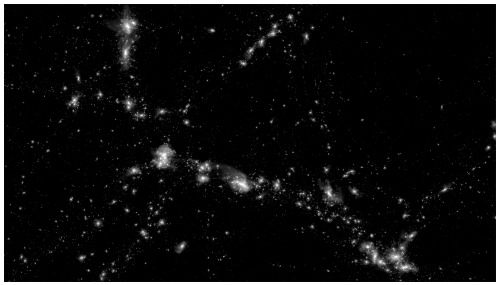
Kinetic (Lattice) Monte Carlo for Helical Molecules and Magnetic Substrates

Jeffrey Kelling

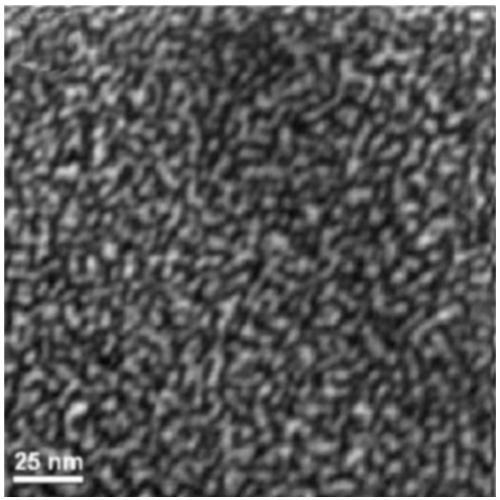
13th November 2020

Applications for Monte Carlo: Stochastic Prosesses

Phase Separation



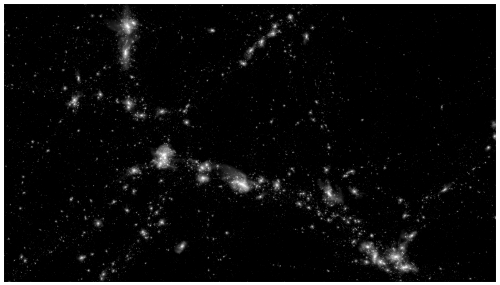
IllustrisTNG



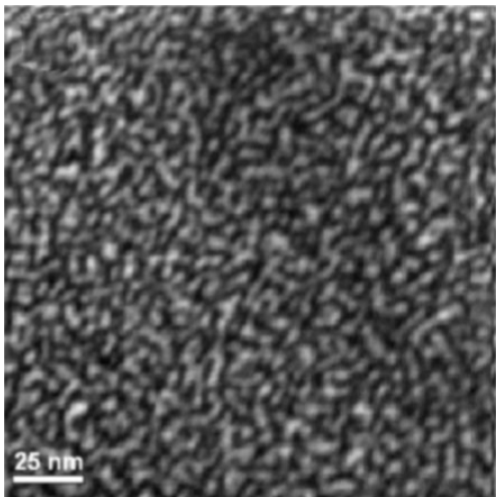
Müller, T., Heinig, K.-H. et al. *Appl. Phys. Lett.* **85** 2373 (2004)

Applications for Monte Carlo: Stochastic Prosesses

Phase Separation



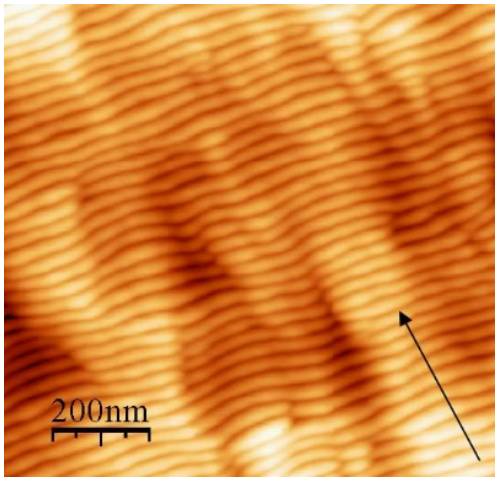
IllustrisTNG



Müller, T., Heinig, K.-H. et al. *Appl. Phys. Lett.* **85** 2373 (2004)

Driven Systems

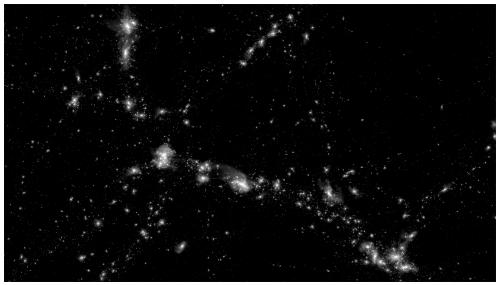
http://en.wikipedia.org/wiki/File:Rub_al_Khali_002.JPG



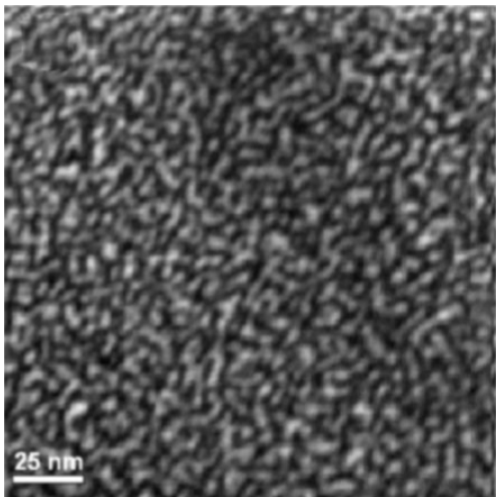
https://www.hzdr.de/db/Cms?pOid=24344&pNid=2707

Applications for Monte Carlo: Stochastic Prosesses

Phase Separation



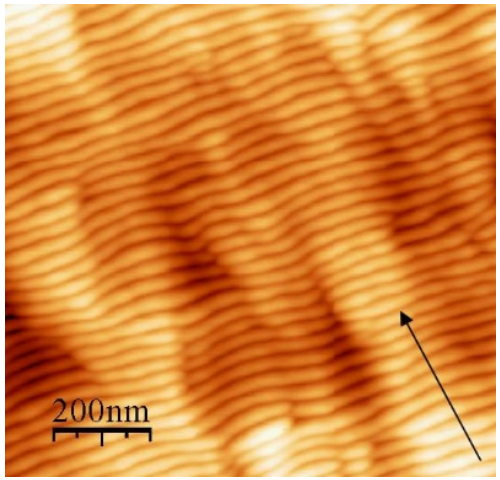
IllustrisTNG



Müller, T., Heinig, K.-H. et al. *Appl. Phys. Lett.* **85** 2373 (2004)

Driven Systems

http://en.wikipedia.org/wiki/File:Rub_al_Khali_002.JPG



https://www.hzdr.de/db/Cms?pOid=24344&pNid=2707

- game theory
  e. g.: Perc, Matjaž *Eur. J. Phys.* **38**(4) 045801 (2017)
  - sociology
  - finance
  - ...

