MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

Trap-Diffusion Equations in Constrained Geometries

ModPMI 2025

IAEA -Vienna

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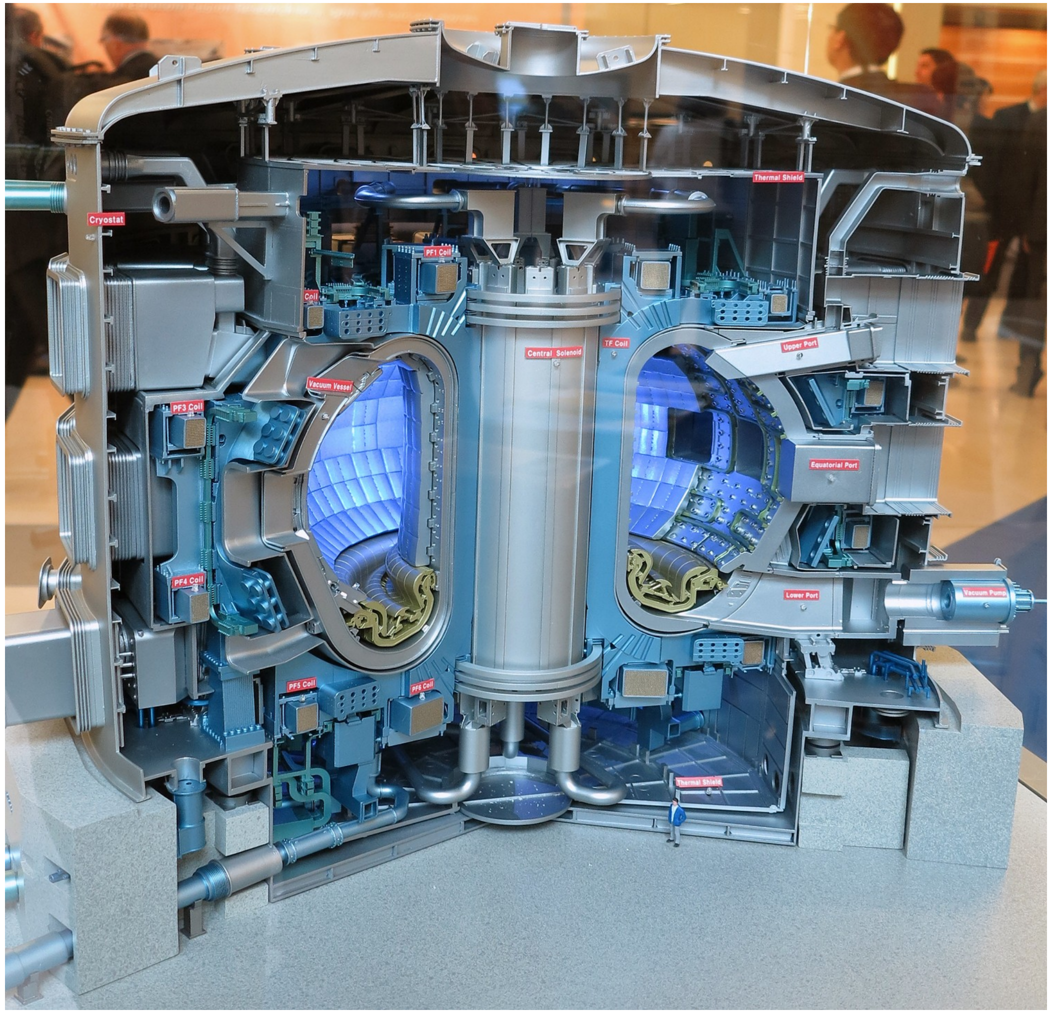
CONTENT

I. Motivation

- Modelling of hydrogen isotope (D, T) and He transport crucial for ITER & DEMO :
  - T retention
  - Isotope exchange
  - Influx to coolant
  - He bubble formation
  - Density control
  - ...



Source: Conleth Brady / IAEA

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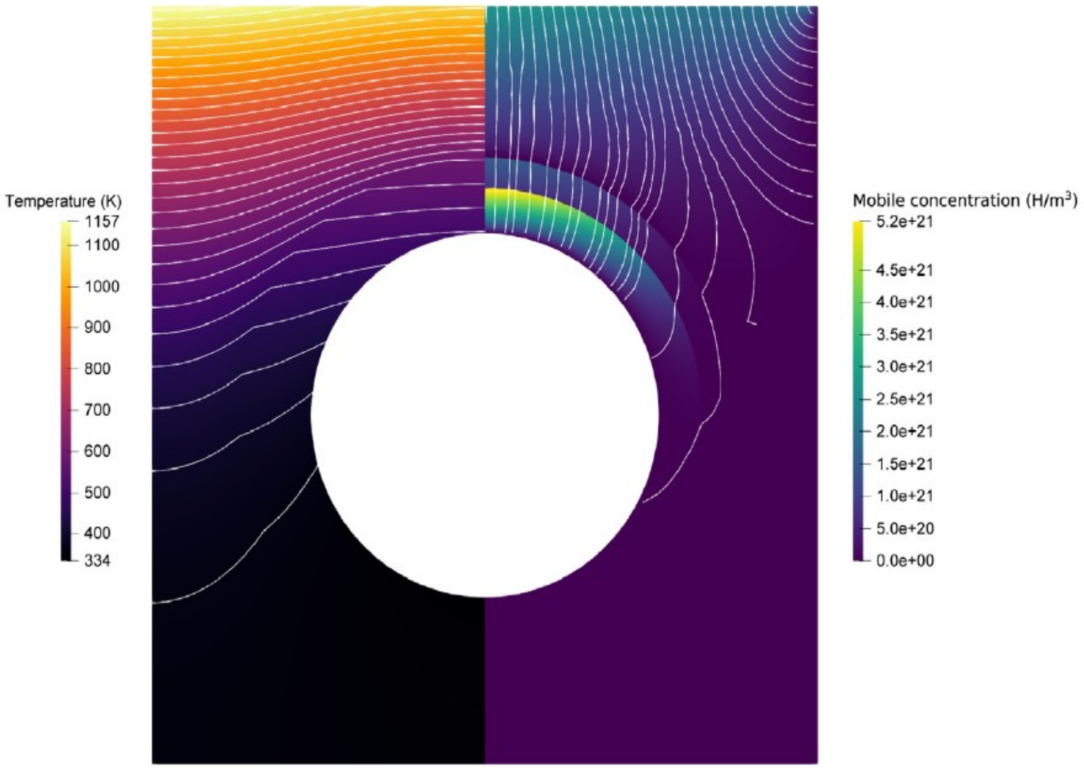
- Main modelling tool: Trap-Diffusion Codes, e.g.
  - TESSIM
  - FESTIM
  - MHIMS
  - RAVETIME
  - TMAP
  - …



Int. J. Hydrogen Energy 63 (2024) p. 786 :FESTIM

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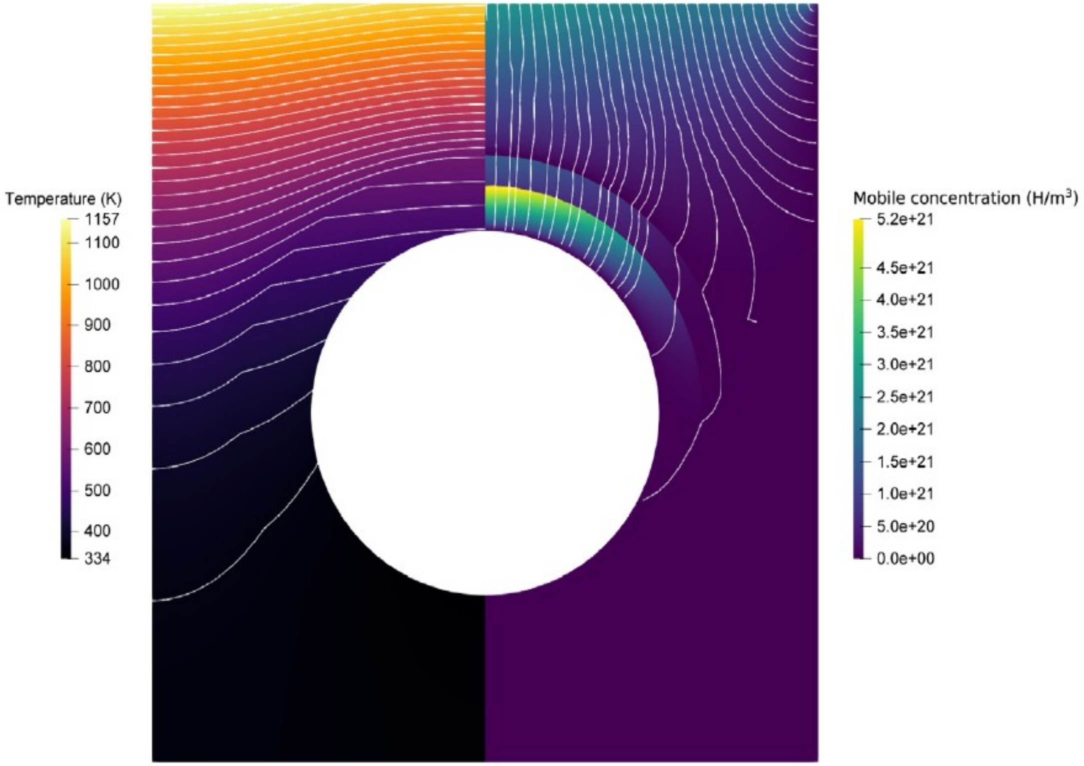


