Plasma-Wall Interaction – A Multi-Scale Problem

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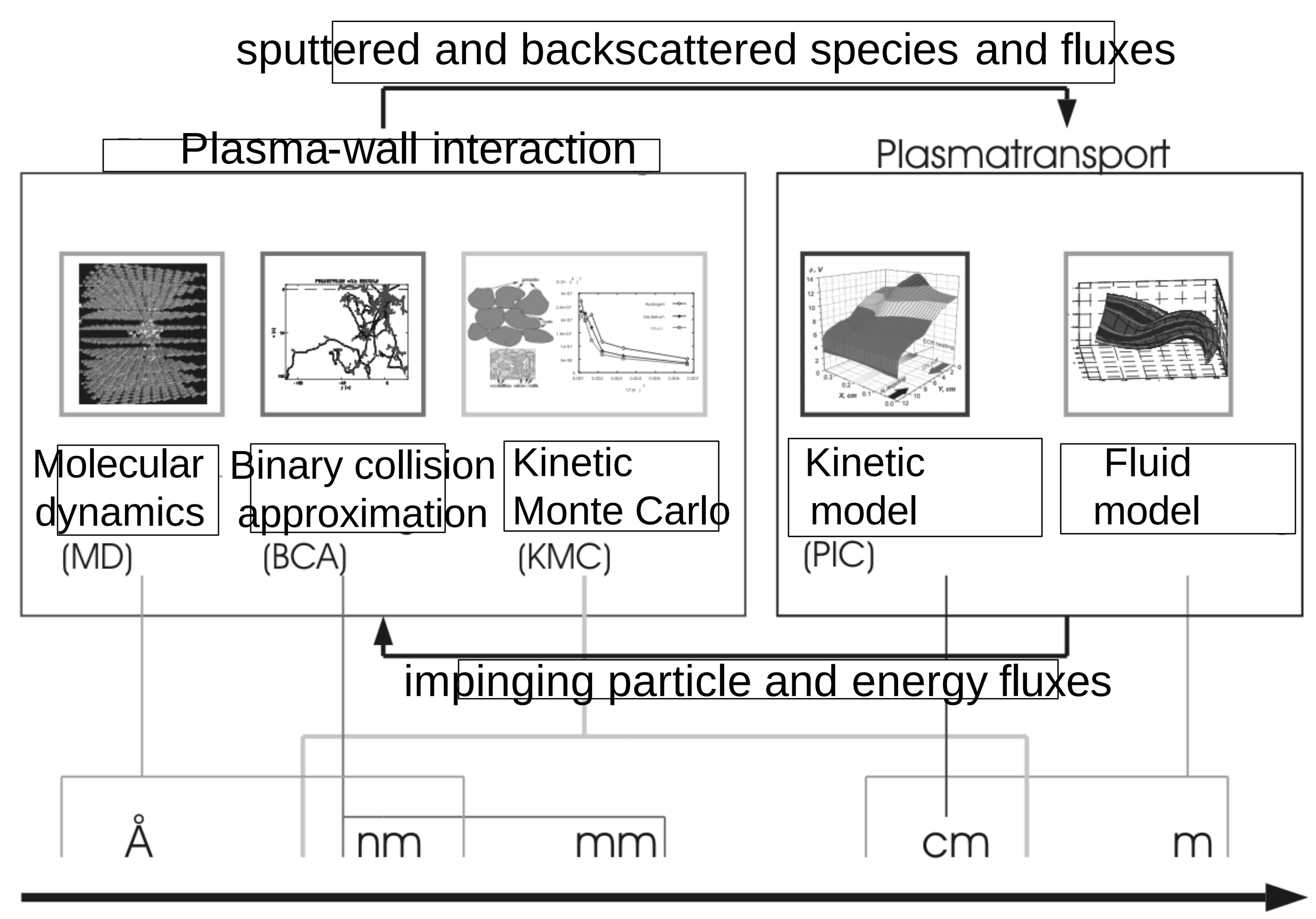
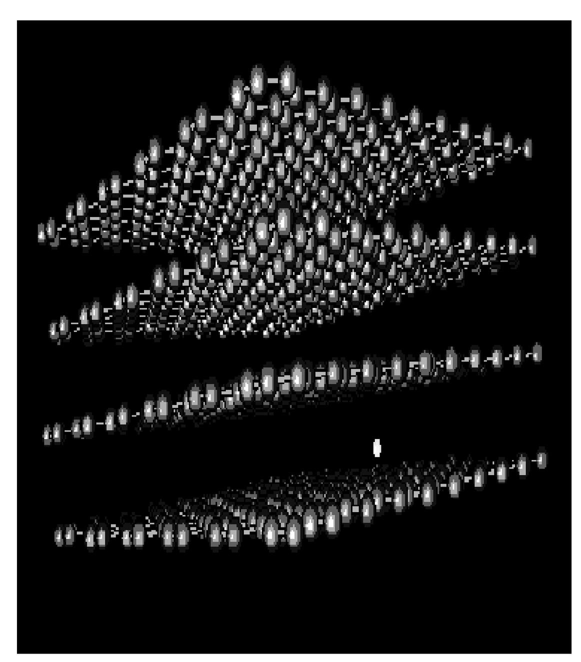
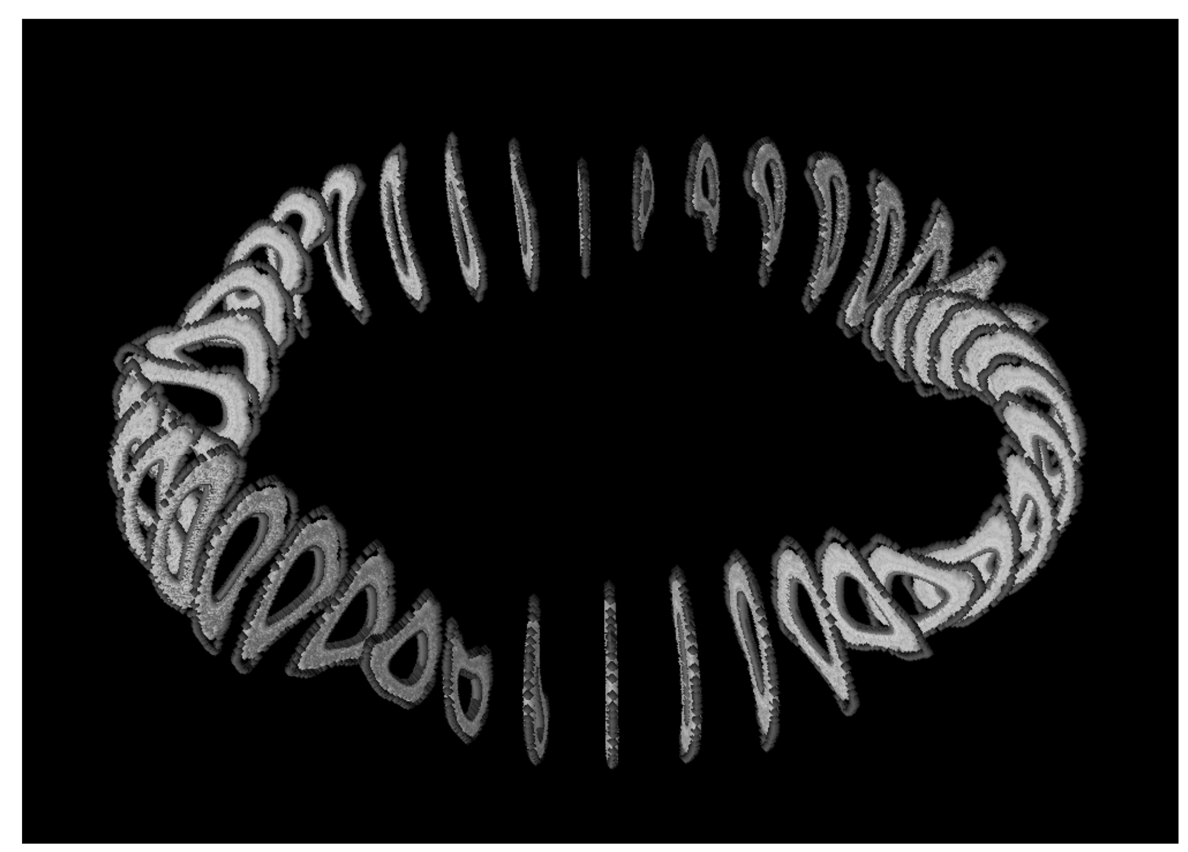
Multi-scales

