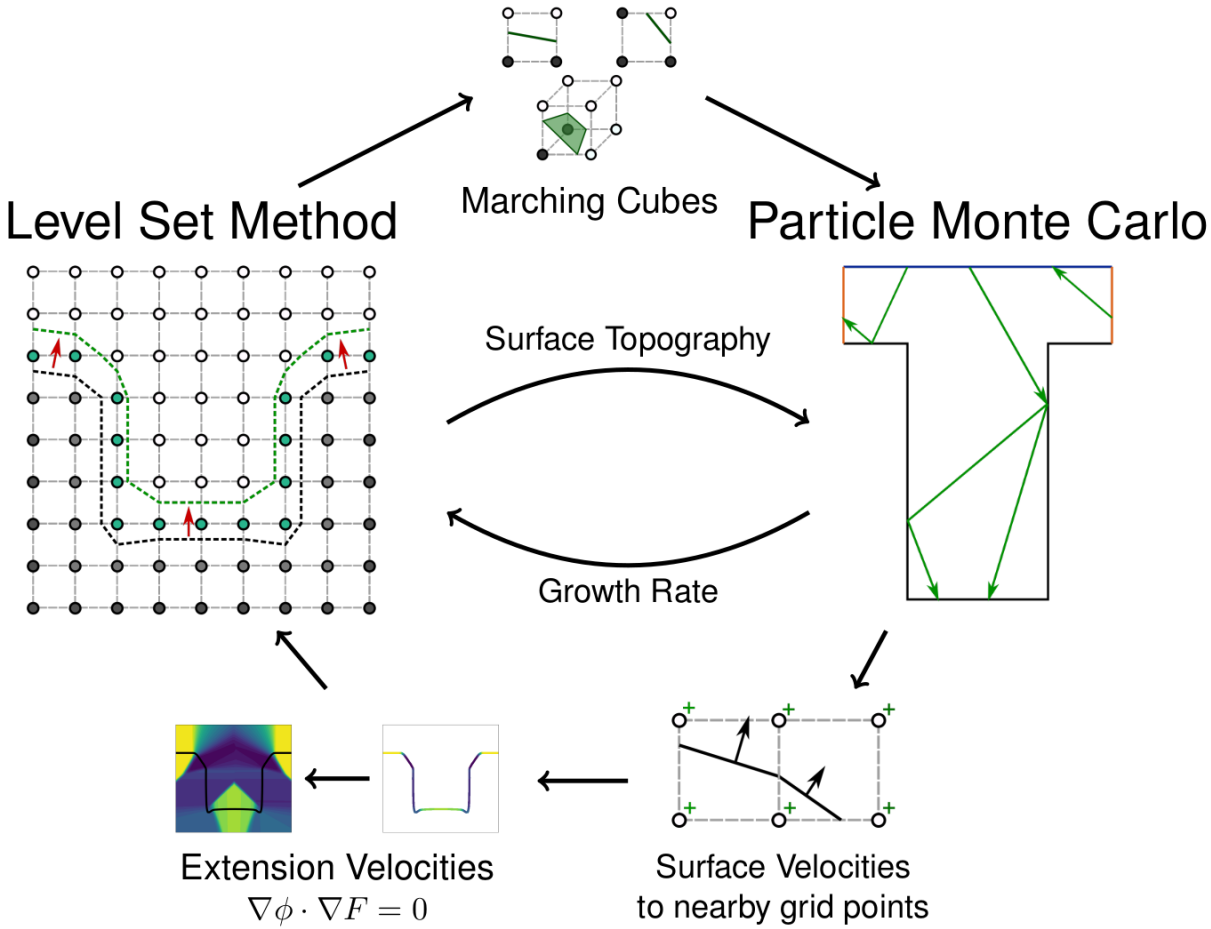


100 s

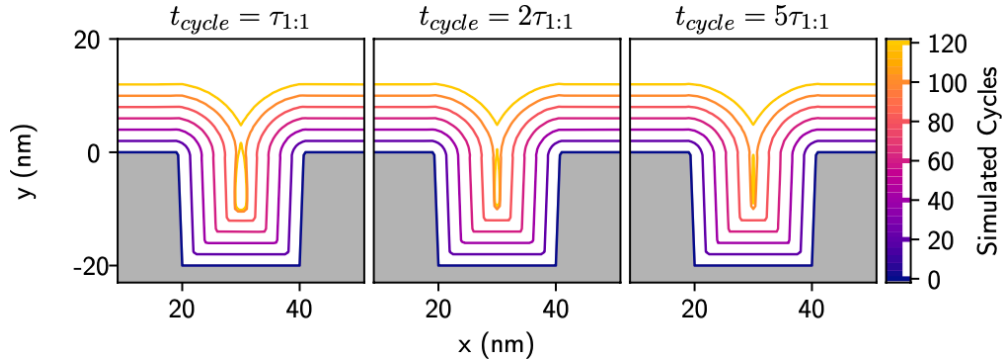


Surrounding topography: Yet another coupling method

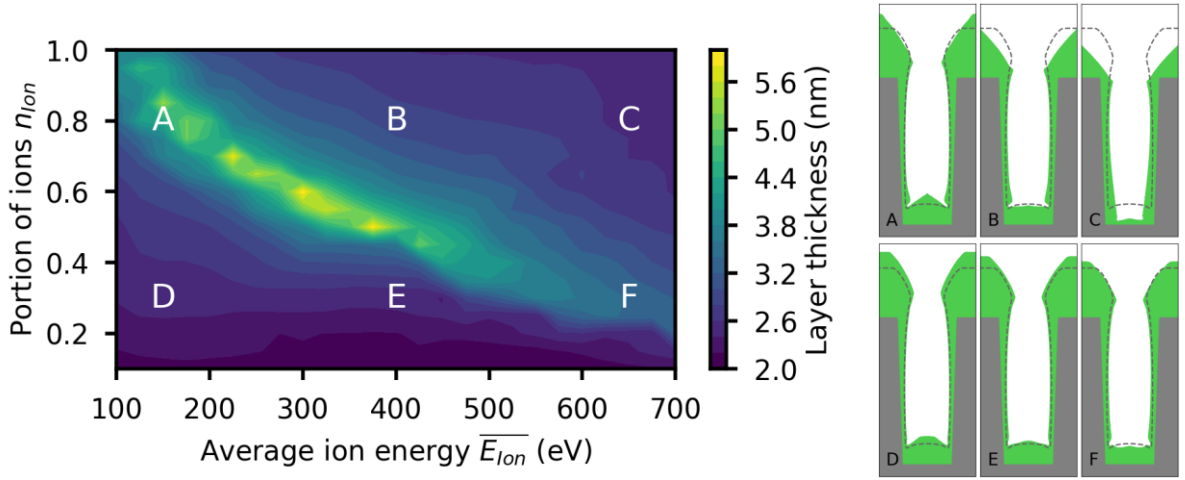
Level Set surface growth + Raytracing growth rate sampling



Coupling scheme ”Geosect” at ENAS



Ex. 1: Economically avoiding void formation during ALD trench fill through feature-adaptive cycle times
t_{cycle} – cycle time, τ time to 99% saturation on initial substrate



Ex. 2: Topography-dependent process optimization for PVD resputter process