Int. J. Hydrogen Energy 63 (2024) p. 786 :FESTIM

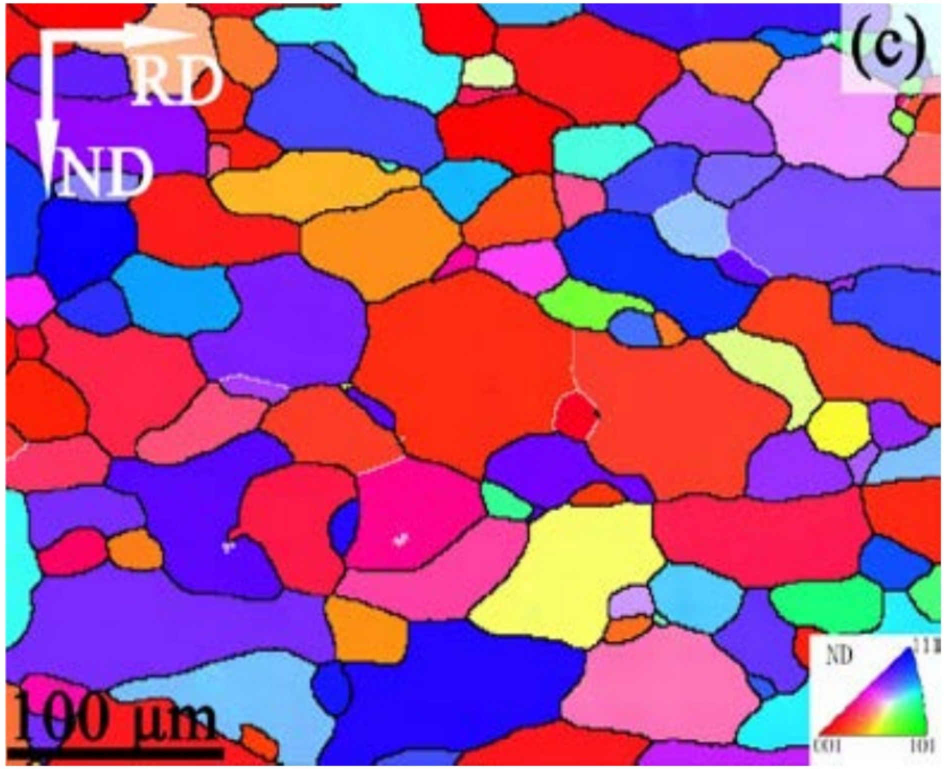
- All rely on the same mathematical loss model [1]: (with variations in the trap handling)

$$\frac{\partial c_H^S}{\partial t} = D\frac{\partial^2 c_H^S}{\partial x^2} - b\, c^T c^S + \gamma * c_t$$

[1] McNabb A, Foster PK. A new analysis of the diffusion of hydrogen in iron and ferritic steels. Trans Metall Soc AIME 227 (1963) p. 618–627

I. Motivation

Trap-Diffusion models are quite successful - but many relevant materials have structure which influences/dominates transport (e.g. via GB)



EBSD-orientation map of rolled W [1]

[1] Wang, K et al, JNM 540 (2020) p. 152412

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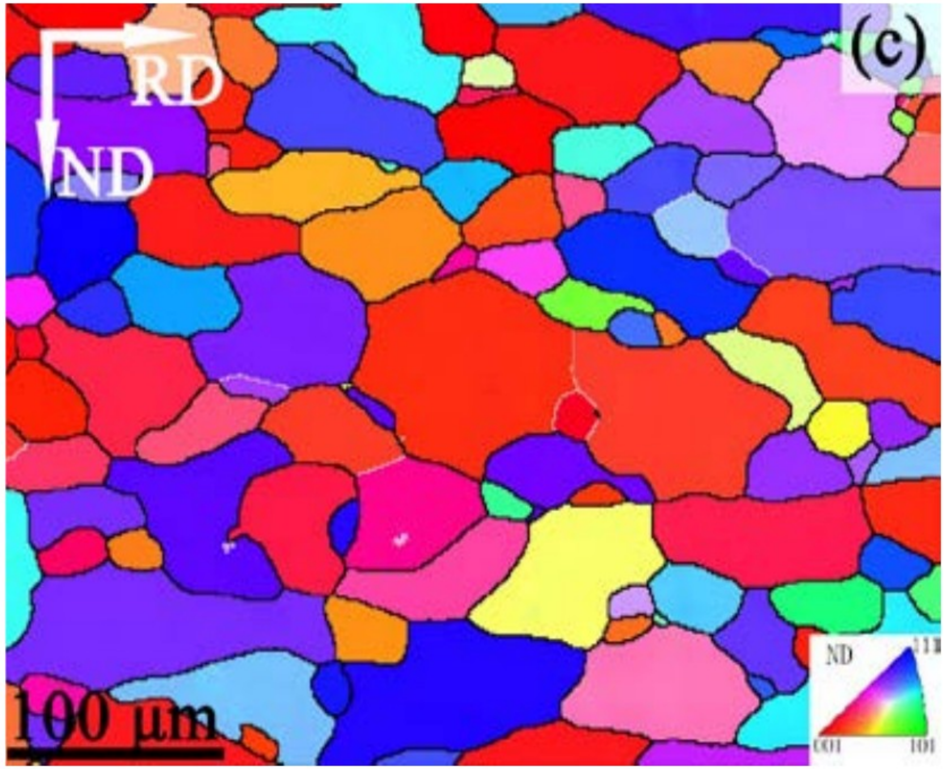

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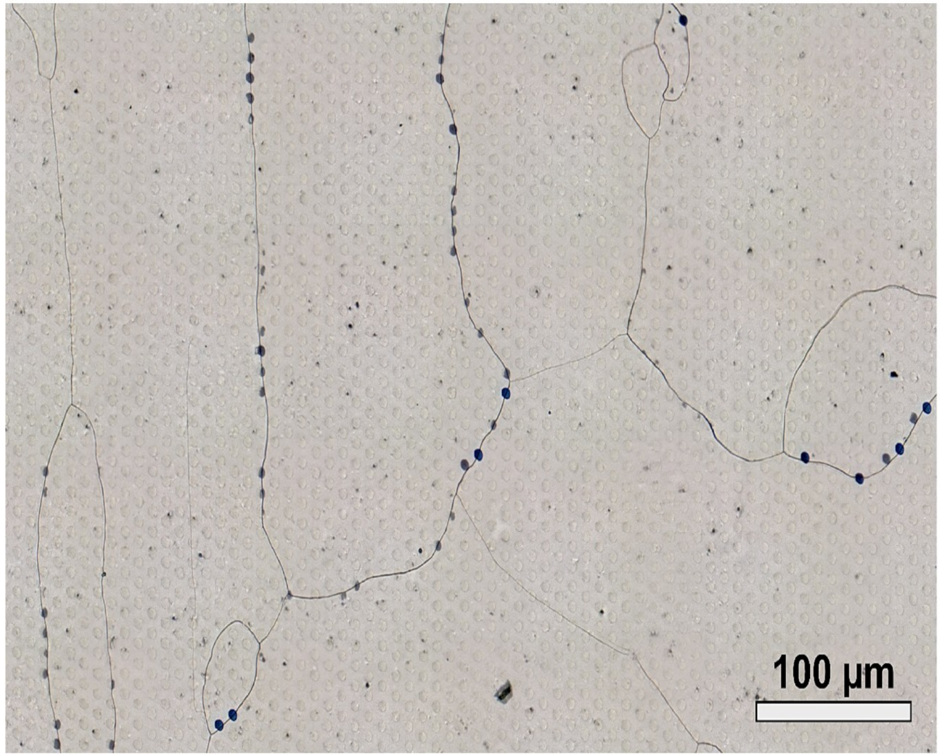


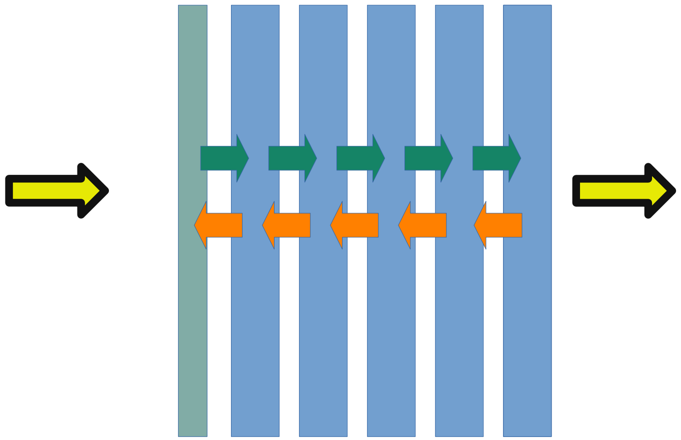
Hydrogenography: D permeating through some GBs [2,3]

→ Trap-diffusion models need to be adapted

[1] JNM 540 (2020) 152412,
[2] NME 36 (2023) 101498, [3] PhysScripta T145 (2011) 014036

I. Motivation

- ‘Obvious’ approach: use McNabb-model and generalize geometry



‘Standard’ sample profile

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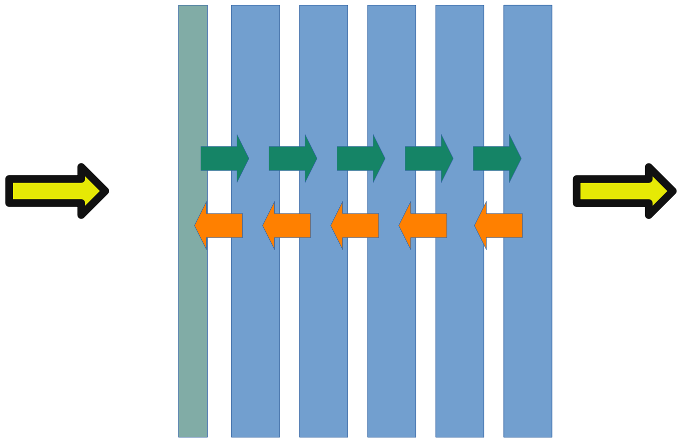