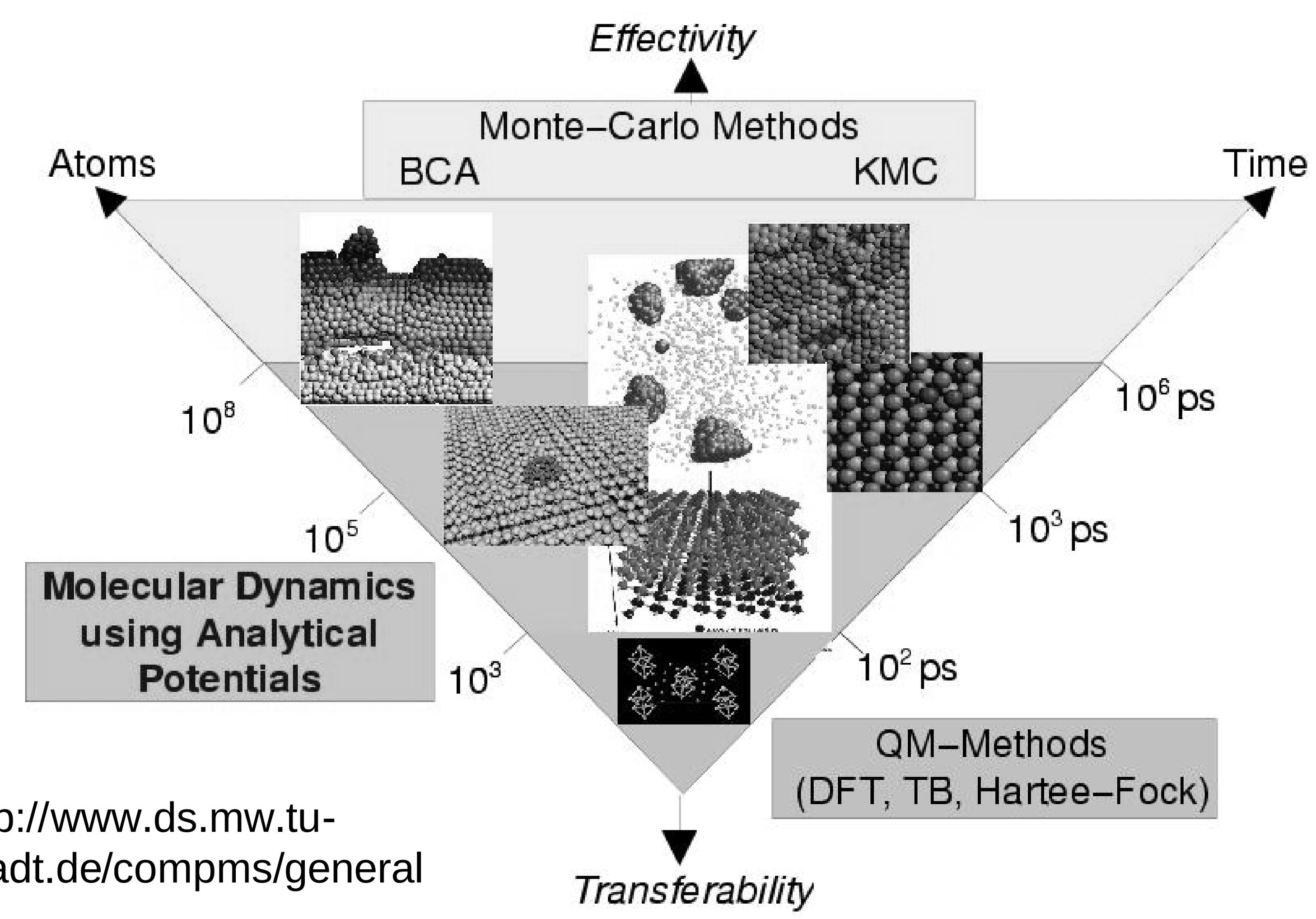


From atoms to W7-X





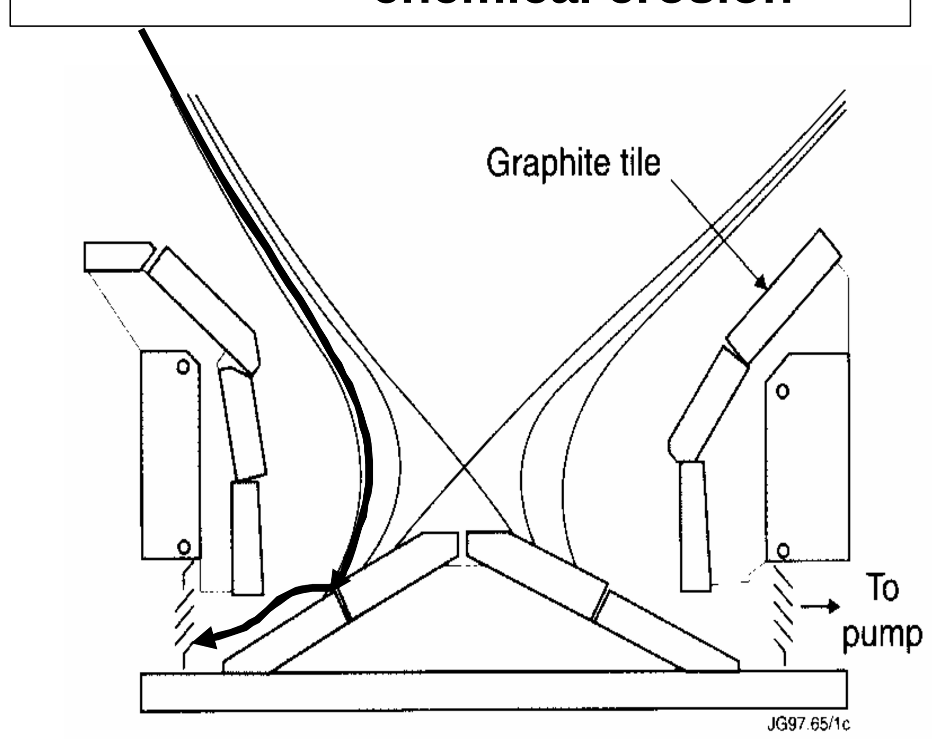
Multi-scale physics needs a combination of methods! But how???



http://www.ds.mw.tu-darmstadt.de/compms/general

Carbon deposition in divertor regions of JET and ASDEX UPGRADE

Major topics: tritium codeposition
chemical erosion

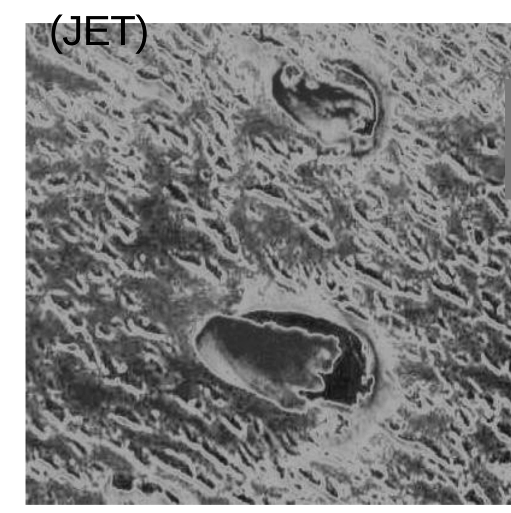


Achim von Keudell (IPP, Garching)

JET

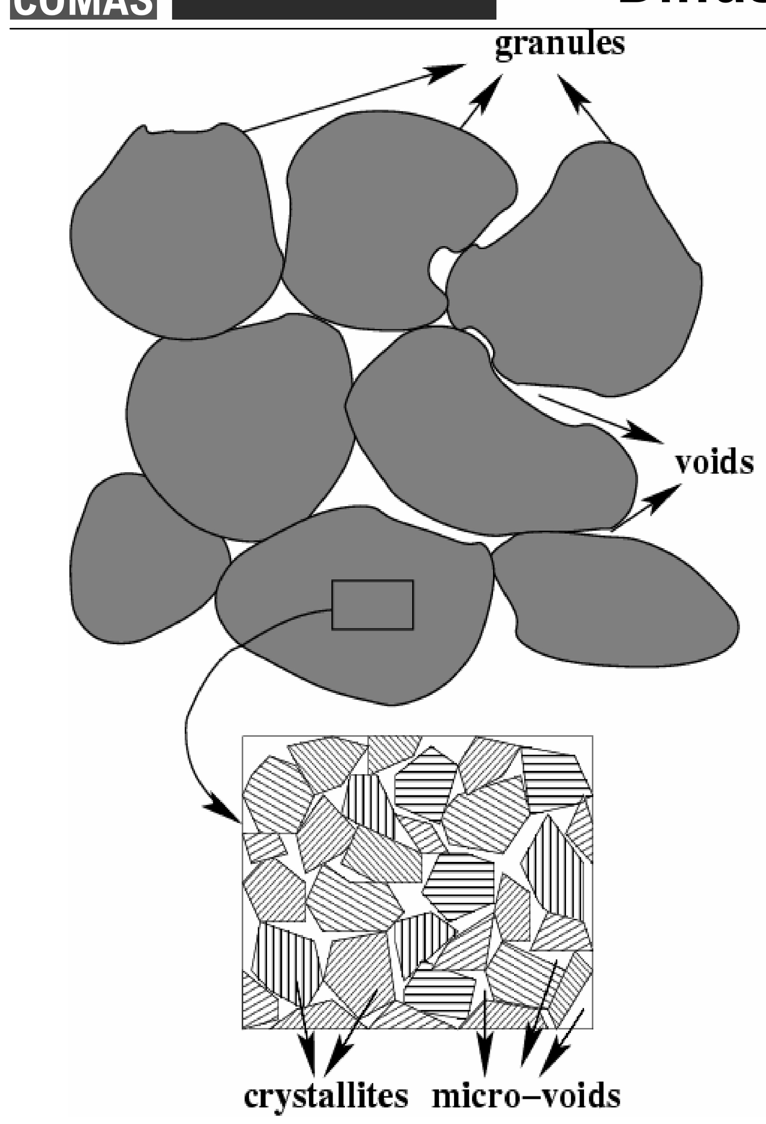
Paul Coad (JET)

ASDEX UPGRADE



V. Rohde (IPP, Garching)

Diffusion in graphite



Real structure of the material needs to be included

Internal Structure of Graphite

Granule sizes ~ microns

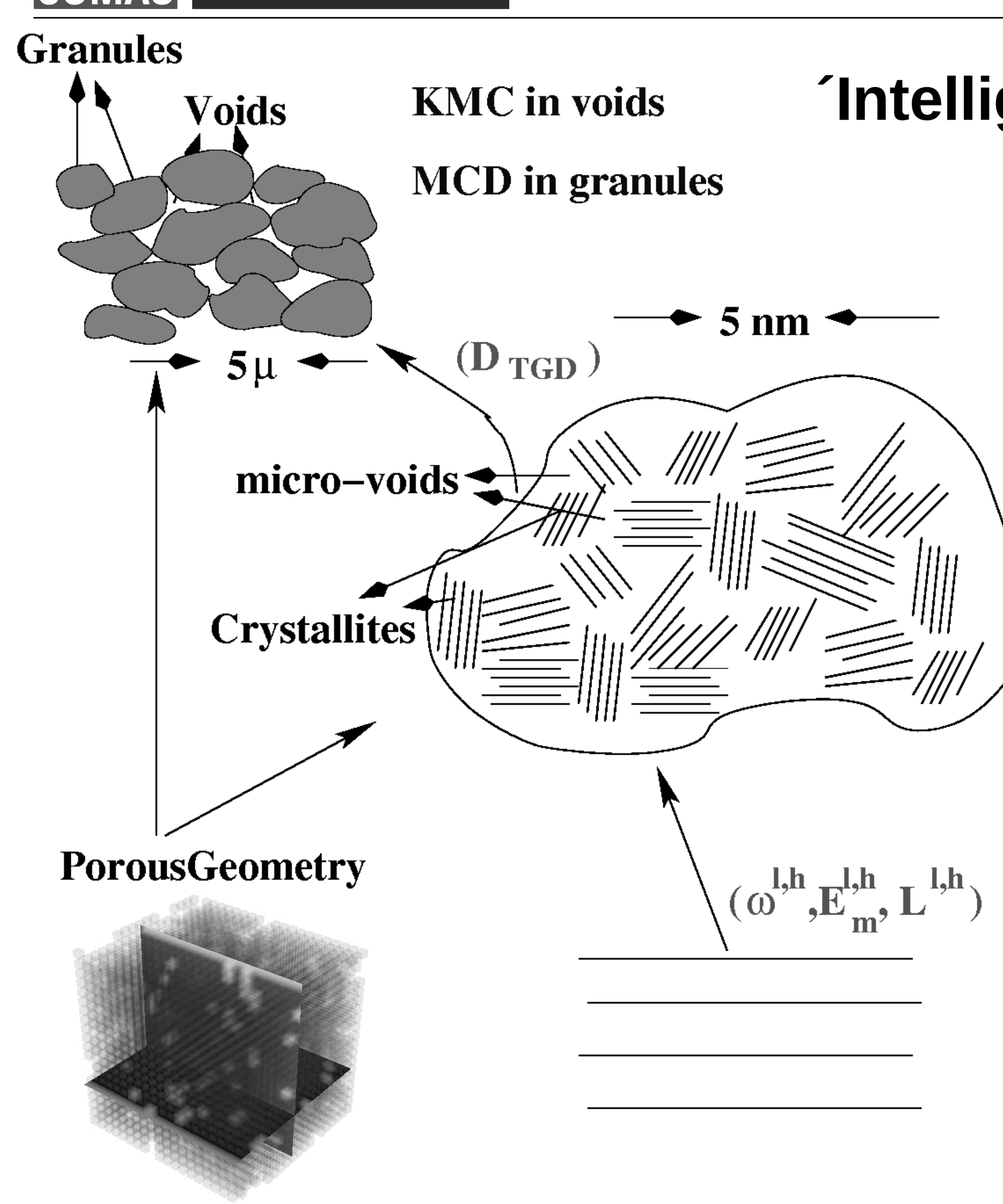
Void sizes ~ 0.1 microns

Crystallite sizes ~ 50-100 Ångstroms

Micro-void sizes ~ 5-10 Ångstroms

Multi-scale problem in space (1cm to Ångstroms) and time (pico-seconds to seconds)