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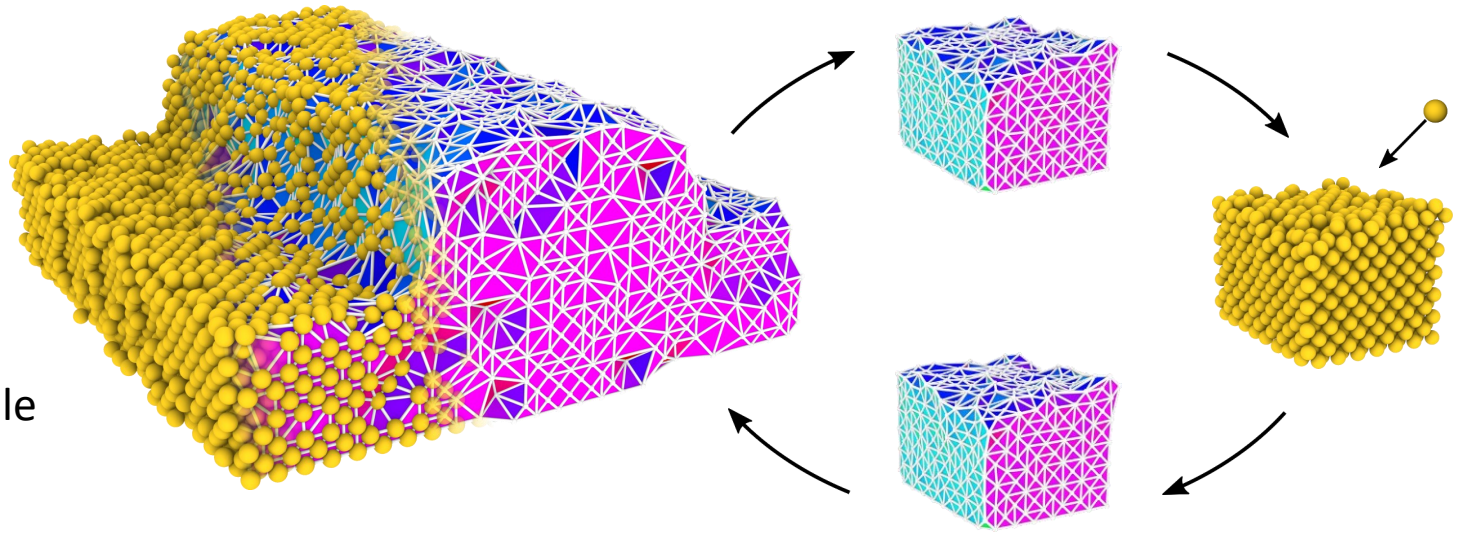
Conclusion



Summary

- Atomistic micrometer-scale method for vapor deposition process simulations
- Links to intermediate scale and reactor scale

Next Steps

- Increased use of available hardware accelerators (NVidia A100 GPUs, Xilinx VCK5000 FPGAs, *Anton3?)*
- Support for moment tensor potentials
- Triangulation-based direct coupling to intermediate scale, and to electronic methods

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