1 Kinetic Metropolis Lattice Monte Carlo (KMC)
- Multi-Surface Simulations

2 Example I: Phase separation in inhomogeneous systems

3 Example II: Structure formation under ion irradiation

4 Modeling in B2

Kinetic Metropolis Lattice Monte Carlo (KMC)

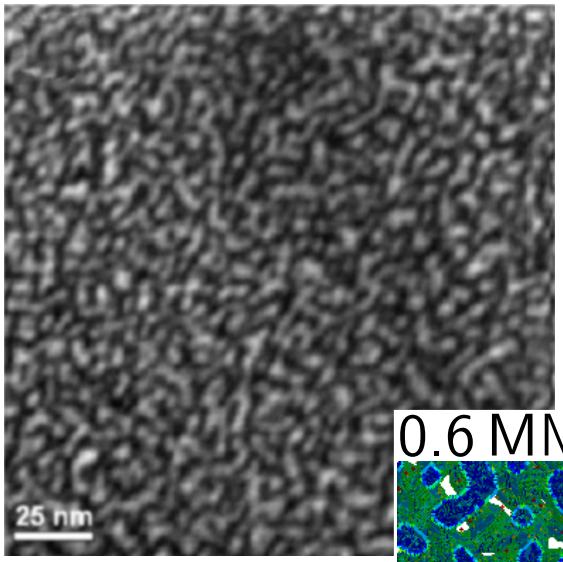
1 Kinetic Metropolis Lattice Monte Carlo (KMC)
- Multi-Surface Simulations

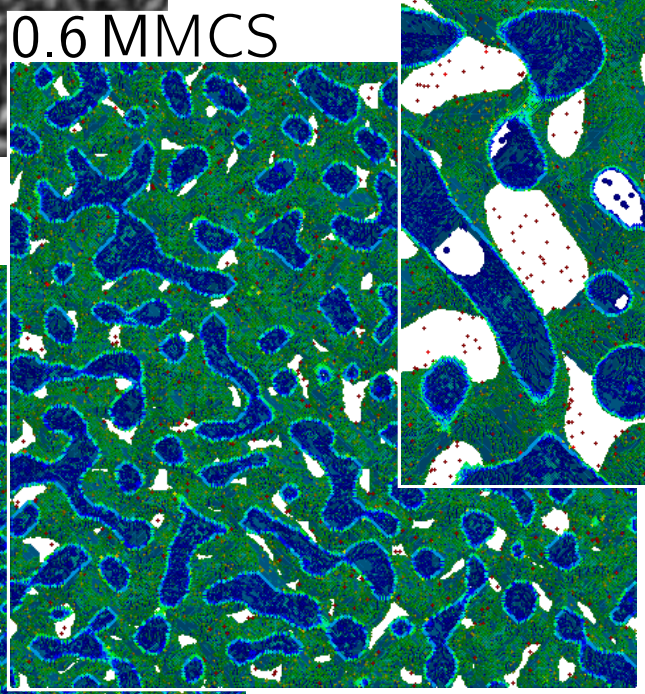
2 Example I: Phase separation in inhomogeneous systems

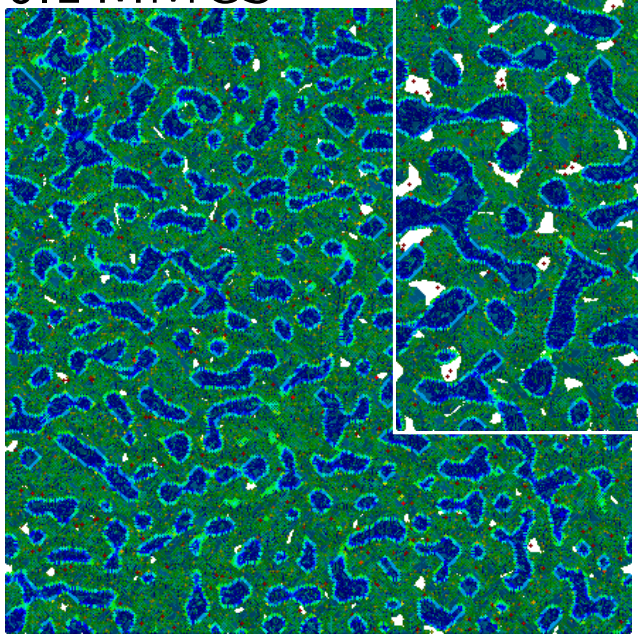
3 Example II: Structure formation under ion irradiation