Multi-scale approach



´Intelligent´ coupling necessary

Macroscales

KMC and Monte Carlo Diffusion (MCD)

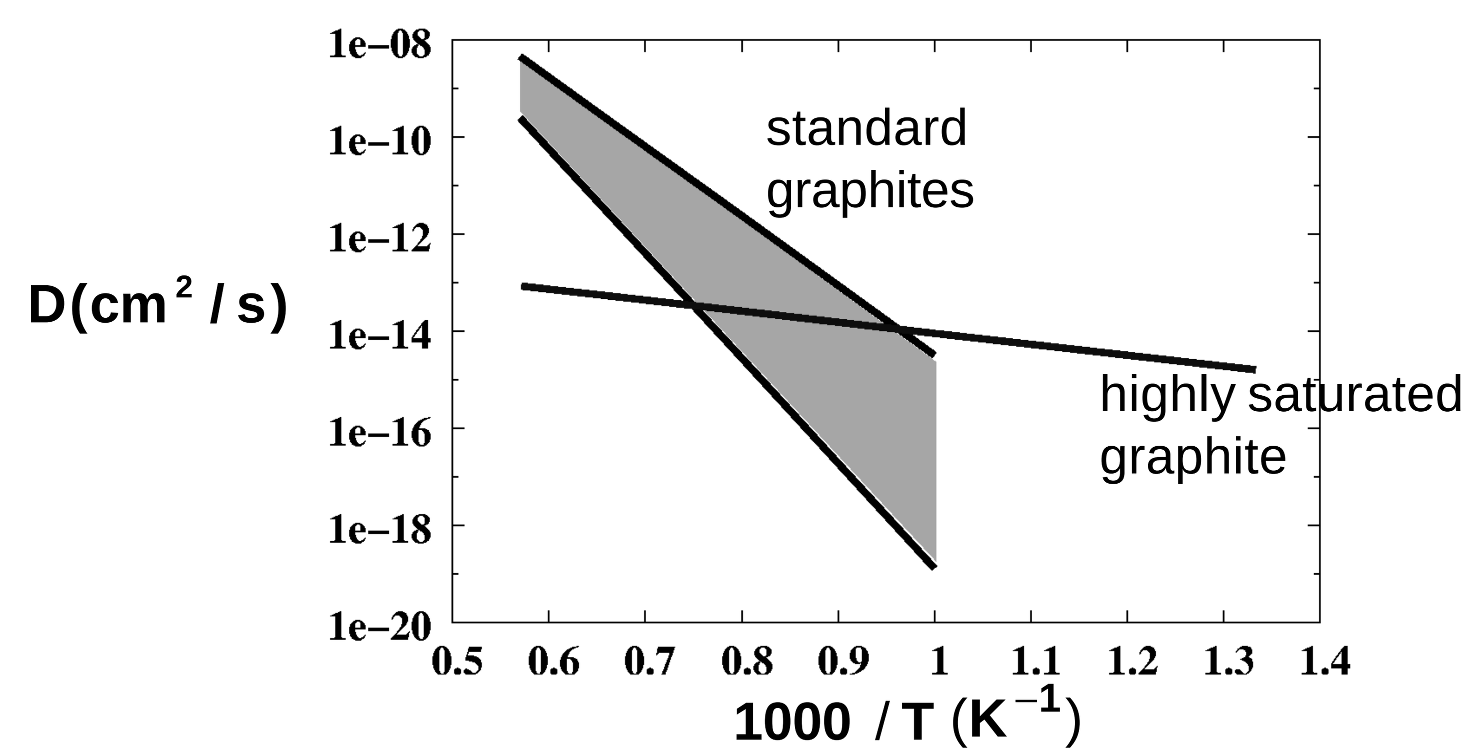
Mesoscales

Kinetic Monte Carlo (KMC)

Microscales

Molecular Dynamics (MD)

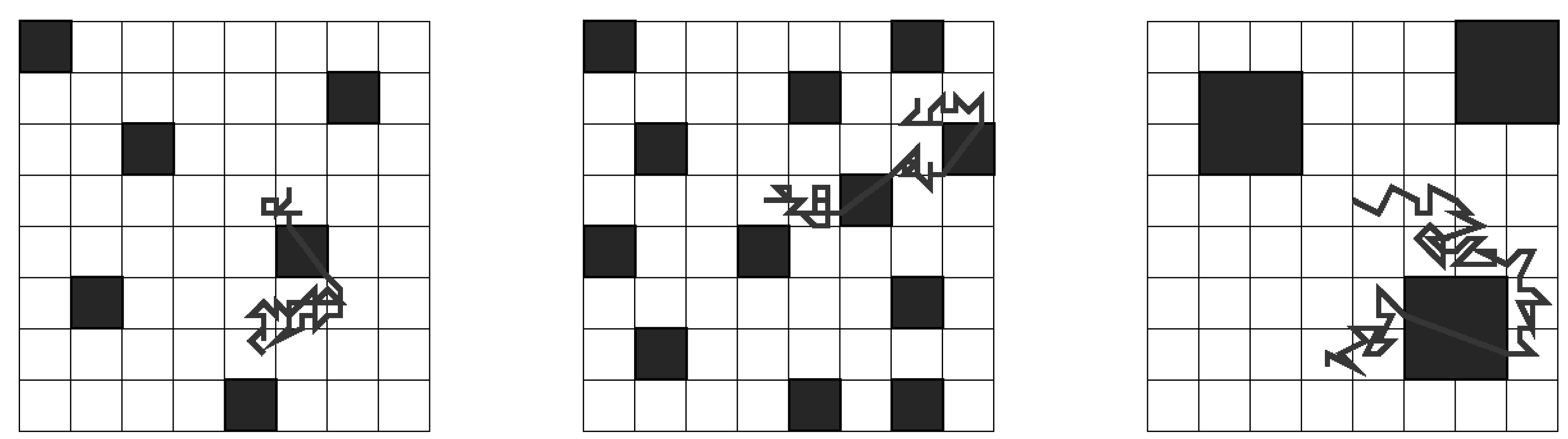
Mesoscales



Large variation in observed diffusion coefficients

- **Strong dependence on void sizes and not void fraction**
- **Saturated H:** w_0**~$10^5 s^{-1}$ and step sizes ~1Å (QM?)**

Effect of voids

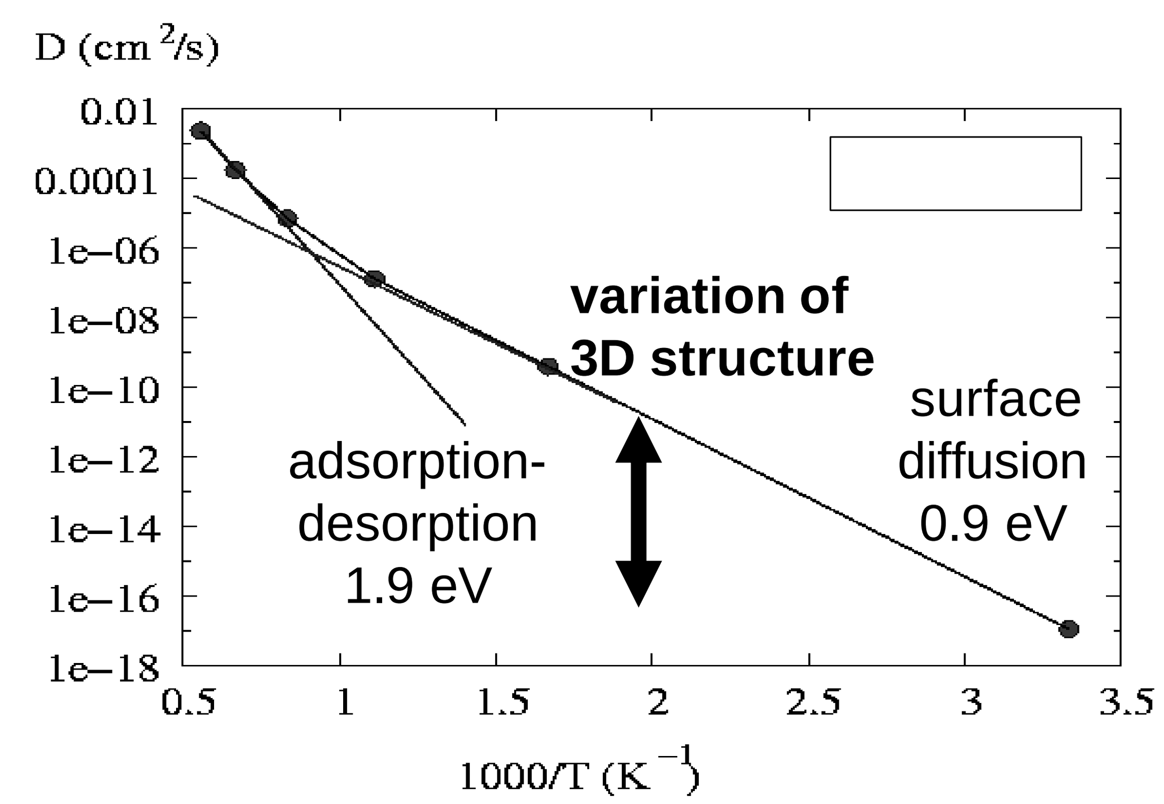


A: 10 % voids **B: 20 % voids** **C: 20 % voids**

$$\mathbf{D}_{\mathrm{TGD}} = \frac{\mathbf{N}}{\mathbf{6}} \left(\frac{\mathbf{P}^{\mathbf{void}}(\mathbf{L}^{\mathbf{void}})^2 + \mathbf{P}^{\mathbf{cryst}}(\mathbf{L}^{\mathbf{cryst}})^2}{\Sigma_{\mathbf{i=1}}^{\mathbf{N}}(-\mathbf{ln}(\mathbf{U}))} \right) \omega^{\mathbf{detrap}}$$