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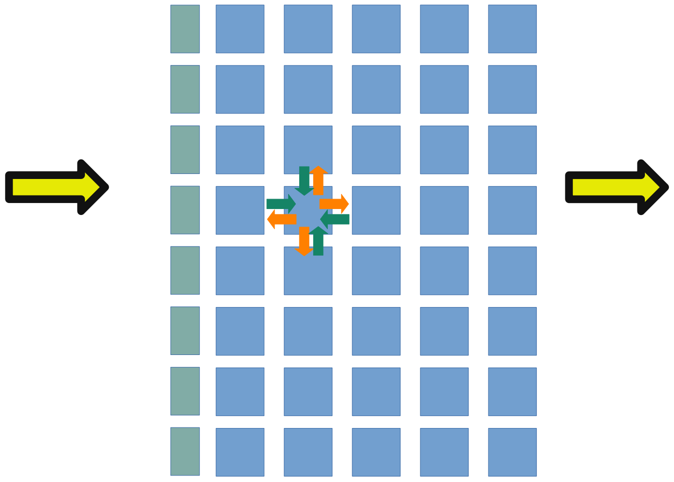

Extension to 2D/3D sample profile

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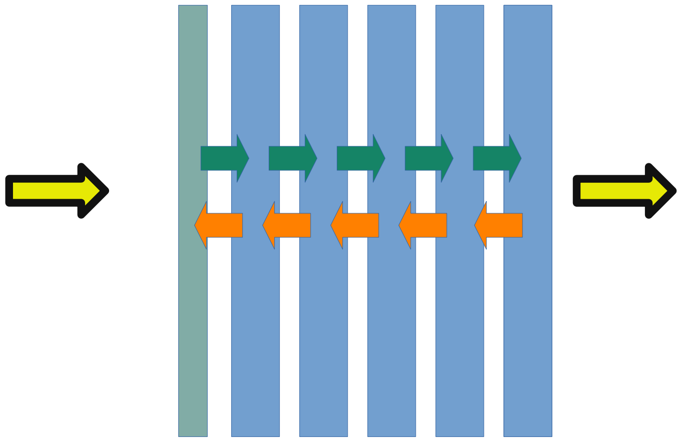

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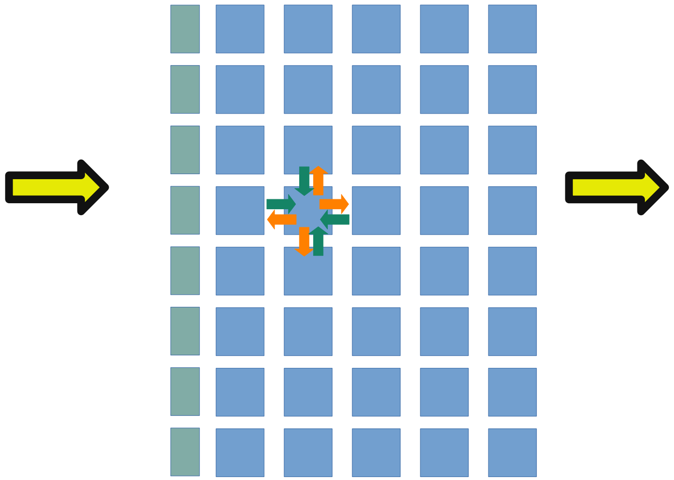

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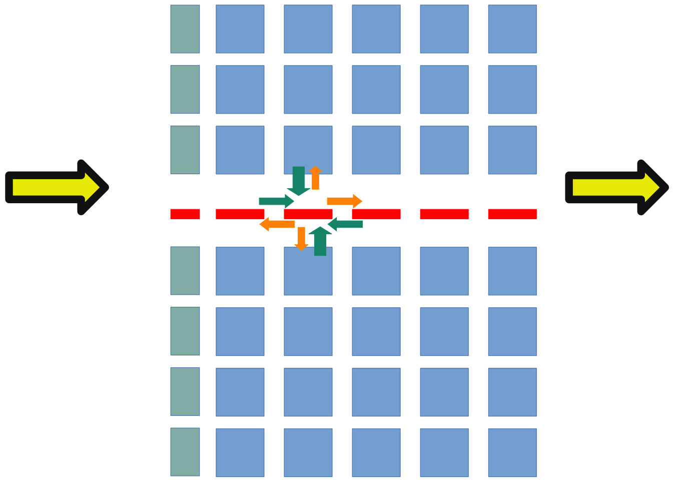

Represent GBs as ‘thin’ cells

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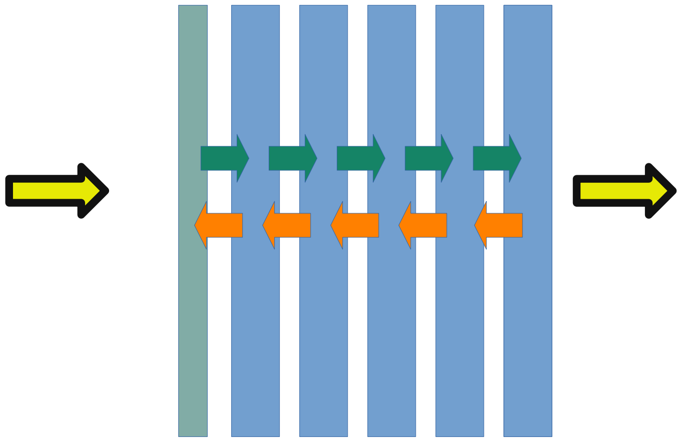

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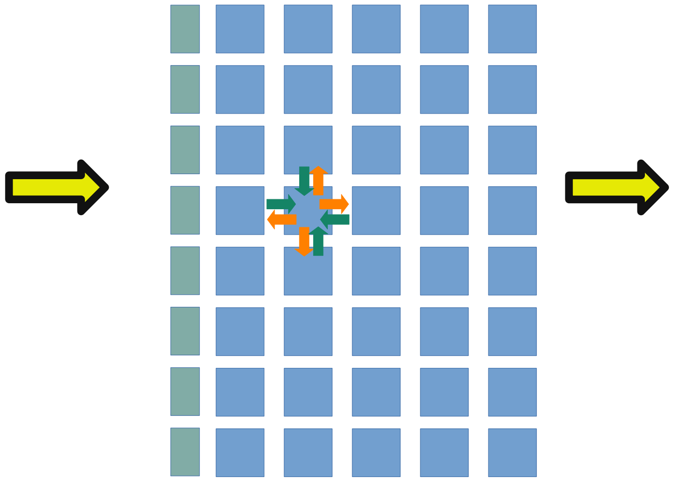

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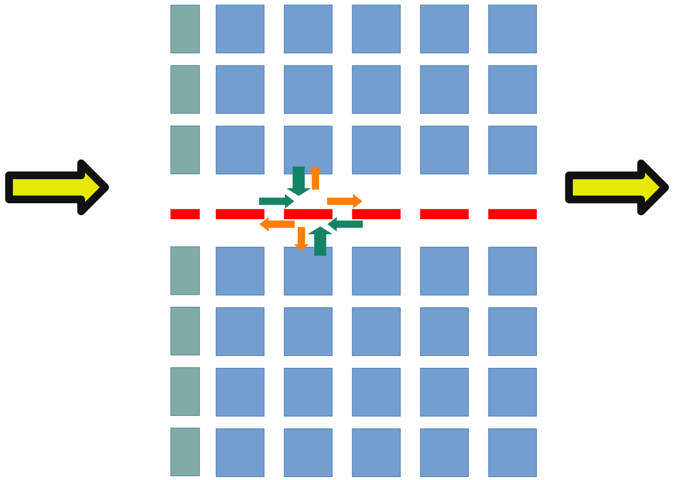


Represent GBs as ‘thin’ cells

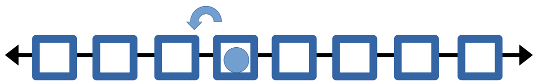
Given the correct parameters (e.g. from DFT) : Does this yield the correct answer?