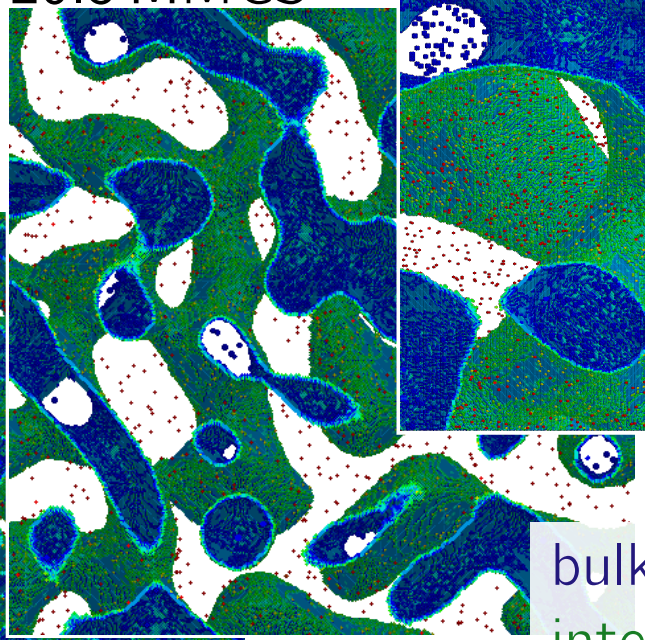
4 Modeling in B2

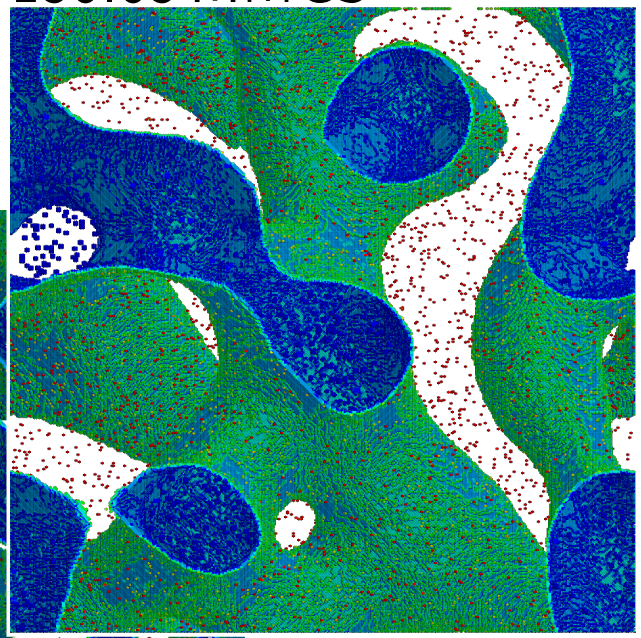
Simulation of Nano Structure Self-Organization





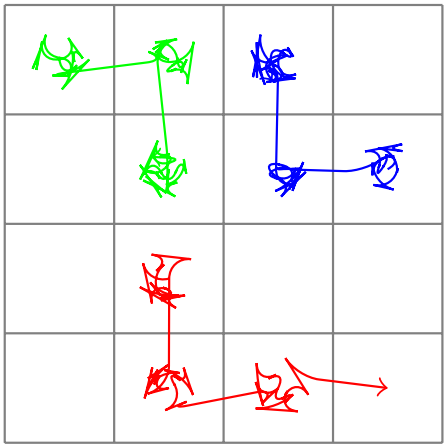






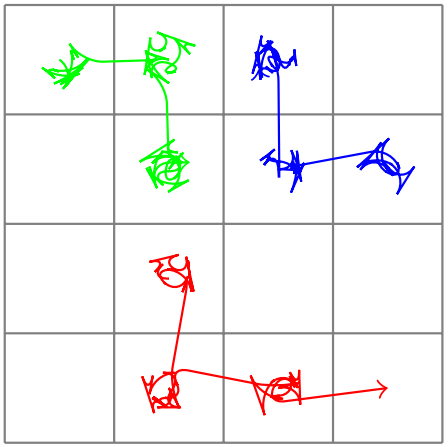
bulk particle
interface particle
dissolved particle
empty space:
embedding matrix

Molecular Dynamics



movement of impurity atoms

Molecular Dynamics



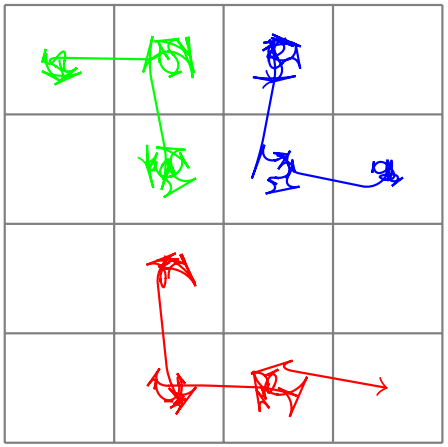
movement of impurity atoms

solve Hamilton's equations

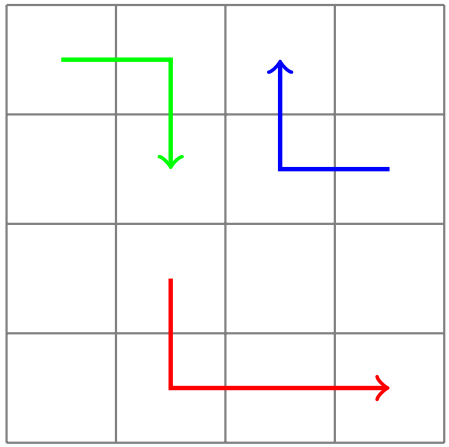
$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \text{ and } \dot{q}_i = \frac{\partial H}{\partial p_i}$$

$\Rightarrow$ "nature's random number generator"

Molecular Dynamics $\rightarrow$ Cellular Automaton



movement of impurity atoms



on–lattice movement of impurity atoms

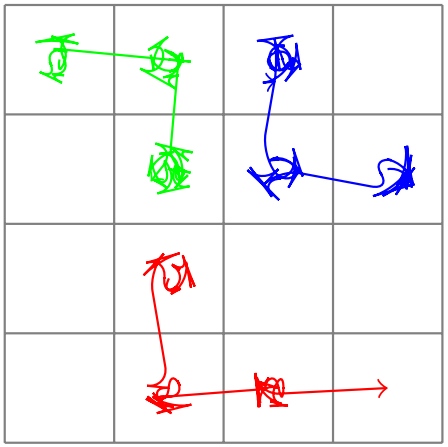
solve Hamilton's equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \text{ and } \dot{q}_i = \frac{\partial H}{\partial p_i}$$

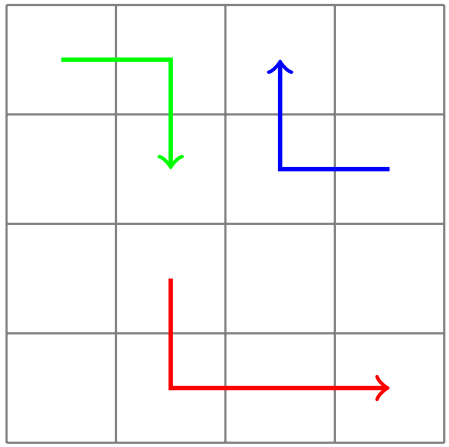
$\Rightarrow$ "nature's random number generator"

$\Rightarrow$ just use simple RNG

Molecular Dynamics → Cellular Automaton



movement of impurity atoms



on–lattice movement of impurity atoms

solve Hamilton's equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \text{ and } \dot{q}_i = \frac{\partial H}{\partial p_i}$$