Larger voids ⟶ **Longer jumps** ⟶ **Higher diffusion**

Results at macroscales

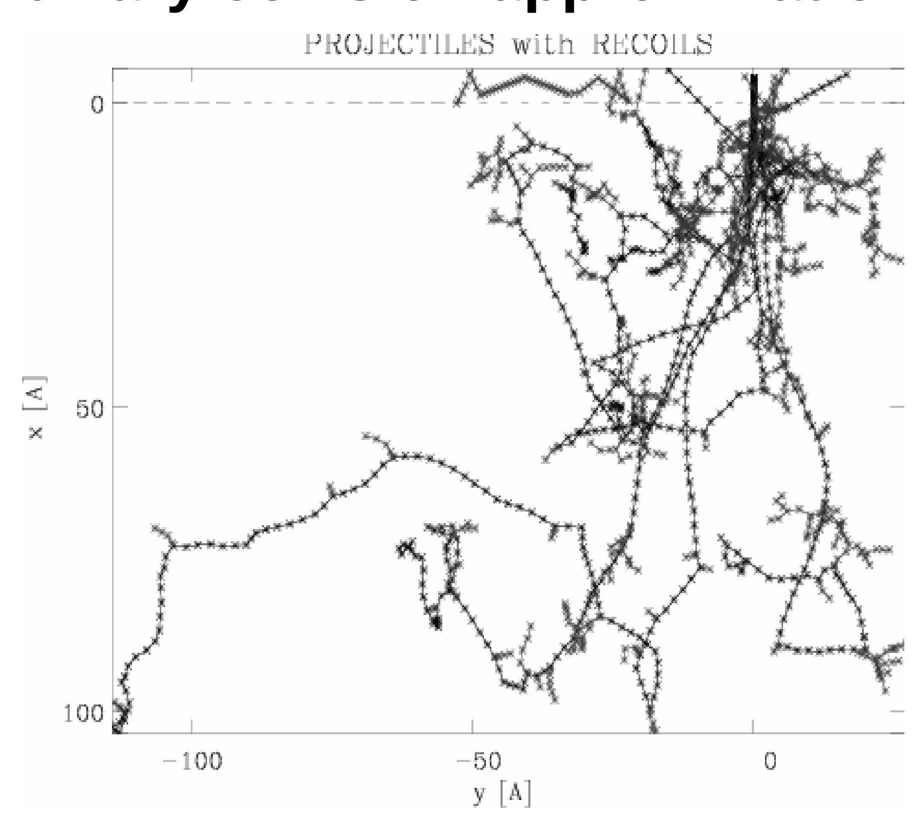


- Different processes dominate at different temperatures
- Diffusion in voids dominates

Diffusion coefficients without knowledge of structure are meaningless

Downgrading

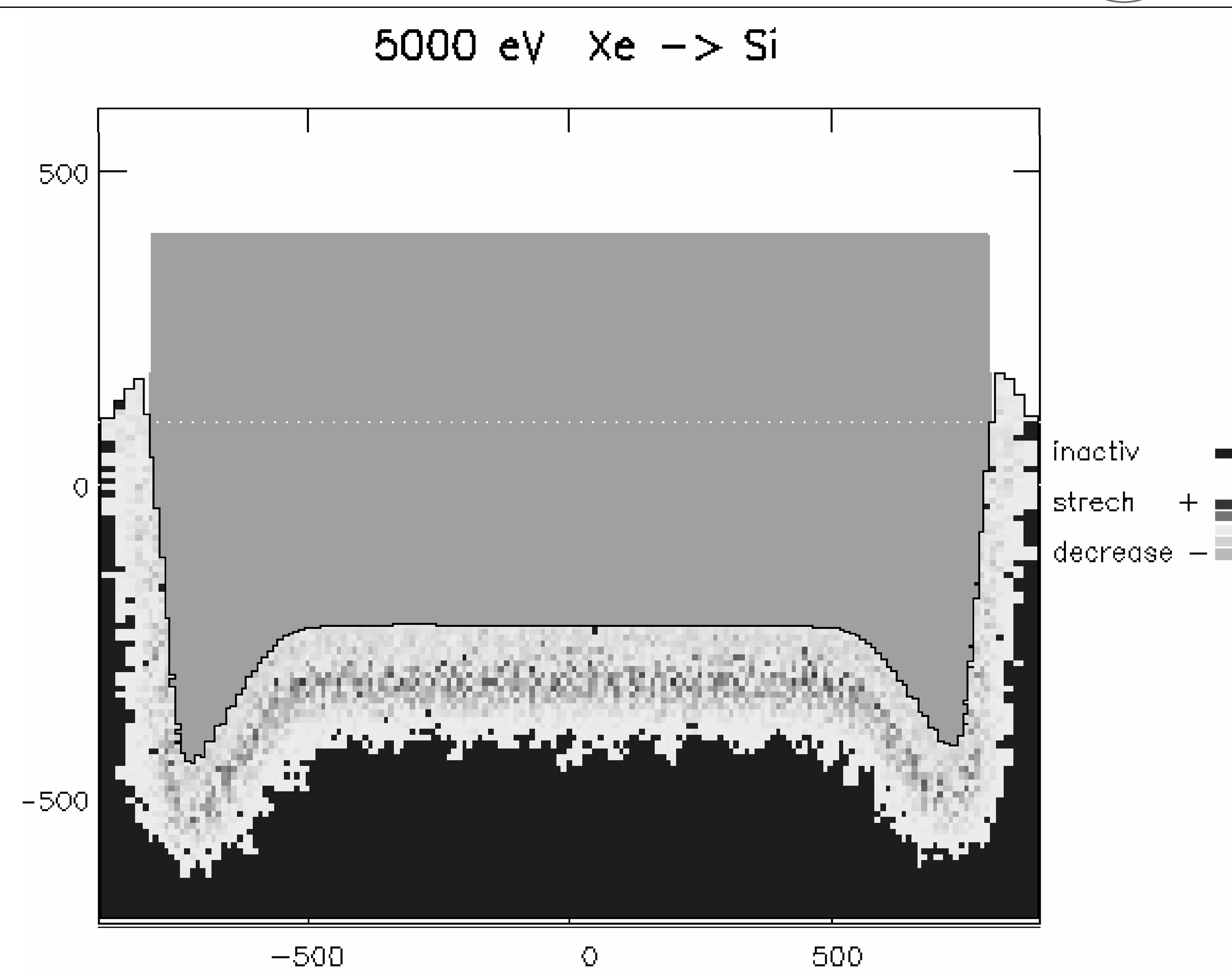
TRIM, TRIDYN: much faster than MD (simplified physics: binary collision approximation)



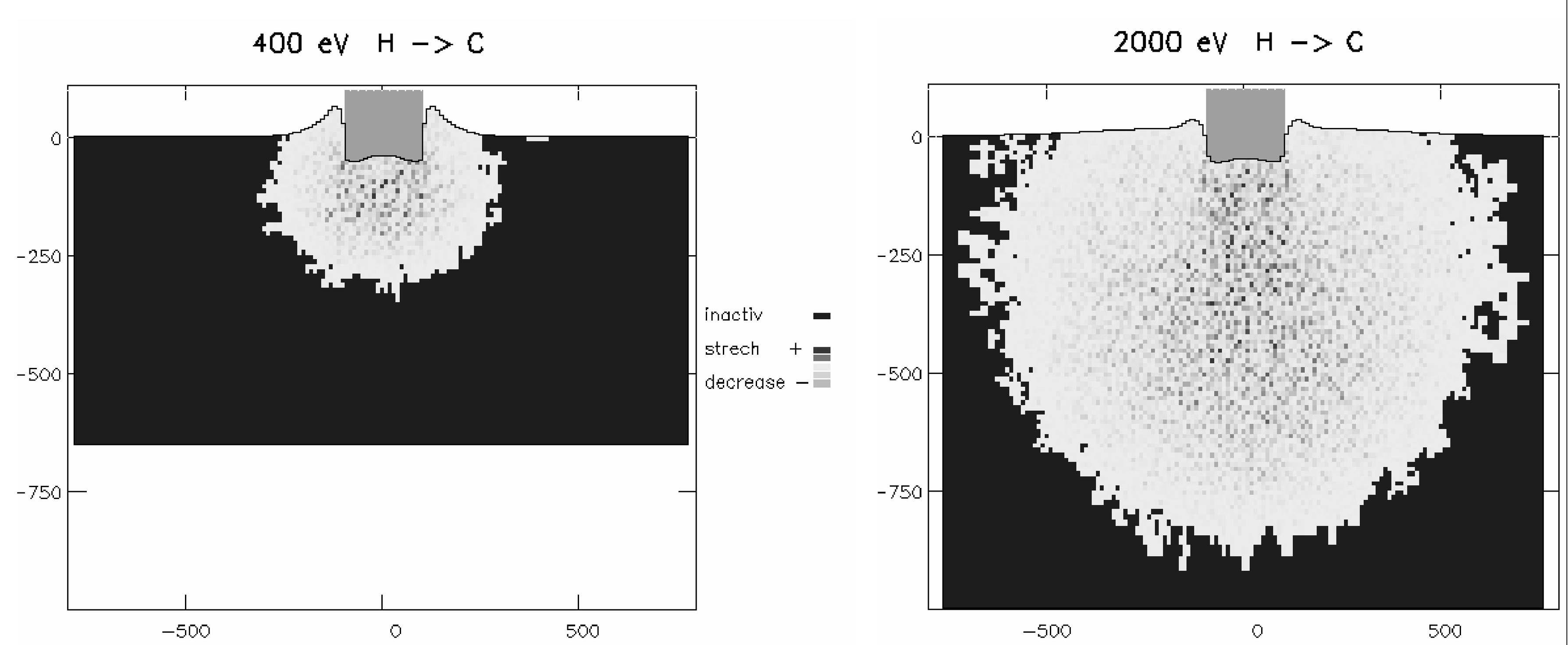
- **very good match of physical sputtering**
- **dynamical changes of surface composition**