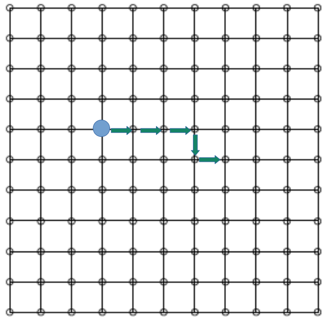
CONTENT

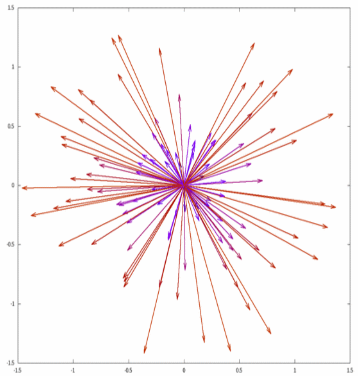
- Motivation
- **From Lattice-RW to Continuum Models**
  - **Diffusion only**
  - **Trapping**
  - **Release**
- Summary

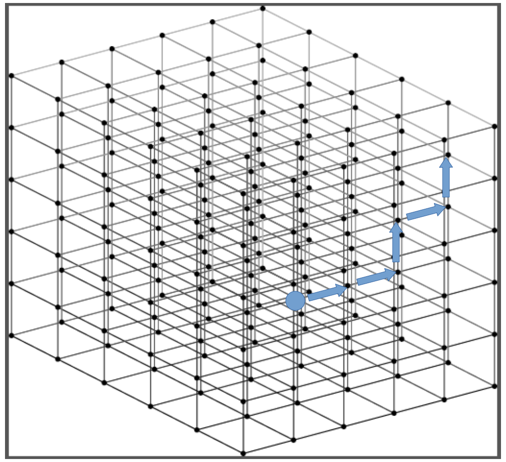
II. From Lattice-RW to Continuum Models

- Diffusion only (e.g. Einstein 1905): $c^T=0$









Atomistic Random Walk
with jump rate a [1/s]
and jump-length l_0 [nm]:

$D_d[nm^2/s] = a * l_0^2 / (2*d)$

$$\frac{\partial c_H^S}{\partial t} = D_d \frac{\partial^2 c_H^S}{\partial x^2}$$

Dimension of random
walk space: d (e.g. d=3)

II. From Lattice-RW to Continuum Models

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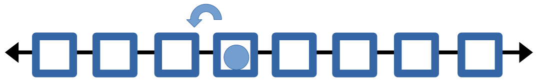

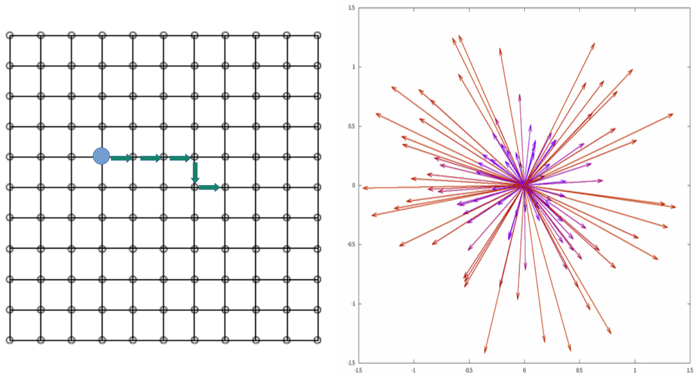

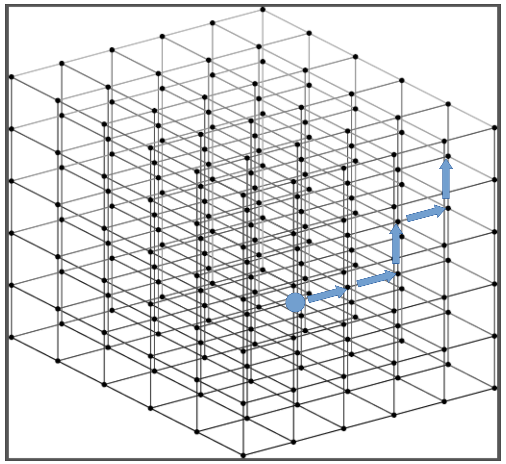

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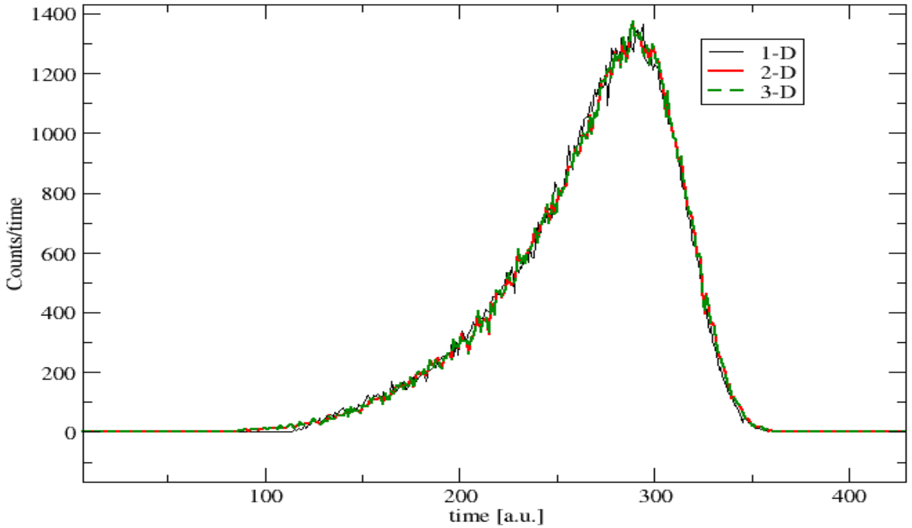
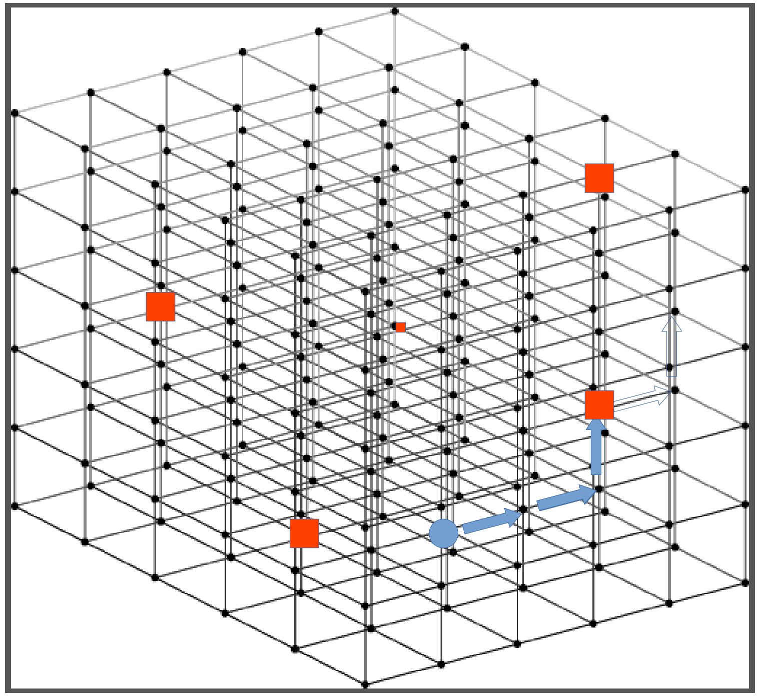


Simulation results of lattice-random-walk and continuum model agree

II. From Lattice-RW to Continuum Models

- Adding traps:



Adding traps : c^T Units: [TS/LS]
Assumption (Foster-McNabb-model):

loss rate ~ **trap concentration** * solute concentration = $c^T * c^S$

$$\frac{\partial c_H^S}{\partial t} = D\frac{\partial^2 c_H^S}{\partial x^2} - b\,c^T * c^S + \gamma * c_t$$

For uniform concentration (no diffusion) and γ=0 :

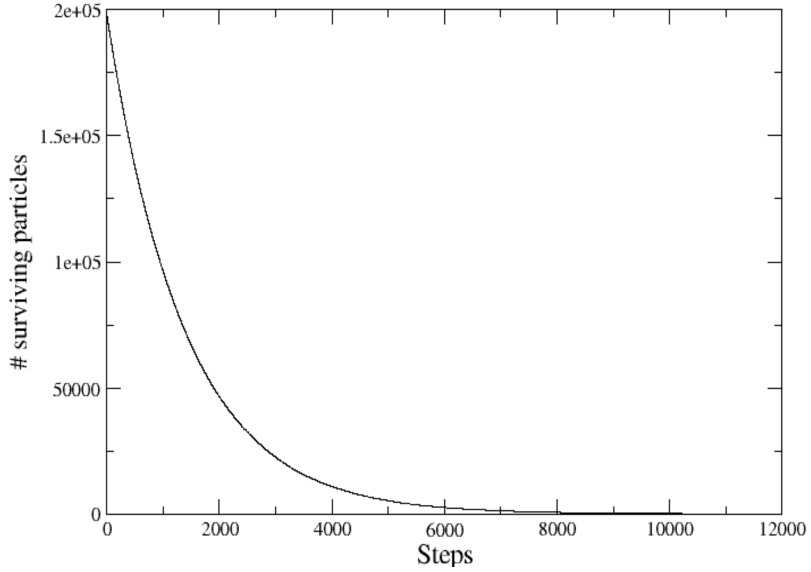
$$c_H^S(t) = C_{H_0}^S * \exp\left(-b * c^T * t\right)$$

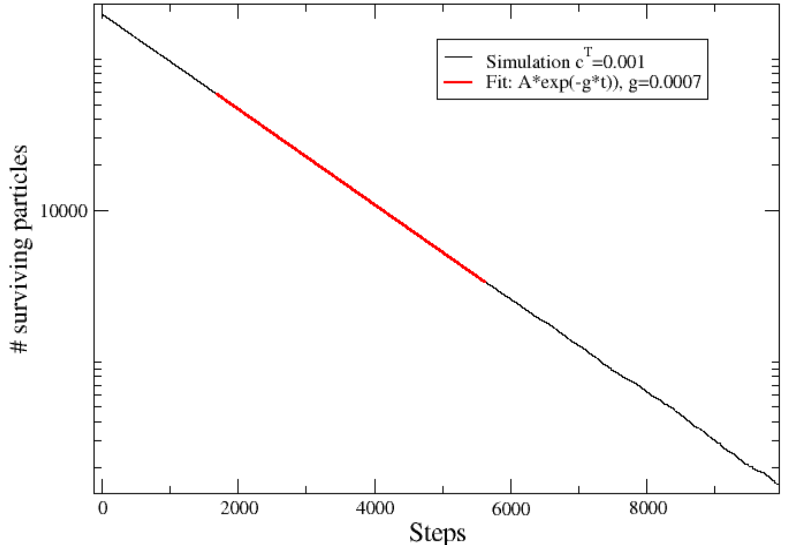
Expectation:

Exponential decay of solute with #steps with c^T as parameter

II. From Lattice-RW to Continuum Models

- Adding traps: **3-D lattice**





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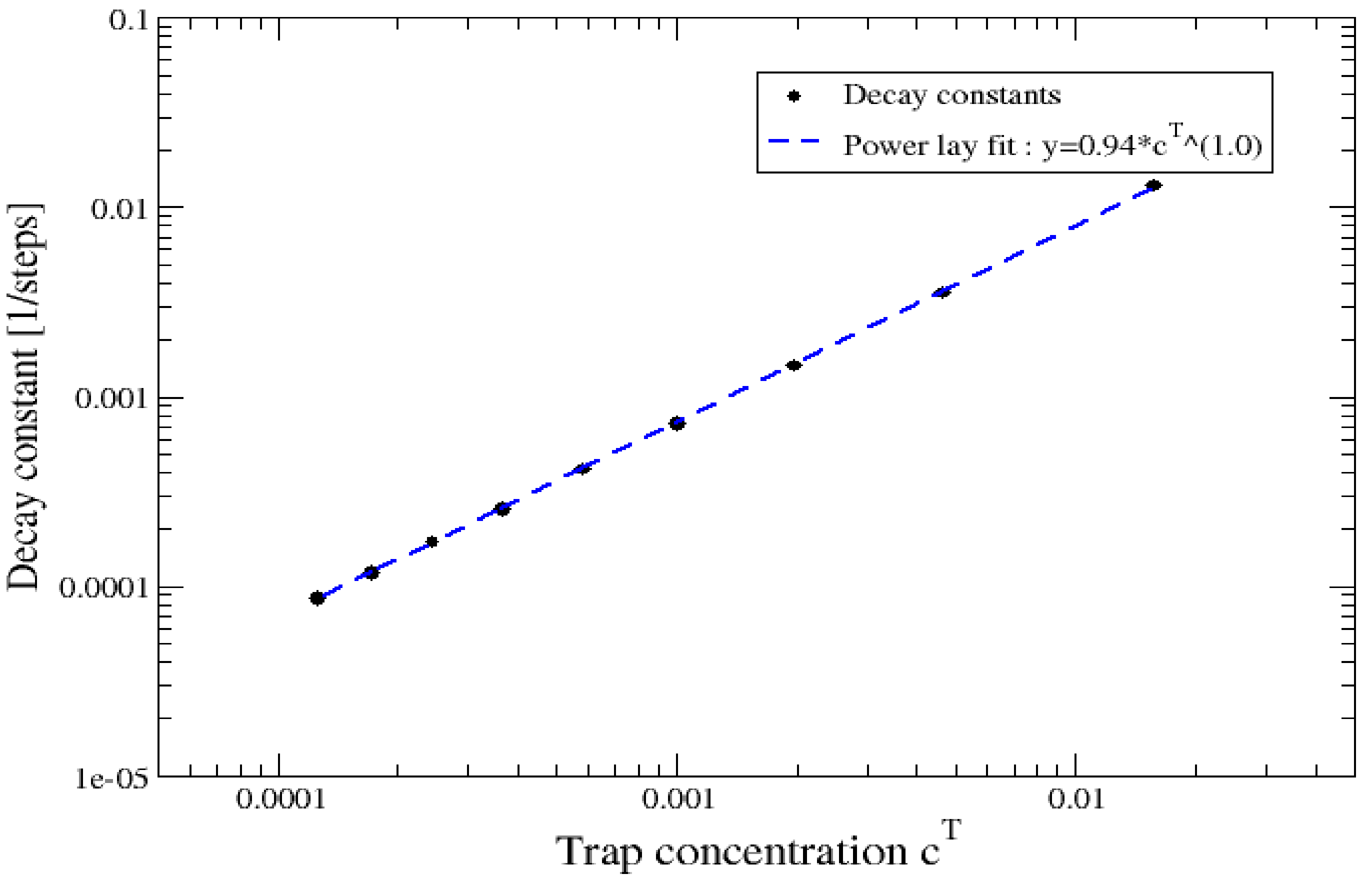
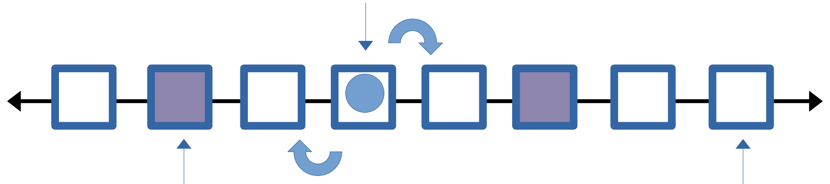


Simulation results of 3D-lattice-random-walk and continuum model agree : $\lambda \sim c_T$

II. From Lattice-RW to Continuum Models

- Adding traps: **1-D lattice**



- Random Walk with nearest-neighbour jumps

- Lattice with (partially) absorbing trap sites

- Periodic boundary conditions (infinite lattice)

- Trap concentration : $c_T = N_T/N$

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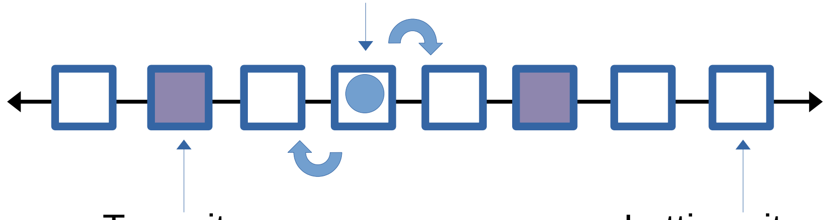

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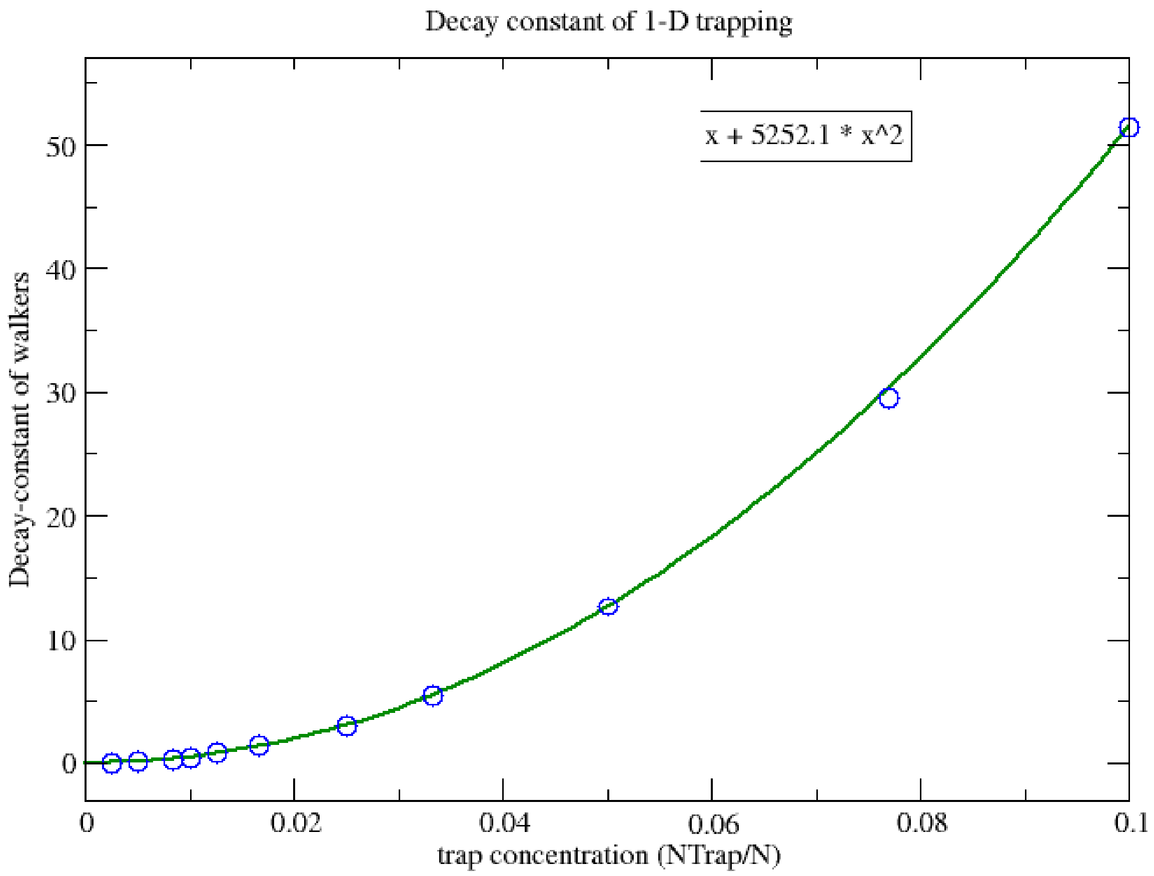
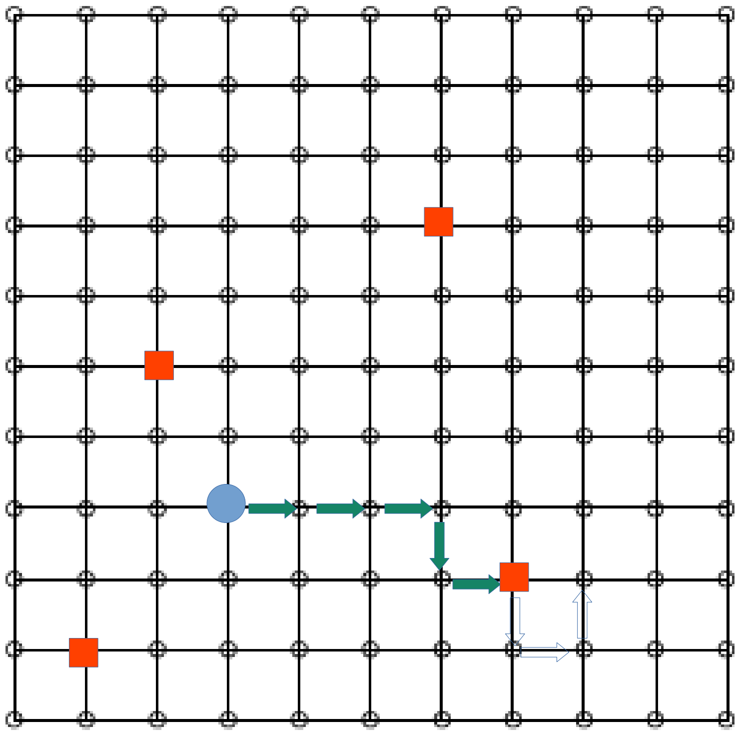