⇒ "nature's random number generator"

⇒ just use simple RNG

- we know how, from *thermodynamics*

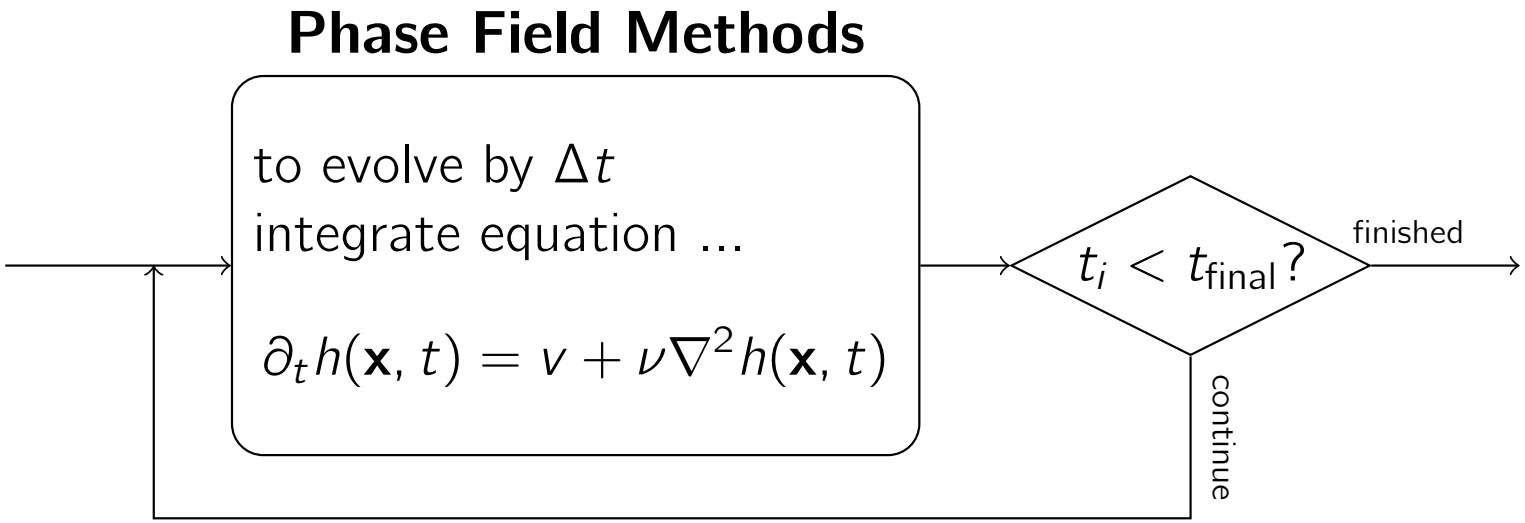
⇒ stochastic process defined by Metropolis algorithm[a]

[a] Strobel, Heing, Möller, *Phys. Rev. B* **64** 245422 (2001)

Simulation

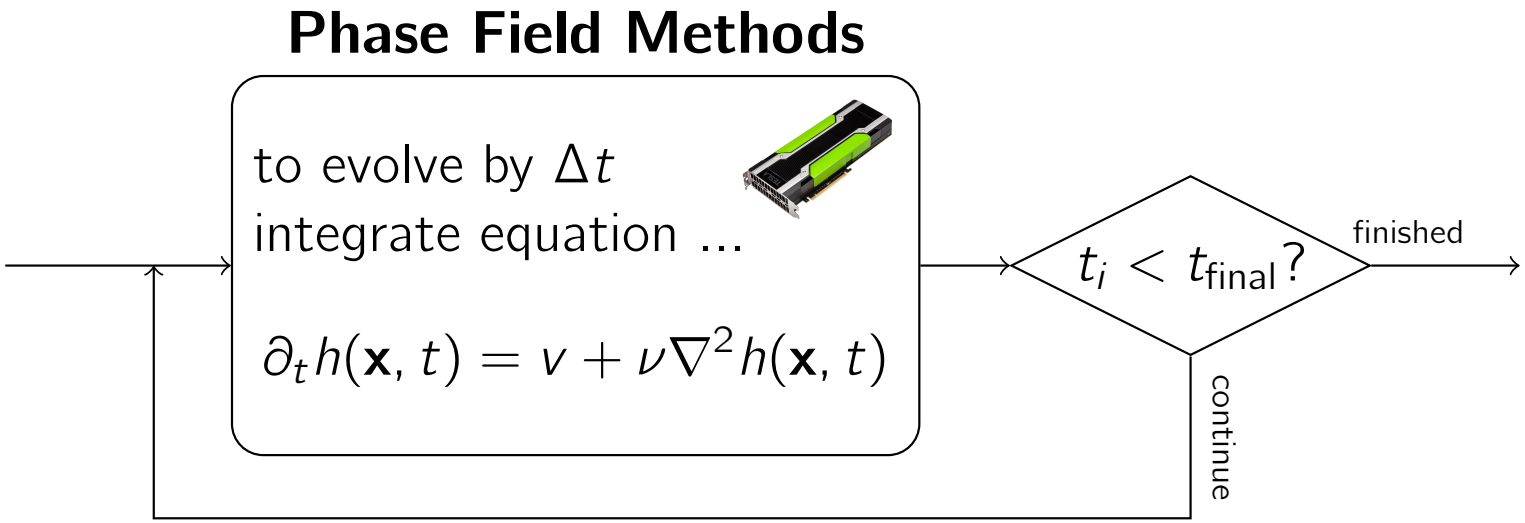
- simulated physical system evolves in discrete time steps Δt