Max-Planck-Institut für Plasmaphysik, EURATOM Association

2D-TRIDYN



2D-TRIDYN


400 eV H -> C
2000 eV H -> C
0
-250
-500
-750
-500
0
500
inactiv
strech +
decrease -

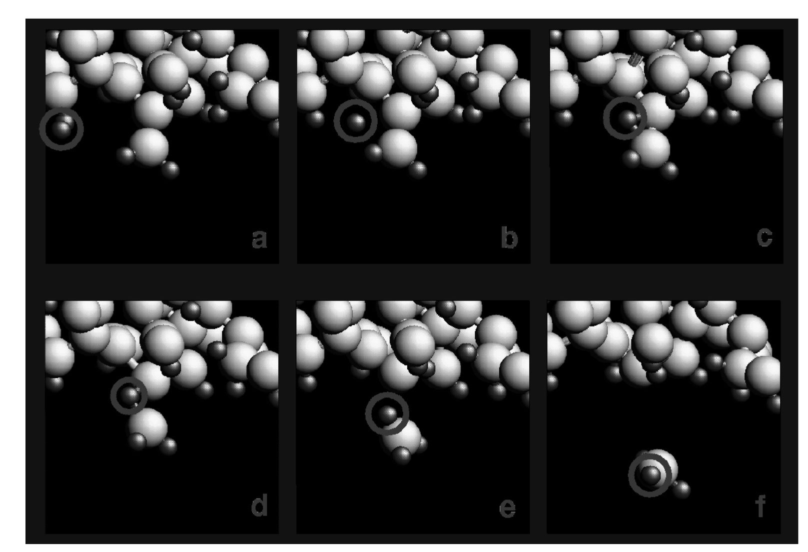
Upgrading

Inclusion of quantum effects

better potentials needed for MD: parametrization of PES (cluster expansion?)

-reaction rates, cross sections

- new methods for many-particle systems: quantum Monte Carlo, quantum MD, quantum kinetics/PIC
  → development of novel hybrid

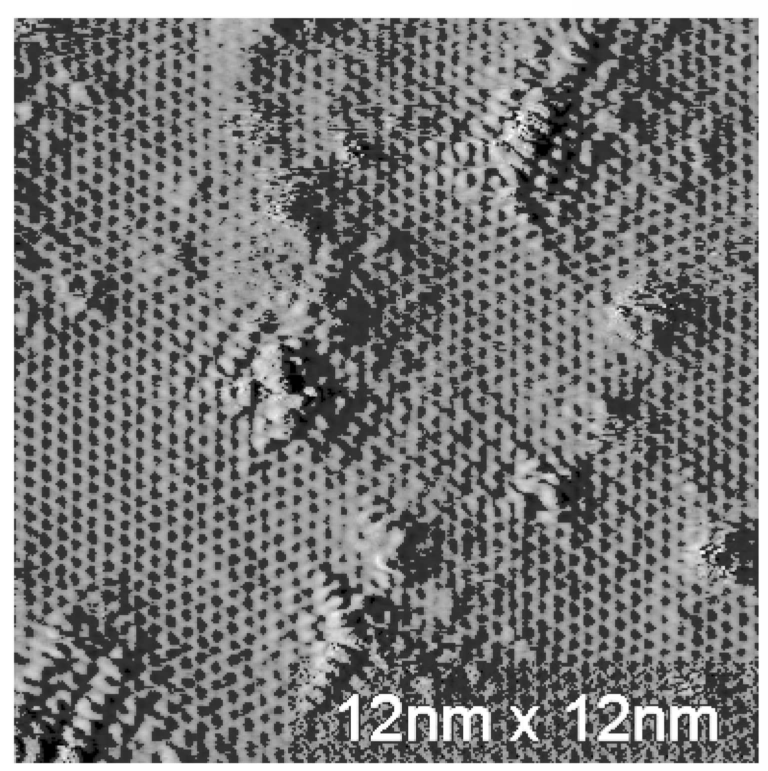


Emppu Salonen, Univ. of Helsinki

Model systems needed

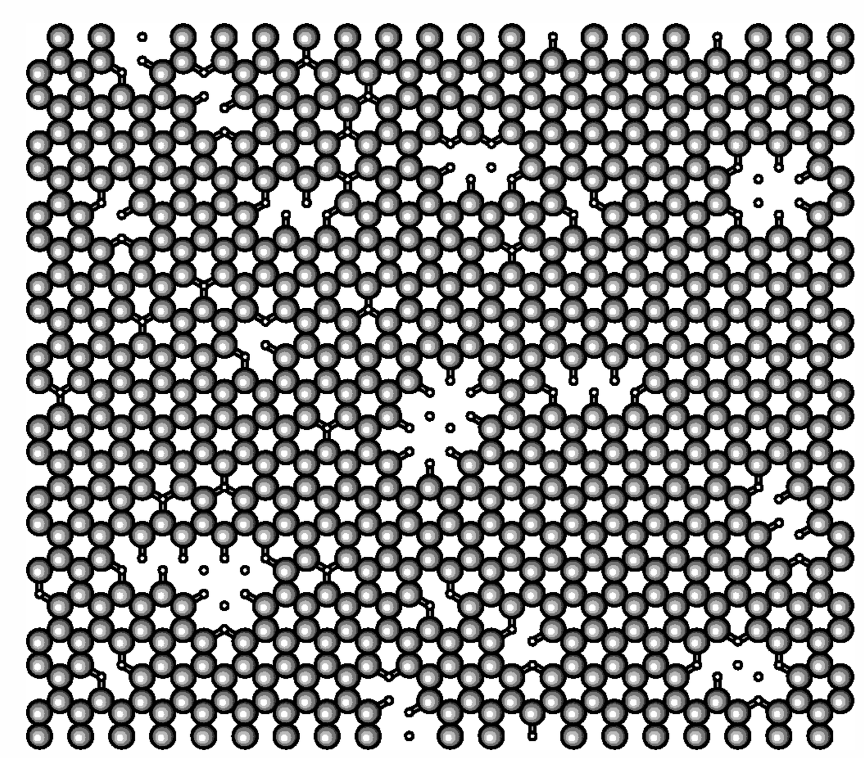
surface science and low-temperature plasma physics

STM of graphite surface



T. Angot et al., University of Provence, Marseille

Simulation

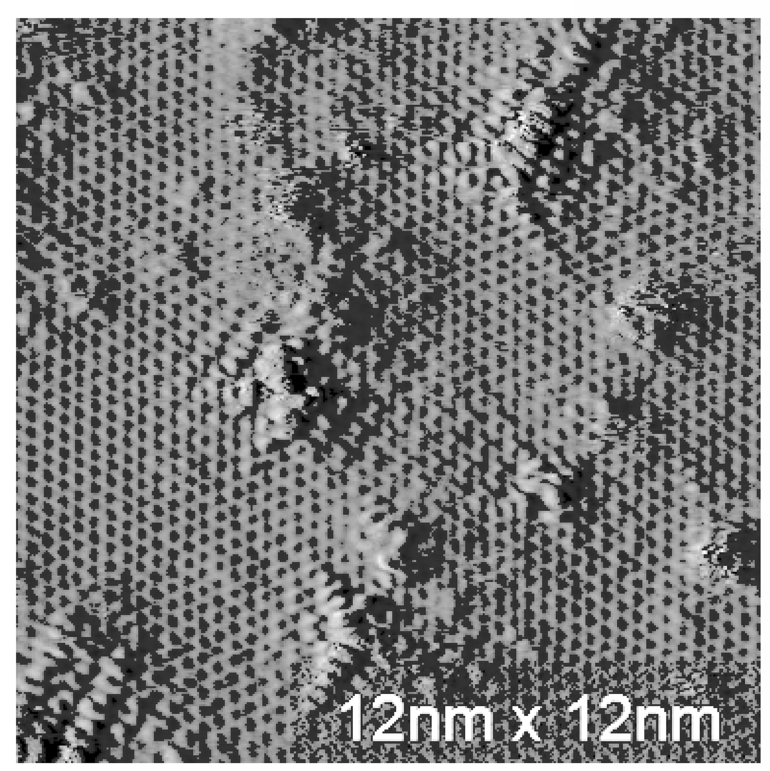


Modelling of Hydrogen bombardement of single crystal

Model systems needed

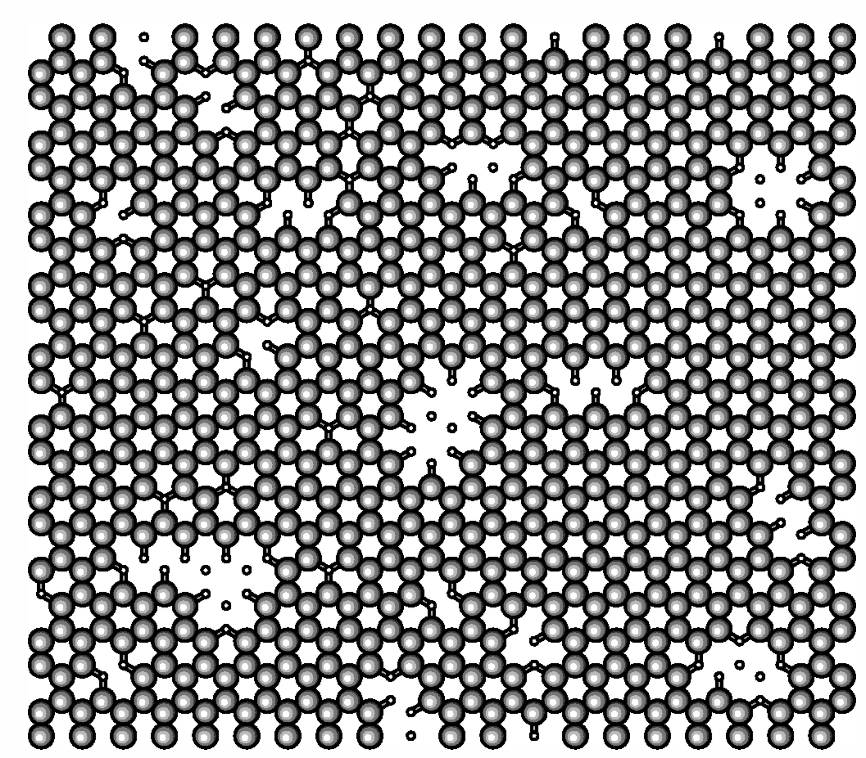
surface science and low-temperature plasma physics