Simulation results of 1D lattice-random-walk and McNabb-continuum model disagree : $\lambda \sim (c_T)^2$

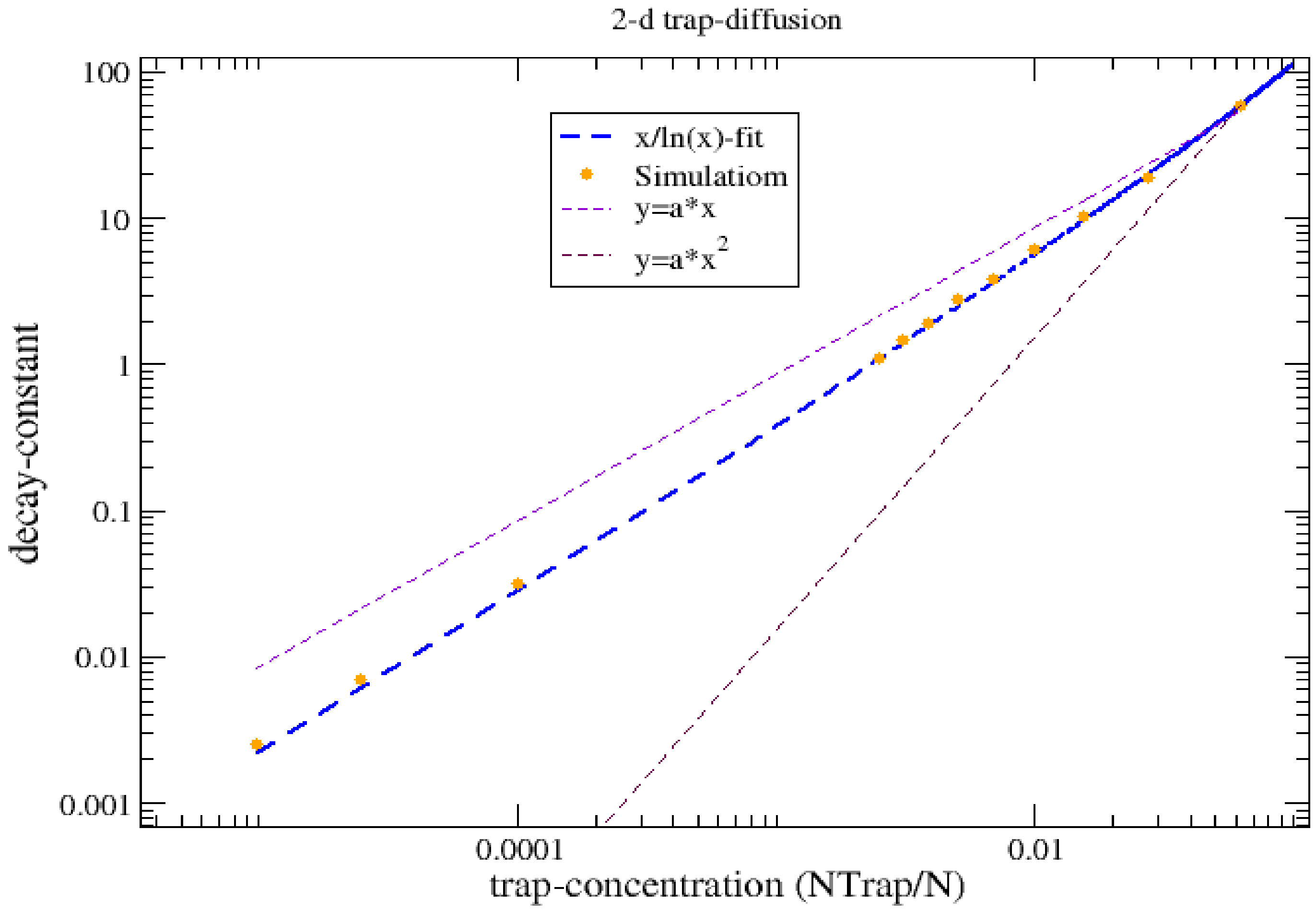
II. From Lattice-RW to Continuum Models

- Adding traps: **2-D lattice**



$$c_H^S(t) = \ldots$$

$$\ldots C_{H_0}^S * \exp\left(-b * c^T / \ln\left(c^T\right) * t\right)$$



Simulation results of 2-D lattice-random-walk and McNabb-continuum model disagree : $\lambda \sim c^T / \ln(c_T)$

II. From Lattice-RW to Continuum Models

- Adding traps:

Dimension	decay-constant
1-D	$\sim (c^T)^2$
2-D	$\sim c^T / \ln(c^T)$
3-D	$\sim c^T$
4-D	$\sim c^T$

Explanation:

survivial probability $p(n) = (1-c^T)^n \sim \exp(-c^T * n)$ but with p_T i.i.d (!)

Leading order correction: n should be the number of *distinct sites* instead, c.f. [1]

[1] H. B. Rosenstock, J. Math. Phys. 21(7) (1980) p. 1643-1645

II. From Lattice-RW to Continuum Models

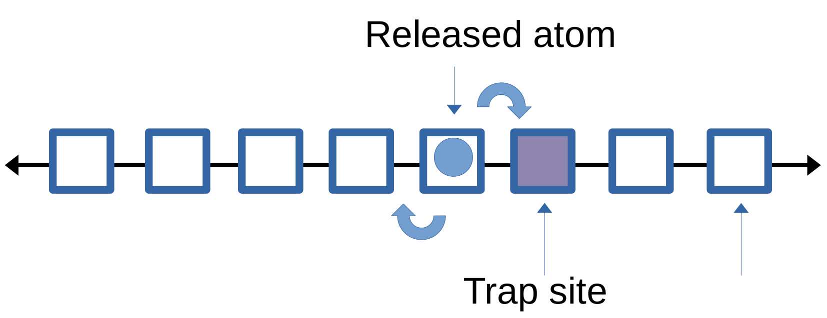
- **Release** from traps:

- Detrapping rate from traps:
  Foster-McNabb : ~ γ_0 c_t
  (independent of c^T !)

- Does this hold ? ↔ Strong spatial correlation of trap site and release site ...

$$\frac{\partial c_H^S}{\partial t} = D \frac{\partial^2 c_H^S}{\partial x^2} - b\, c^T * c^S + \gamma_0 * c_t$$

$$\frac{\partial c_t}{\partial t} = b\, c^T * c^S - \gamma_0 * c_t$$



Related to sink-strength-concept [1,2] : consider also size and shape of traps for effective detrapping rates

[1] Ahlgren, T.; Heinola, K. Improvements to the Sink Strength Theory, Materials 13 (2020), 2621
[2] Brailsford, A.D.; Bullough, R., Theory of sink strengths. Philos. Trans. R. Soc. 302 (1981), p. 87