Simulation



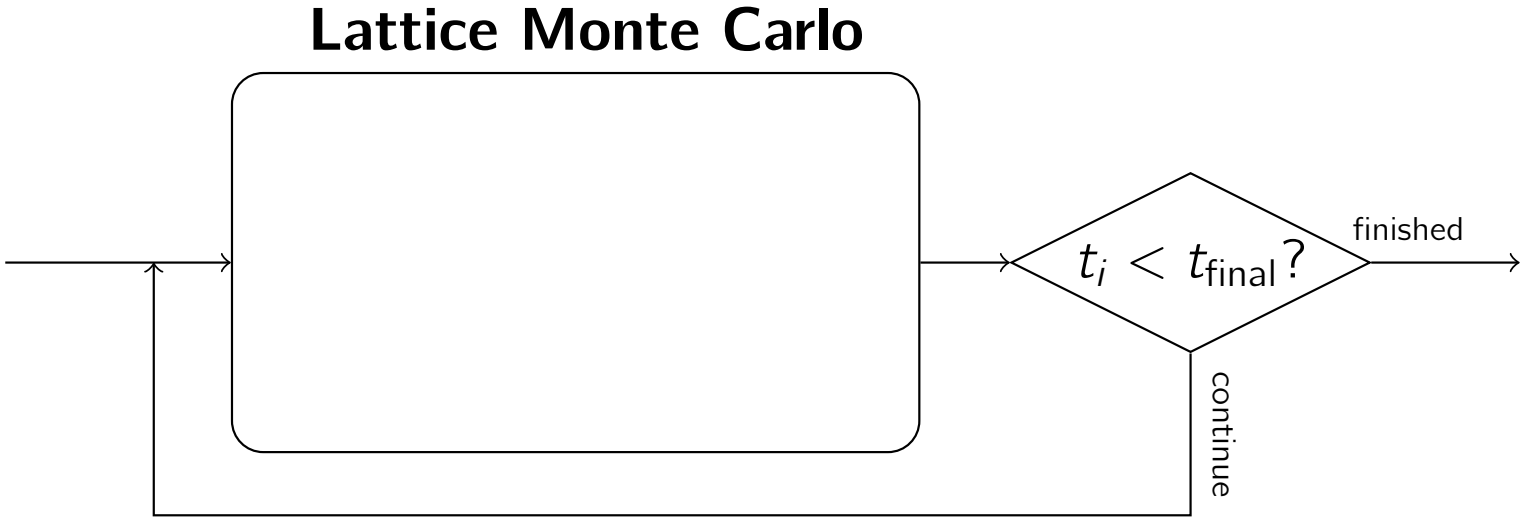
- simulated physical system evolves in discrete time steps Δt
- more accurate the smaller Δt and the larger the system

Simulation



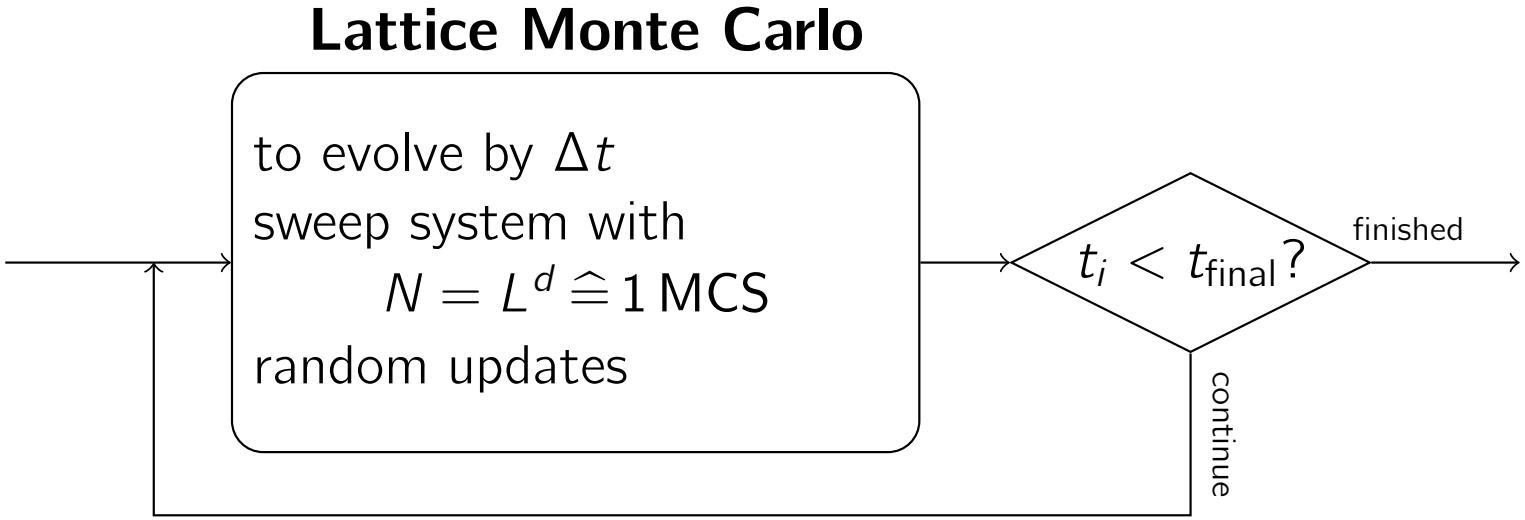
- simulated physical system evolves in discrete time steps Δt
- more accurate the smaller Δt and the larger the system

Simulation



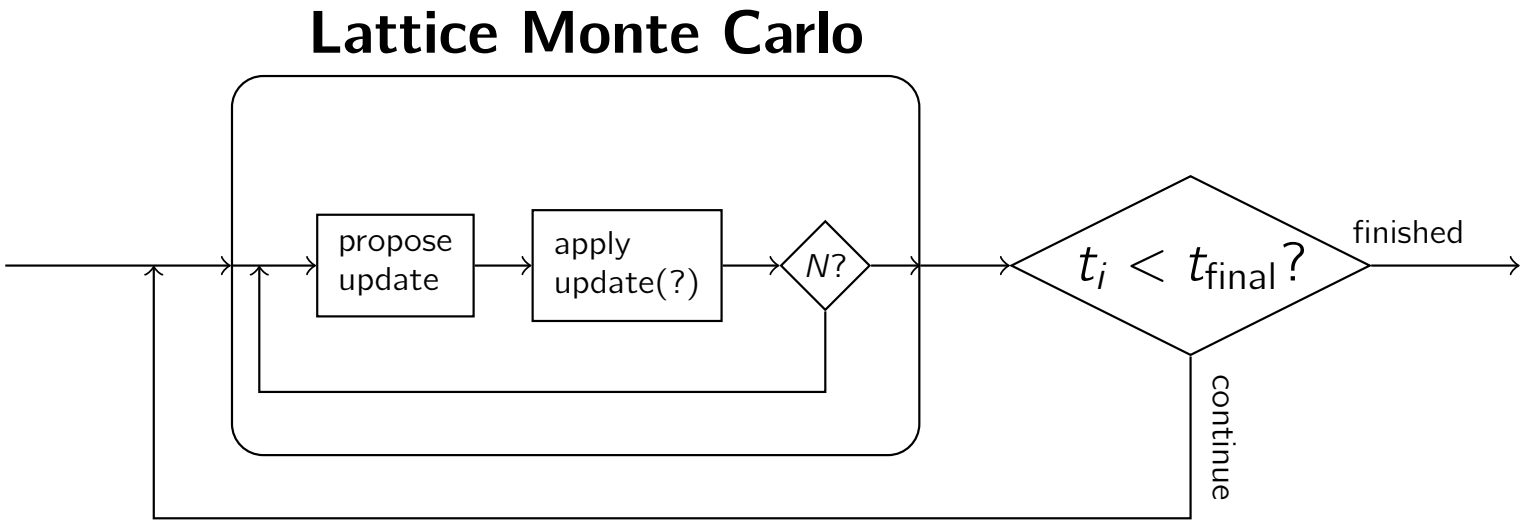
- simulated physical system evolves in discrete time steps Δt
- more accurate the larger the system