STM of graphite surface



T. Angot et al., University of Provence, Marseille

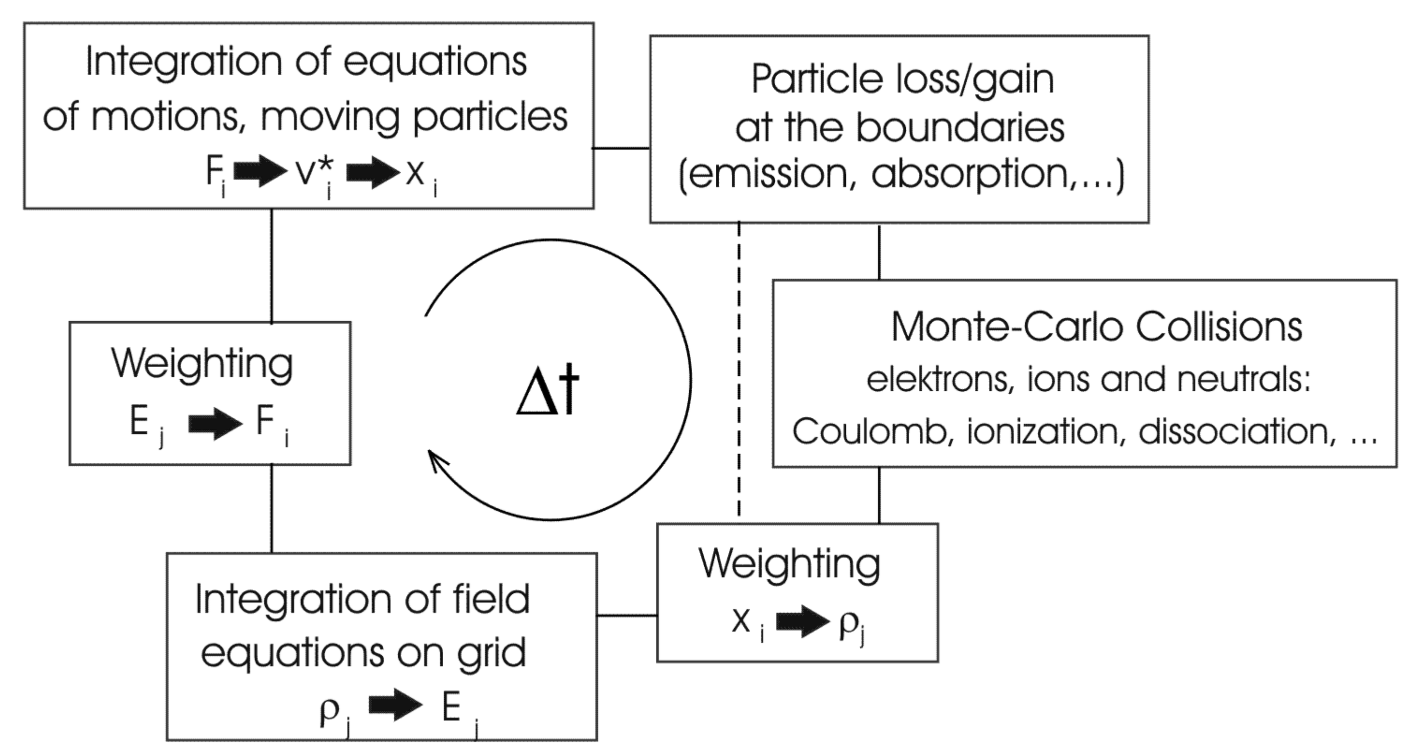
Simulation



Modelling of Hydrogen bombardement of single crystal

Plasma and nanoparticles

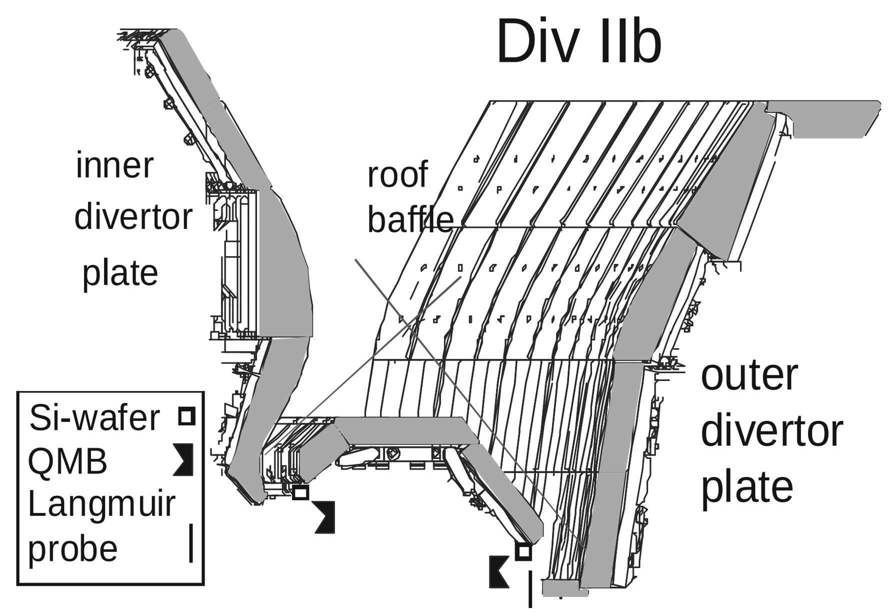
Particle-in-Cell (PIC):

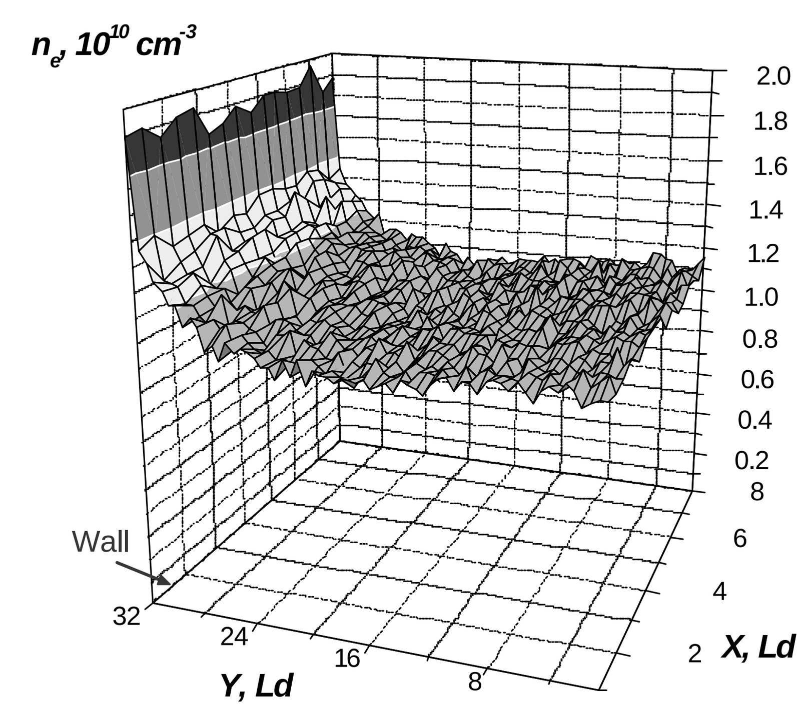


Applications:
Low temperature plasmas (methane, RF discharges)
Complex plasmas (plasma crystals, nanoparticles)
Parasitic plasmas in the divertor (radiative ionization)

PIC application

Parasitic plasma below divertor roof baffle in ASDEX Upgrade Div IIb from *photoionisation or photoeffect*





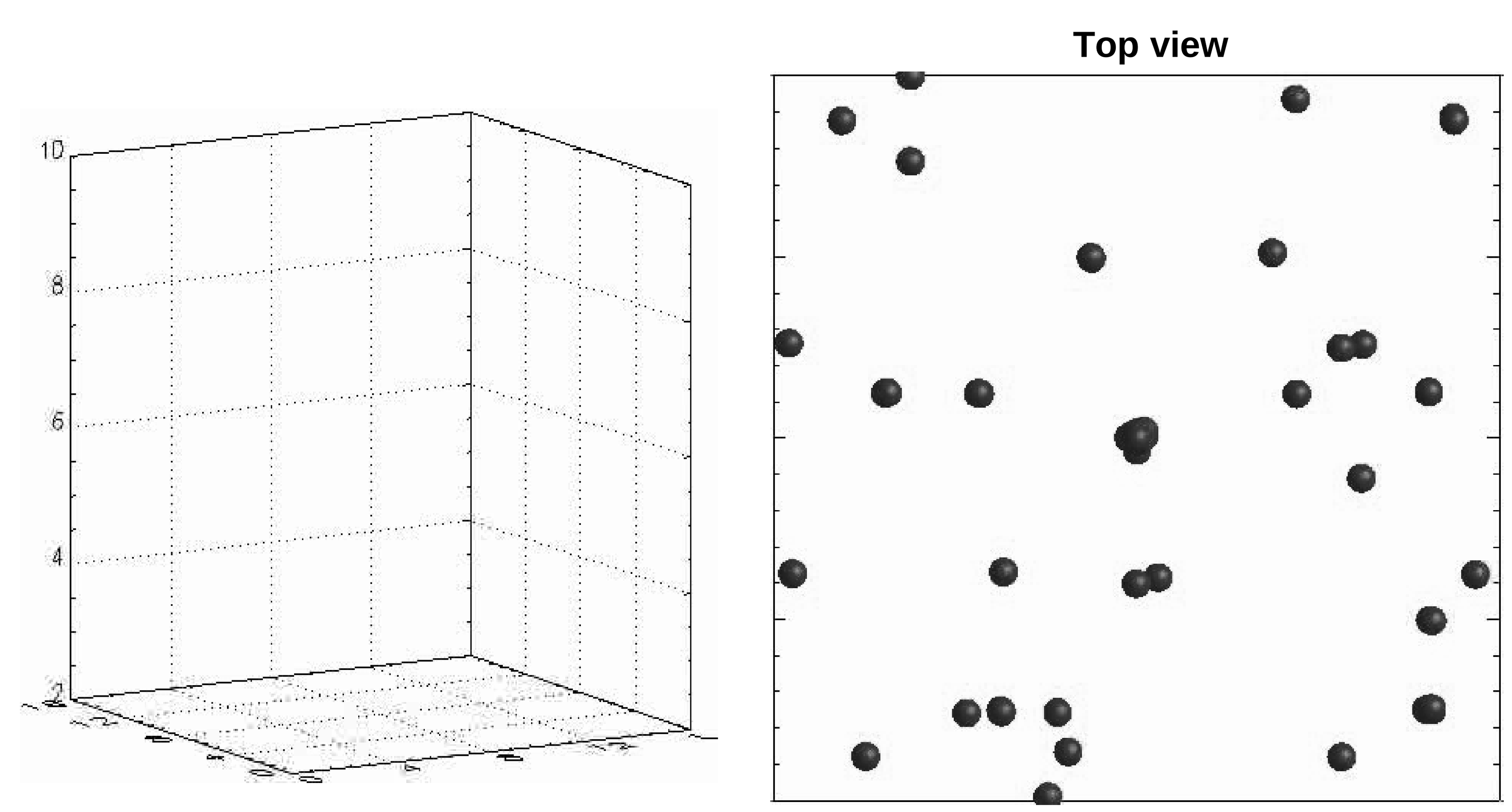
Typical parameters:

$4*10^8 < ne < 7*10^{11}\ cm^{-3}$

$5 < Te < 15\ eV$

Scaling: $ne \sim Radiation^{2.7} * Particle\_flux^{0.7}$

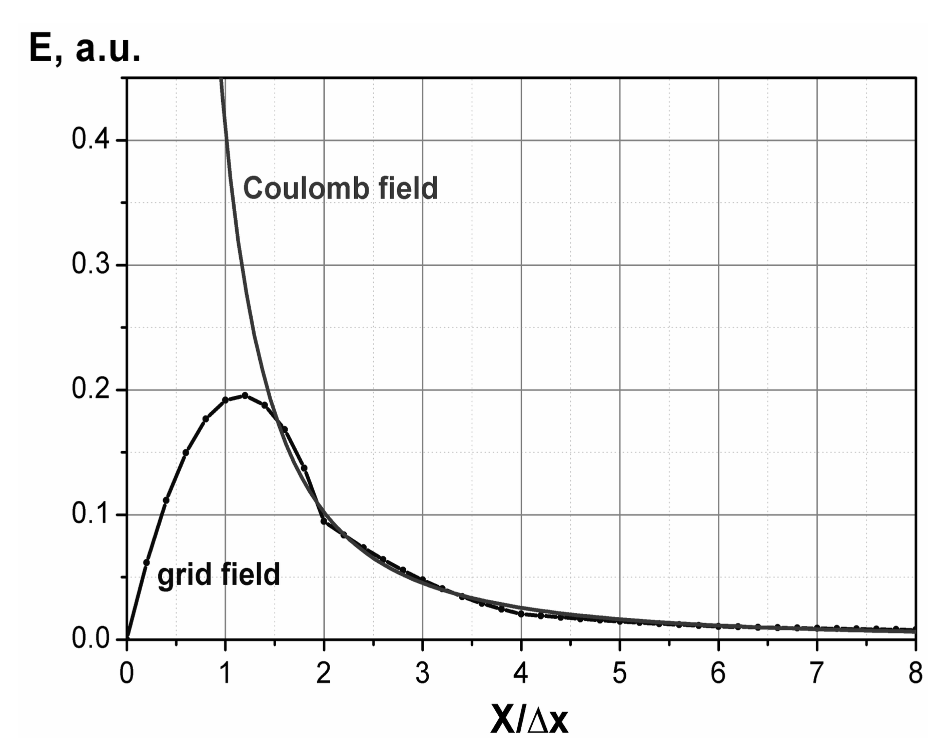
Plasma crystal - full 3D



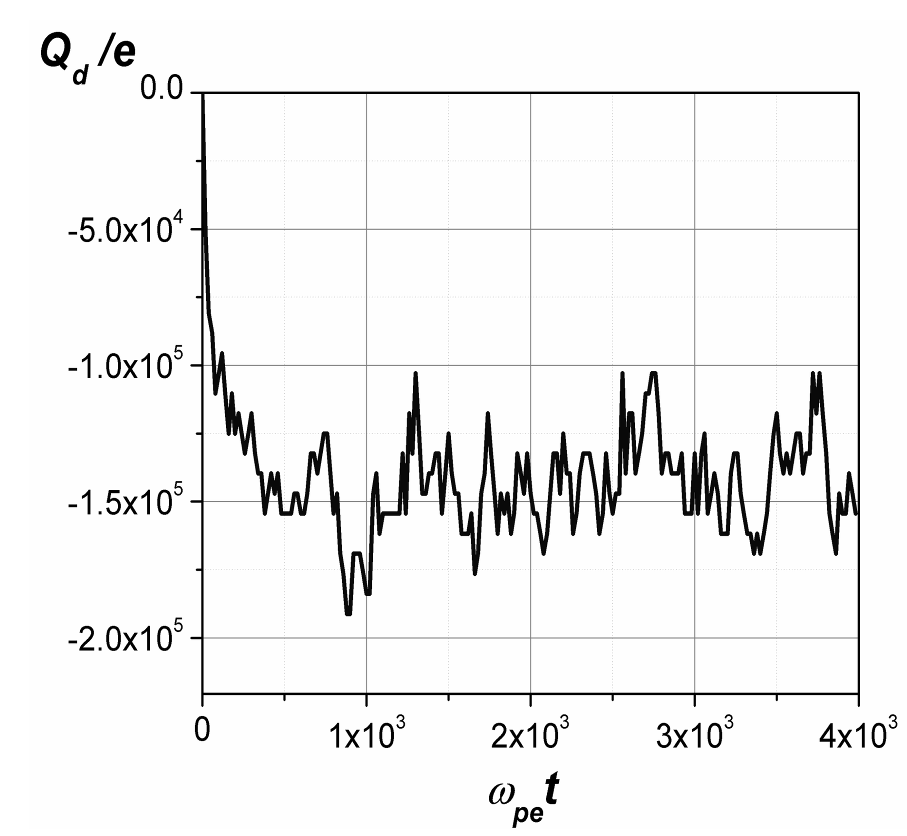
Quasi - ordered 3D structure

P3M model: PIC+MD

inter-particle interaction

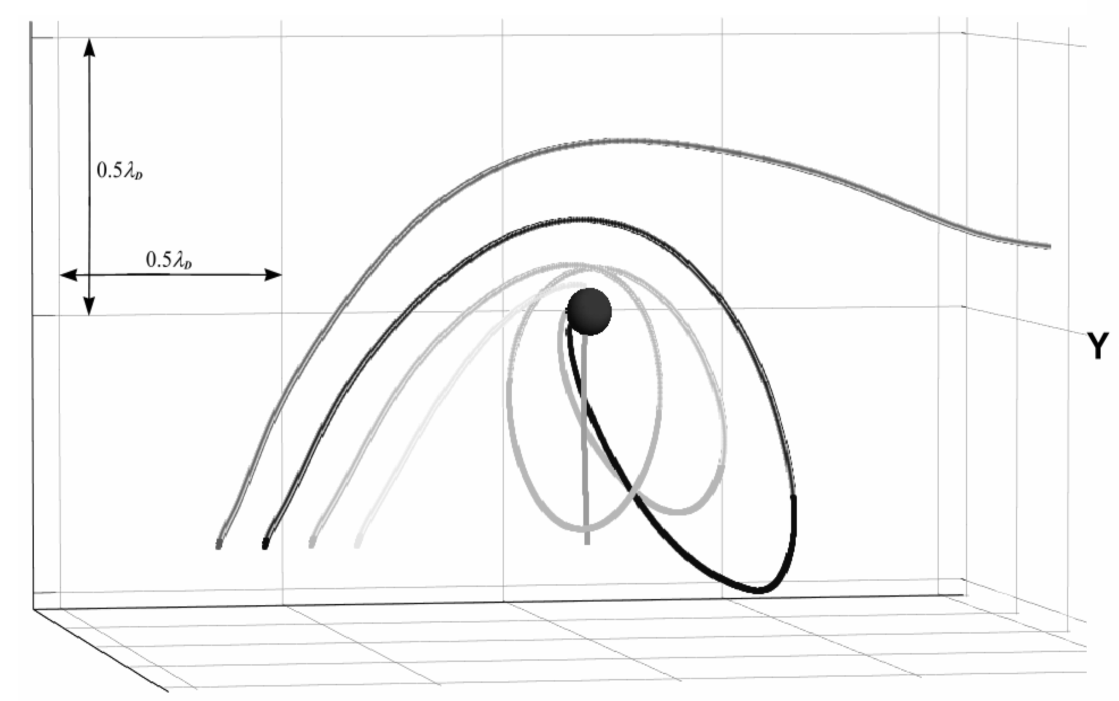


self-consistent dust charging



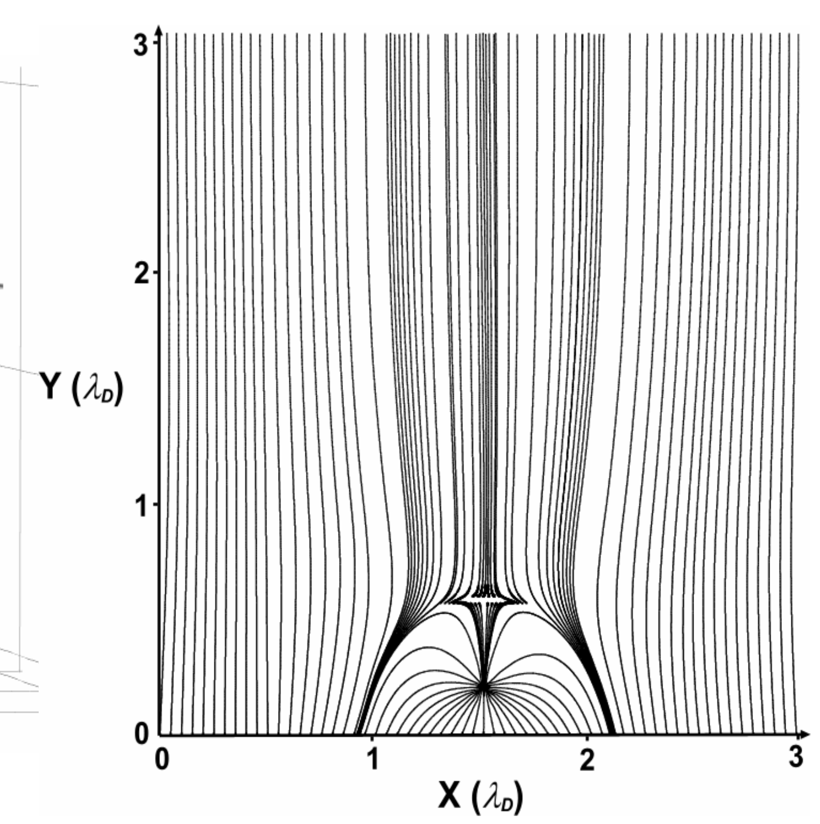
Dust-plasma interaction

ion trajectories close to the dust



trapped ions

electric field flowchart

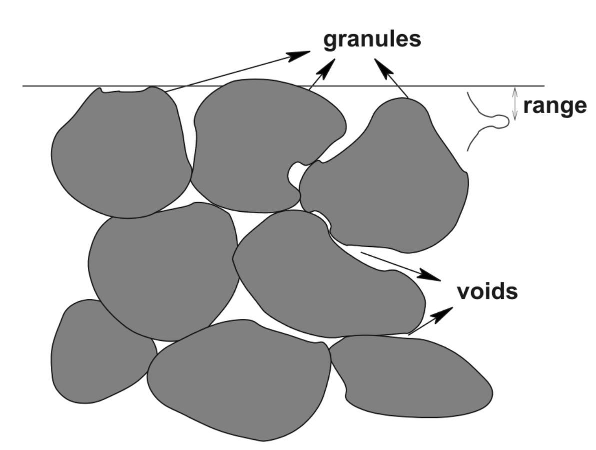


wake field effect

Summary

- Multi-scale physics needs a combination of methods
- ´Intelligent´ coupling necessary !??
- Hierarchy of models needed
  (downgrading, upgrading)
- Real structure of the material needs to be included
- Model systems needed:
  use the experience of the low-temperature
  plasma physics community