II. From Lattice-RW to Continuum Models

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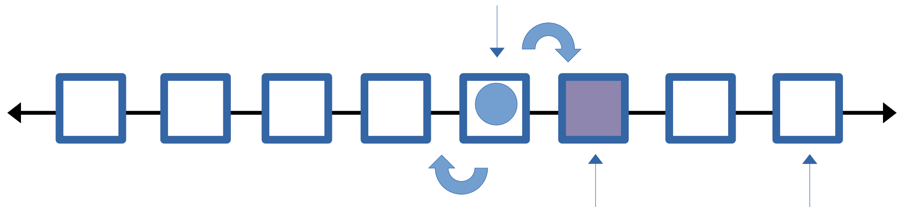
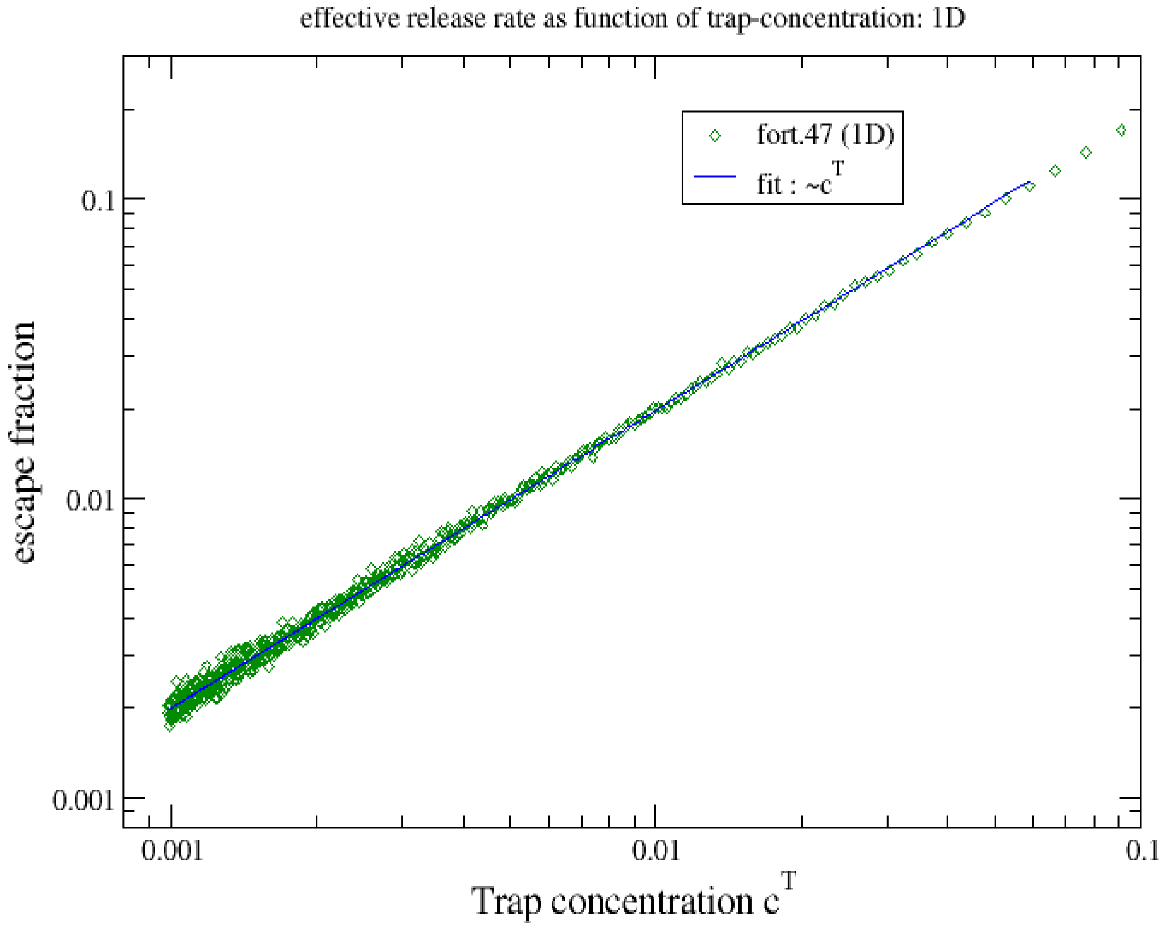


- Atom always starts next to releasing trap:
  prompt retrapping likely

- **Effective release rate**? Definition?

- e.g. p of reaching at least ½ trap distance

- Trap concentration : $c_T = N_T/N$



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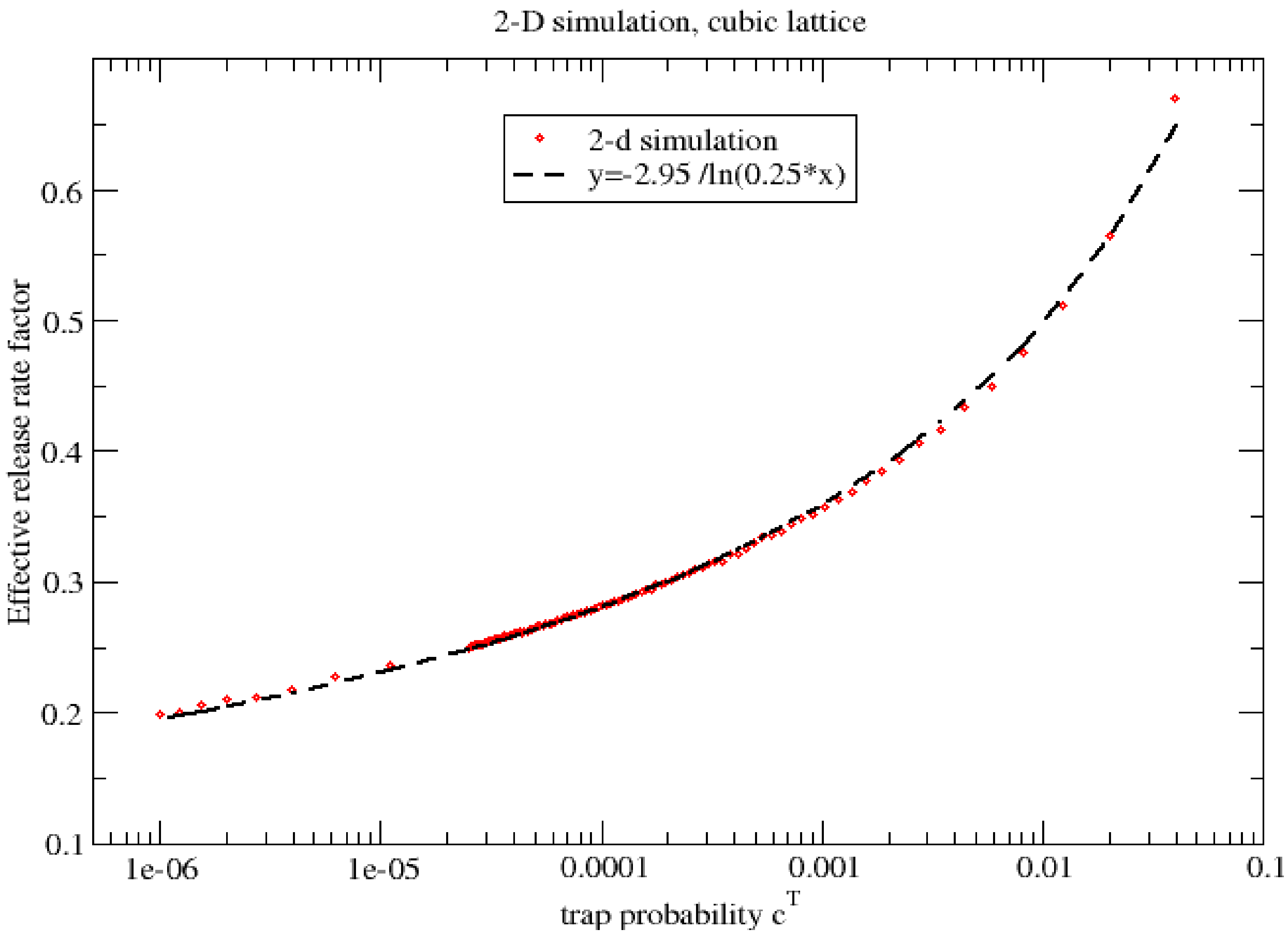
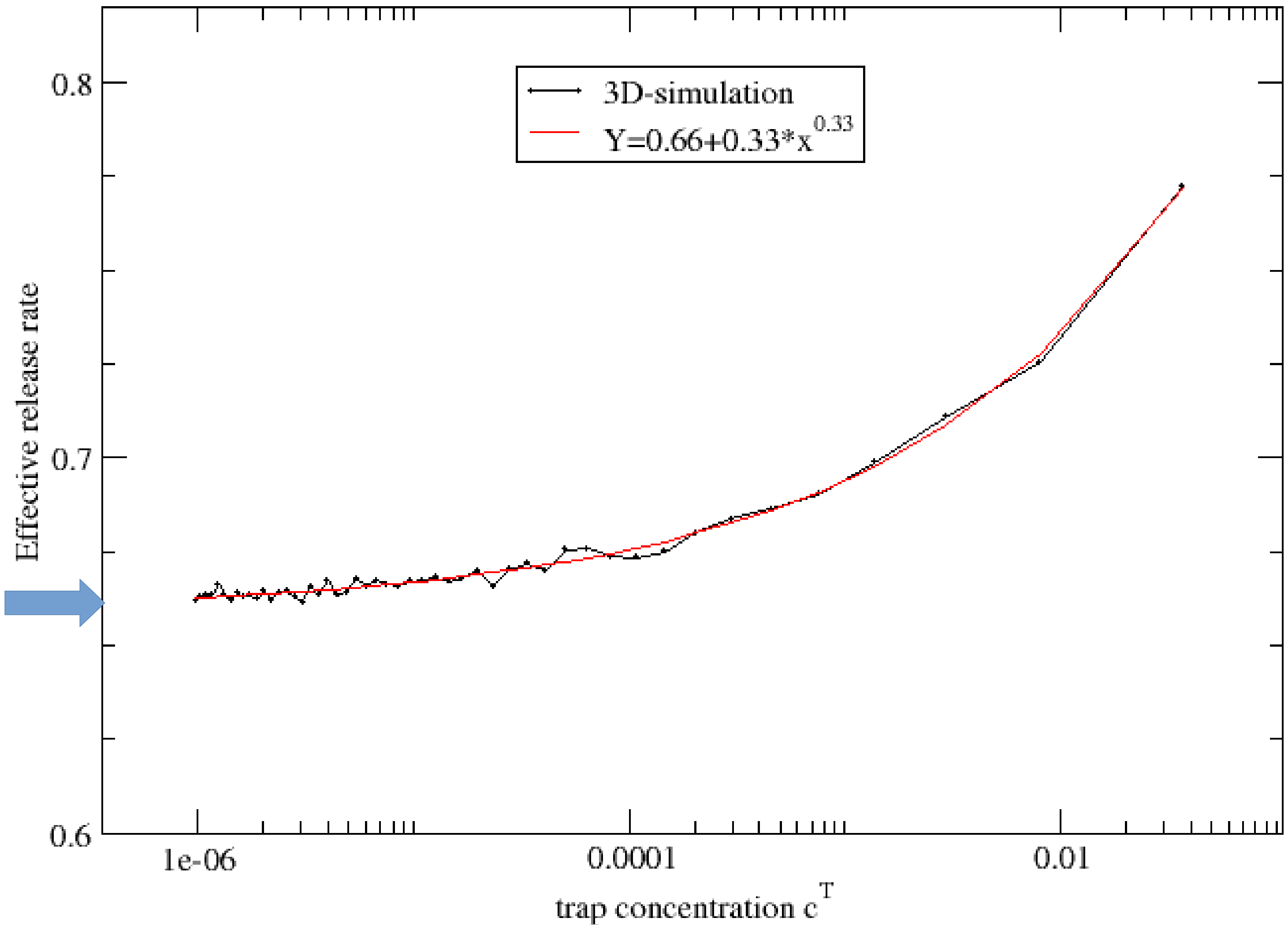