Simulation



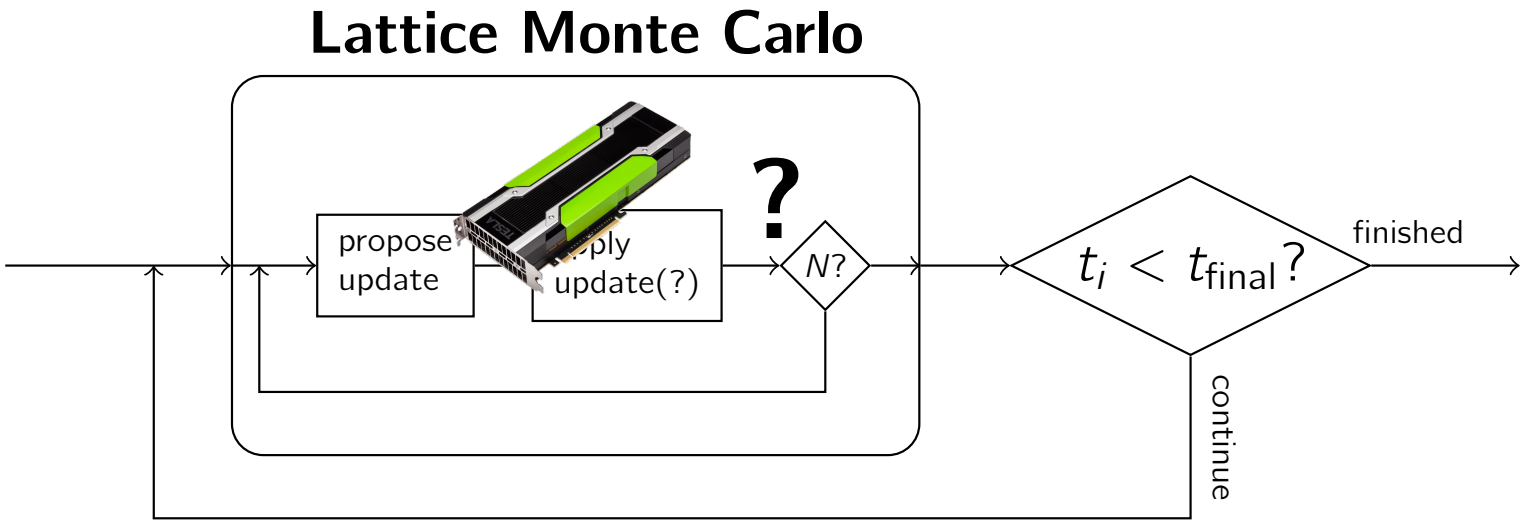
- simulated physical system evolves in discrete time steps Δt
- more accurate the larger the system
- updates are simple, but need to be applied in order
- uncorrelated updates

Simulation



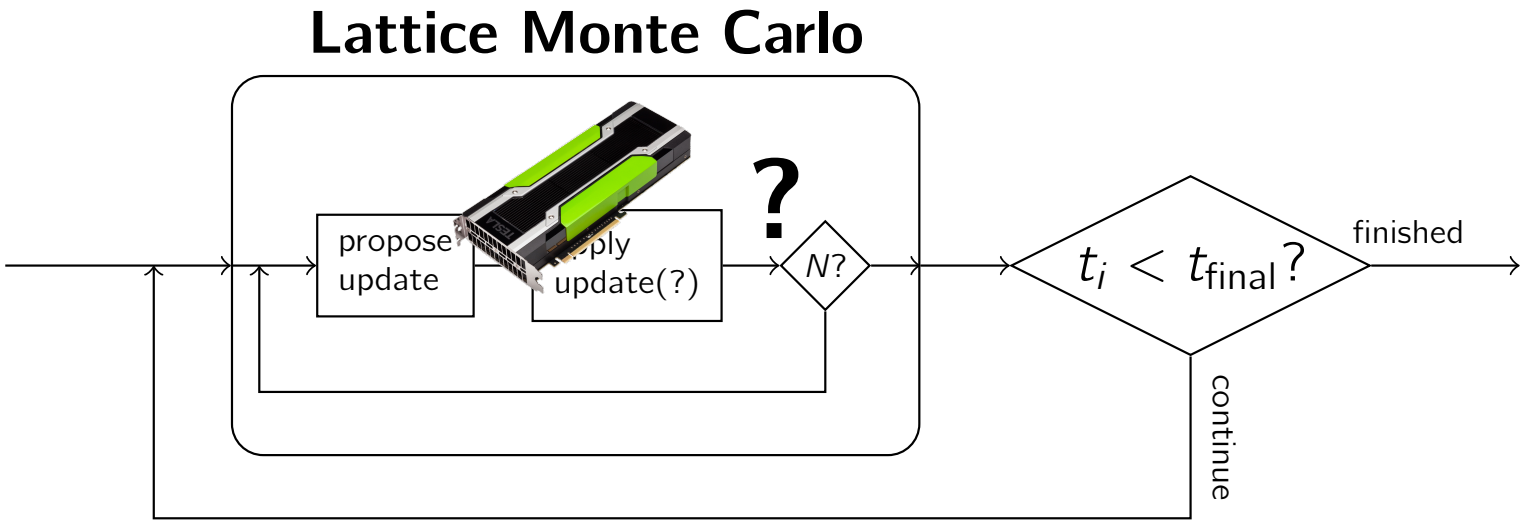
- simulated physical system evolves in discrete time steps Δt
- more accurate the larger the system
- updates are simple, but need to be applied in order
- uncorrelated updates