Multiscale model



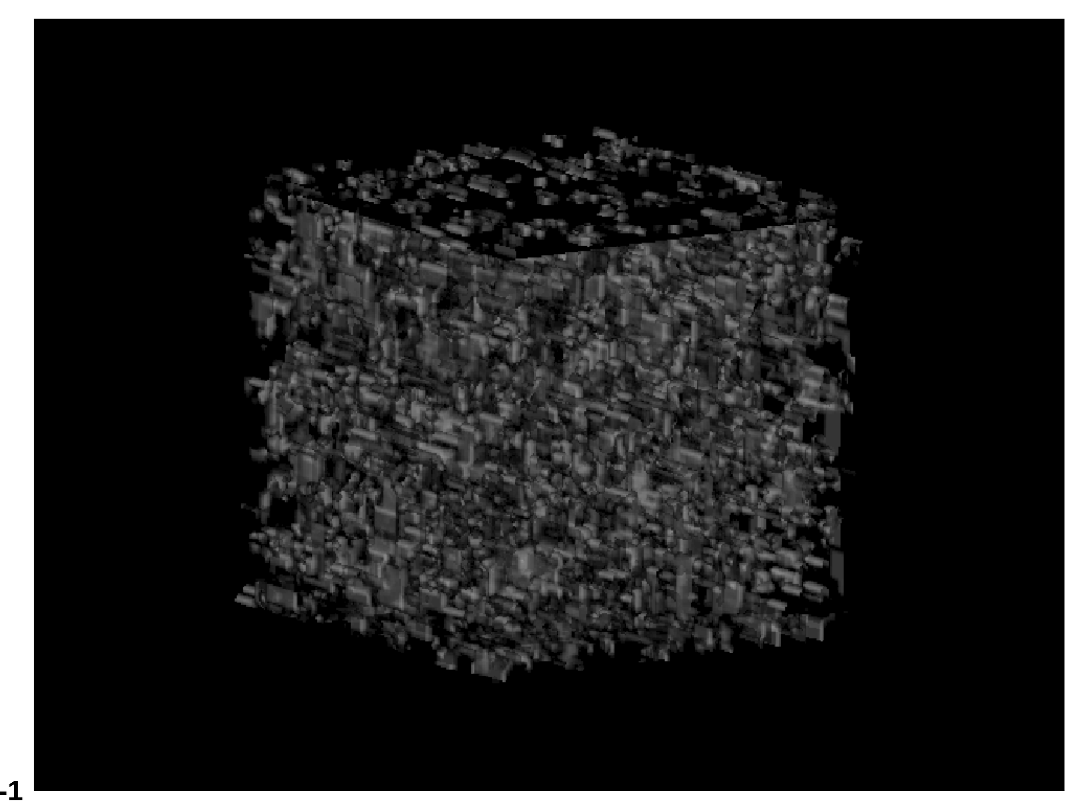
Activation energies:

trapping-detrapping 2.7 eV

desorption 1.9 eV

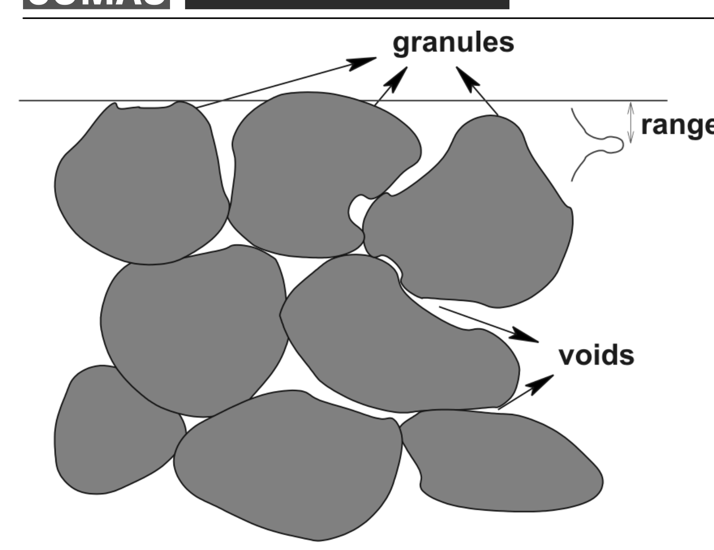
surface diffusion 0.9 eV,
jump attempt frequency w_0**~10^{13}s^{-1}** ,
jump step length **~35Å**

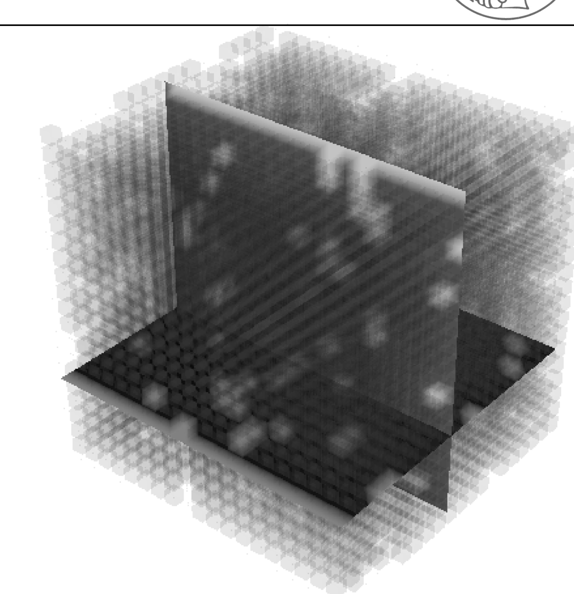
for entering the surface for a solute H atom 2.7 eV



porous graphite structure

Macroscales





Trapping - detrapping (2.7 eV)

Desorption (1.9 eV)

Surface diffusion (0.9 eV)

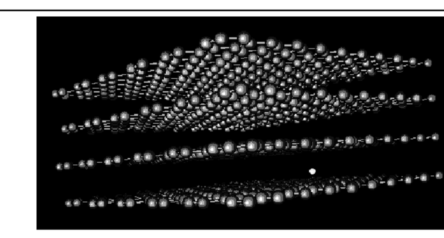
KMC with $\omega_o = 10^{13}\ (\mathrm{sec}^{-1})$

Jump lengths depend on the process

Monte Carlo Diffusion (MCD) used to simulate TGD

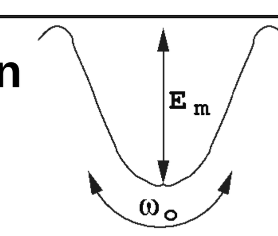
$$\Delta X = \sqrt{2D\Delta t}\,\boxed{?}$$

Molecular dynamics: graphite, hydrocarbons



$$\mathbf{m}\ddot{\vec{\mathbf{r}}}_{\mathbf{i}} = \sum_{\mathbf{j=1,j\neq i}}^{\mathbf{N}} \vec{\mathbf{f}}_{\mathbf{i,j}} = \sum_{\mathbf{j=1,j\neq i}}^{\mathbf{N}} -\vec{\nabla}\mathbf{U}_{\mathbf{i,j}}$$

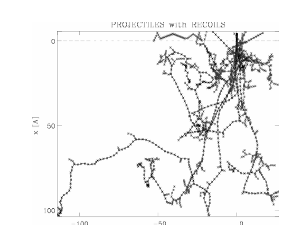
Kinetic MC: hydrogen diffusion

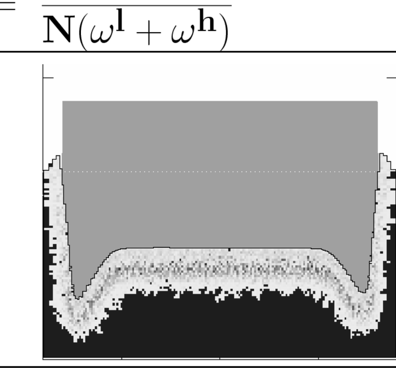


$$\omega^{\mathbf{l,h}} = \omega_{\mathbf{o}}^{\mathbf{l,h}}\, \mathbf{e}^{-\mathbf{E_m^{l,h}}/(\mathbf{k_B T})}$$

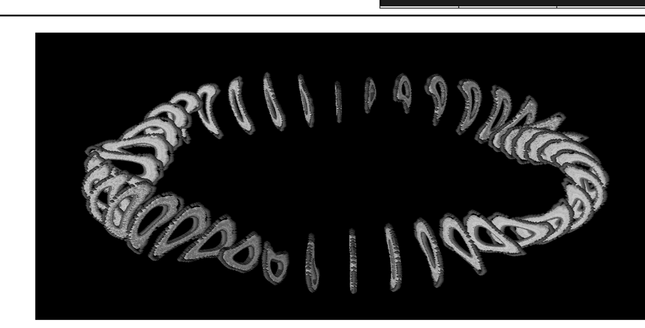
$$\mathbf{\Delta\ t} = \frac{-\ln(\mathbf{U})}{\mathbf{N}(\omega^{\mathbf{l}} + \omega^{\mathbf{h}})}$$

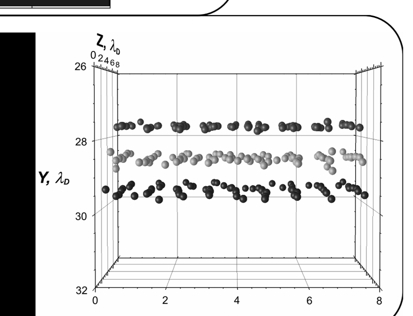
Binary collision approxmation:
2D/3D TRIDYN





Plasma transport: fusion plasmas,
low temperature plasmas





Quantum many particle systems: field theory, exact diagonalization, density matrix renormalization, quantum MC, maximum entropy methods