II. From Lattice-RW to Continuum Models

- **Release** from traps: 3D



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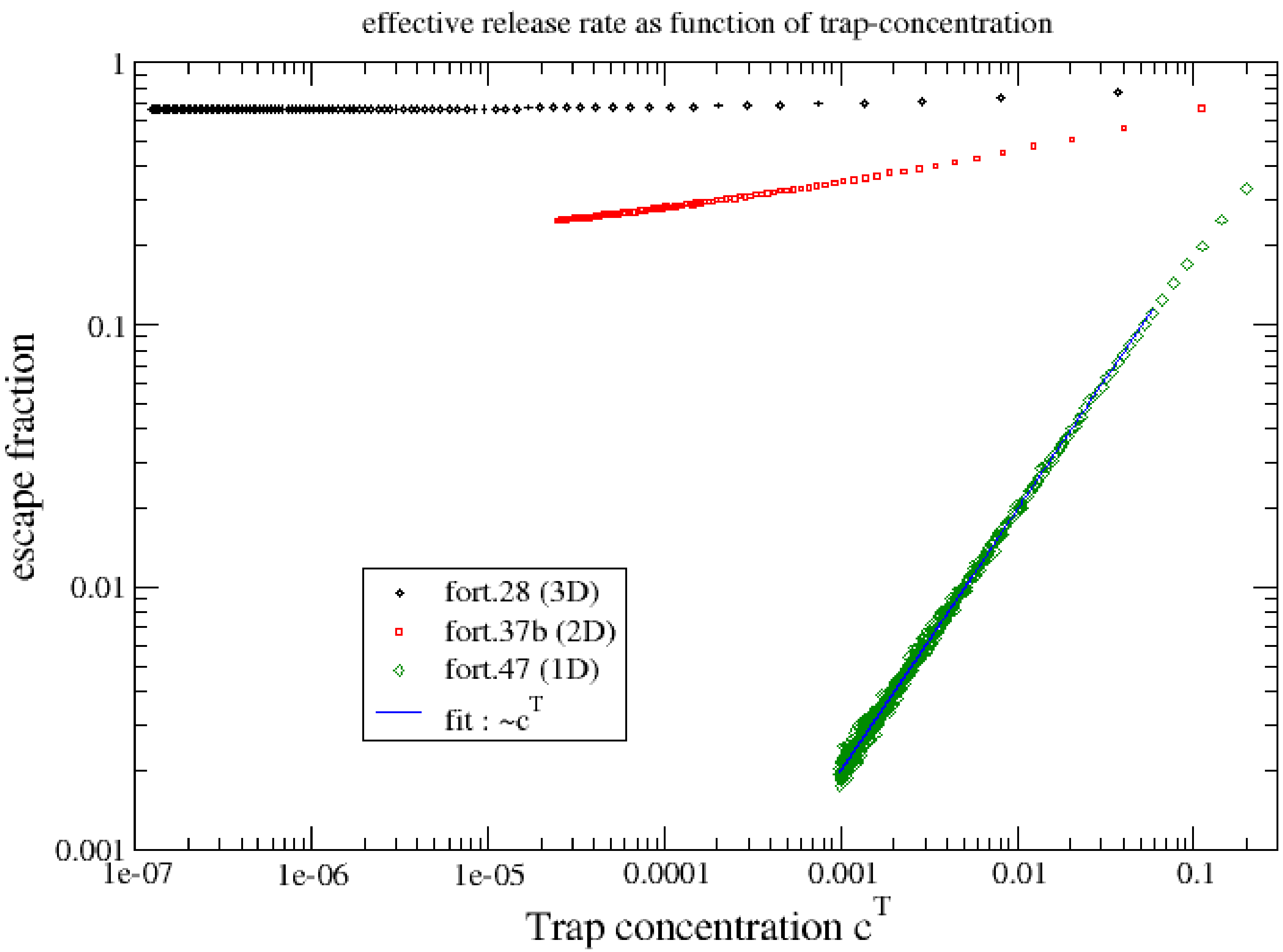


Effective release rate:

- 3D case essentially independent of c^T (→ McNabb oK)
- 1D- and 2D-cases need to consider c^T

II. From Lattice-RW to Continuum Models

- **Summary**:

$$\frac{\partial c_H^S}{\partial t} = D\frac{\partial^2 c_H^S}{\partial x^2} - b\, f_d(c^T) * c^S + \gamma_0 * c_t * g_d(c^T)$$

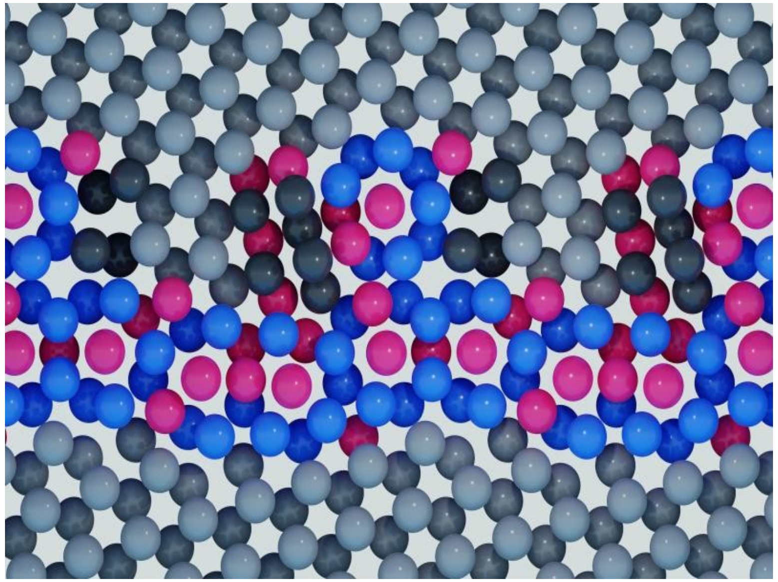
$$\frac{\partial c_t}{\partial t} = b\, f_d(c^T) * c^S - \gamma_0 * c_t * g_d(c^T)$$

Dimension	decay-constant (trapping of solute) $f(c_T)$	escape fraction from traps $g(c_T)$
1-D	$\sim (c^T)^2$	$\sim c^T$
2-D	$\sim c^T / \ln(c^T)$	$\sim 1/\ln(a*c^T)$
3-D	$\sim c^T$	~ const
4-D	$\sim c^T$	~ const

Conclusions

- Trap-diffusion models depend on dimensionality
- Implementation in standard trap-diffusion models feasible (c.f. RAVETIME), provided quantities like
  - Trap-rate
  - Effective detrapping-rate
  - Blocking efficiency
  - ...

  are derived from lattice-calculations
- Not all cases can be mapped into standard form



GB segregation, Fe atoms (red), Ti (blue&grey), Science 386, p. 420-424 (2024)

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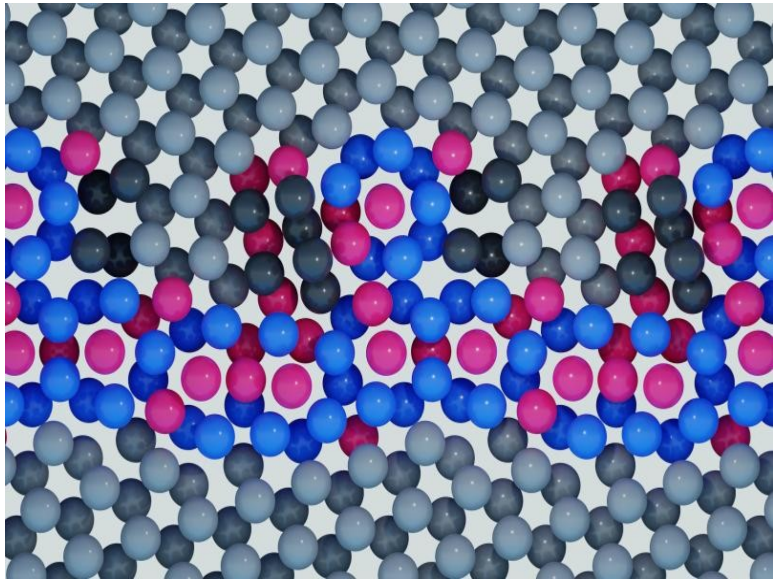

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Thank you! Questions?

Comparison of SDTrimSP and SRIM

‘Simulation of ion beam sputtering with SDTrimSP, TRIDYN and SRIM’
by
H. Hofsäss , K. Zhang and A. Mutzke
Applied Surface Science 310 (2014), p. 134-141

SRIM yields unphysical
sputter yield distribution for non-perpendicular impact

‘Origin of overestimation of vacancies in SRIM’ in Current Opinion in Solid State and Material Science 27(6) (2023) by Lin et al.,
https://doi.org/10.1016/j.cossms.2023.101120

SRIM-2013 vacancy profiles are far too high