Simulation



- simulated physical system evolves in discrete time steps Δt
- more accurate the larger the system
- updates are simple, but need to be applied in order
- uncorrelated updates

Simulation

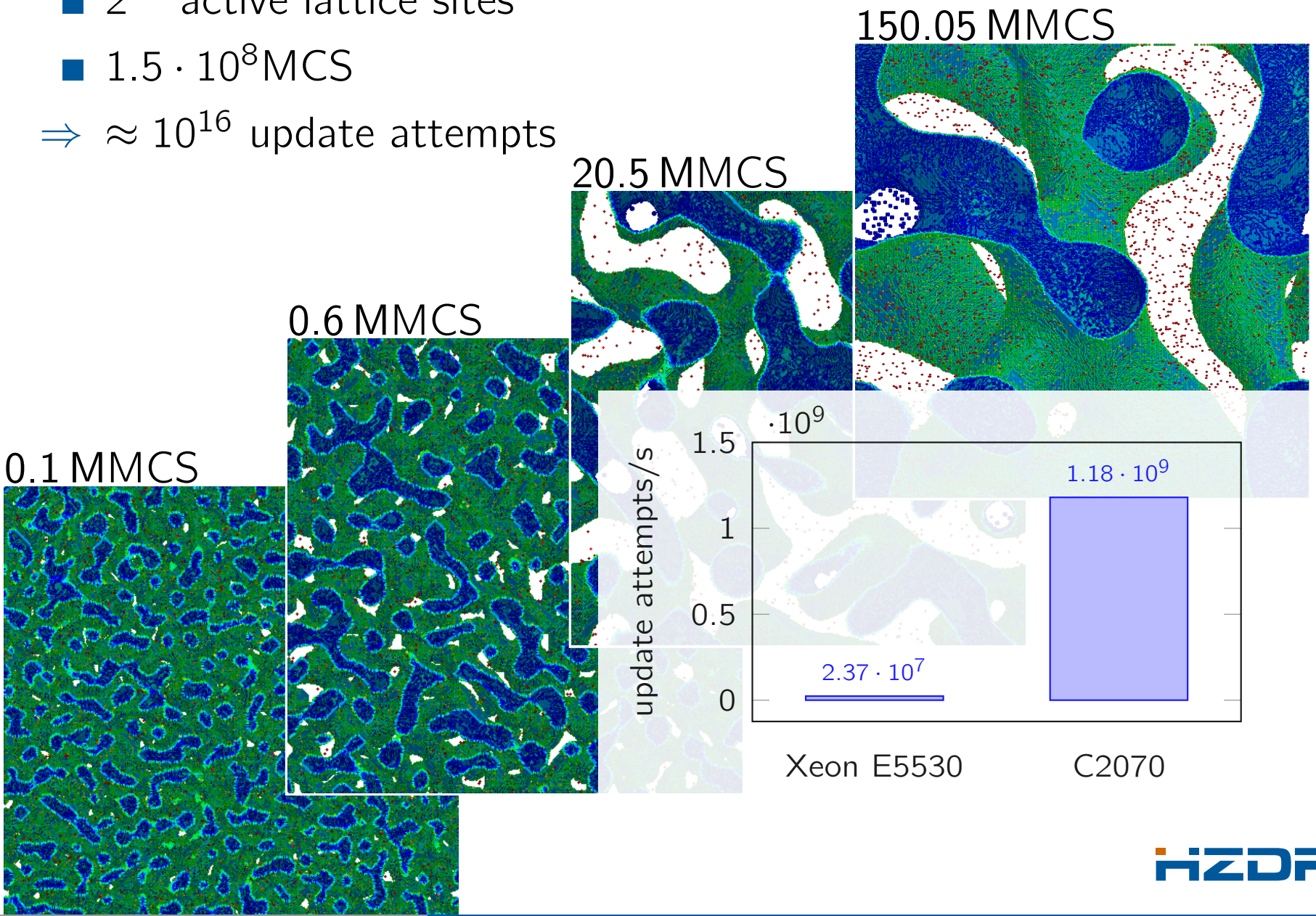


- simulated physical system evolves in discrete time steps Δt
- more accurate the larger the system
- updates are simple, but need to be applied in order
- uncorrelated updates—*We need those out-of-equilibrium.*

Why GPU and Massively Parallel Processing?

- 2^{26} active lattice sites
- $1.5 \cdot 10^8$MCS

$\Rightarrow \approx 10^{16}$ update attempts



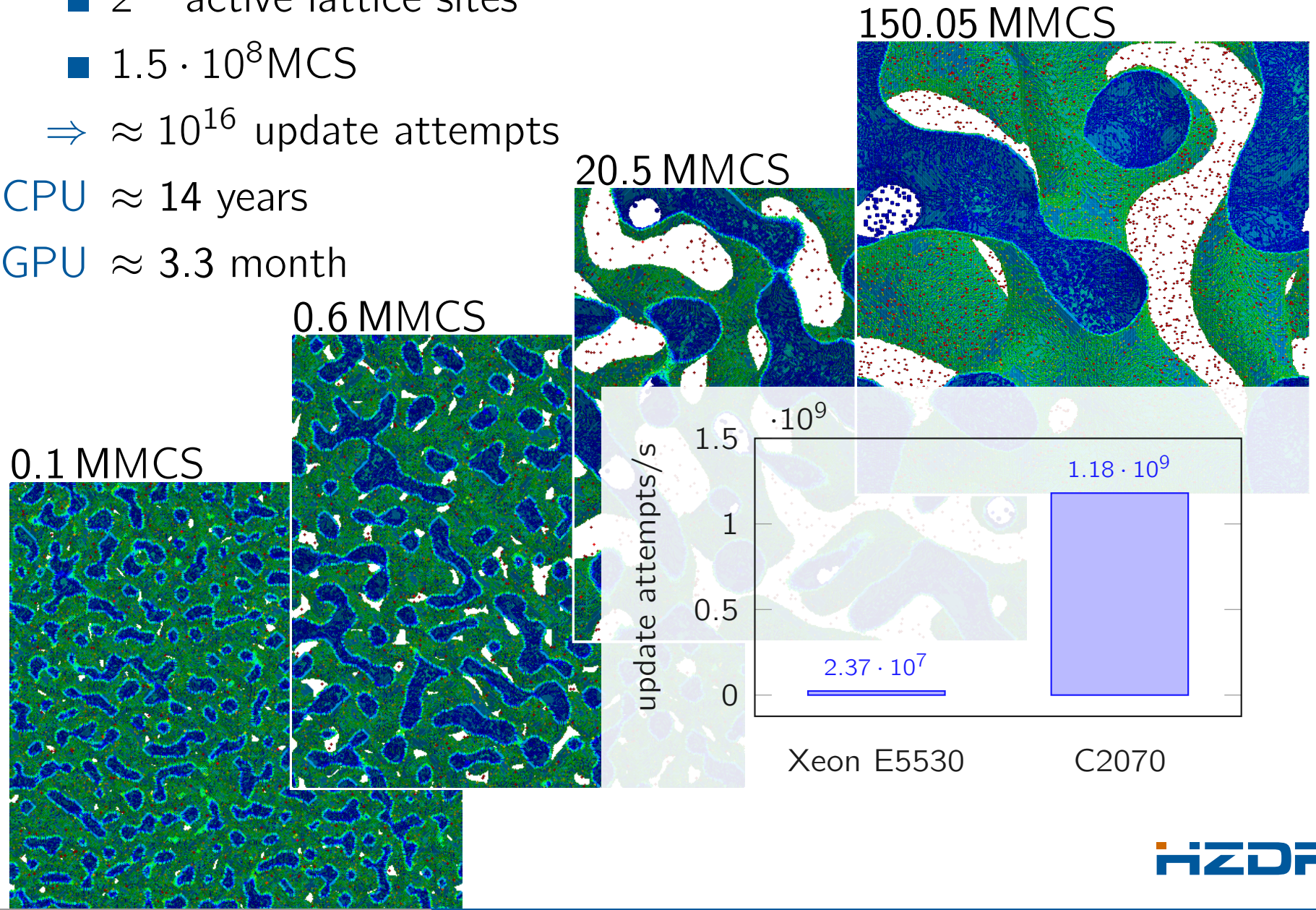
Why GPU and Massively Parallel Processing?

- 2^{26} active lattice sites
- $1.5 \cdot 10^8$MCS

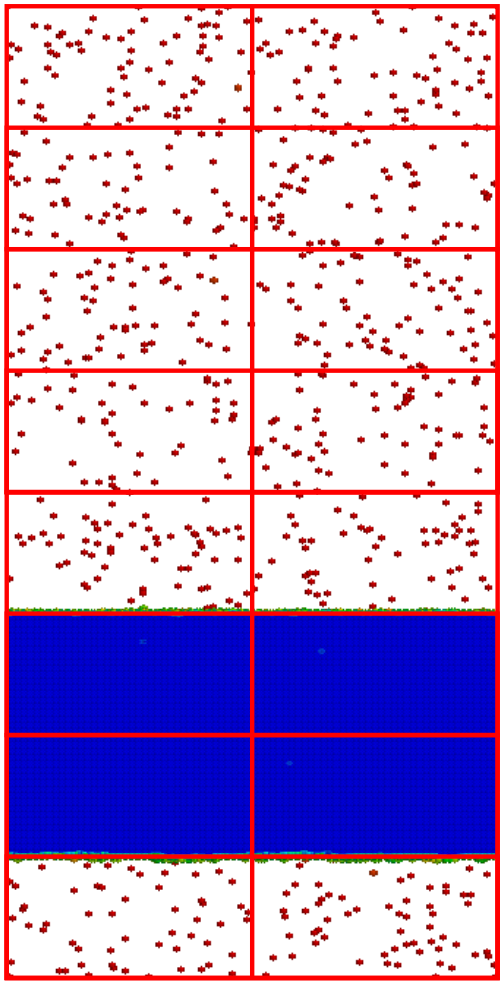
$\Rightarrow \approx 10^{16}$ update attempts

CPU $\approx$ 14 years

GPU $\approx$ 3.3 month



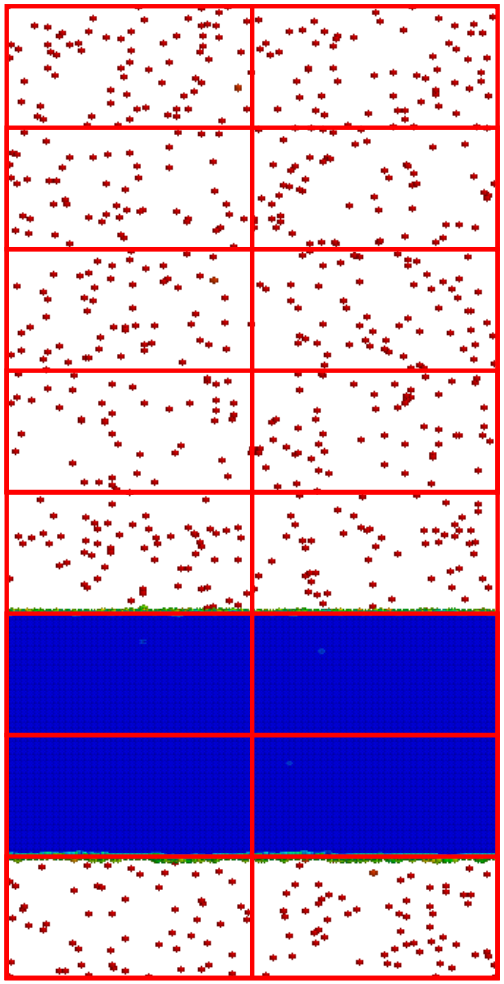
Broken Detailed Balance at Domain Boundaries



particle solubility in KMC

- device-layer domain boundaries break detailed balance:
  - move cannot be reversed at end of sweep
  - slower sweep at boundary

Broken Detailed Balance at Domain Boundaries



particle solubility in KMC

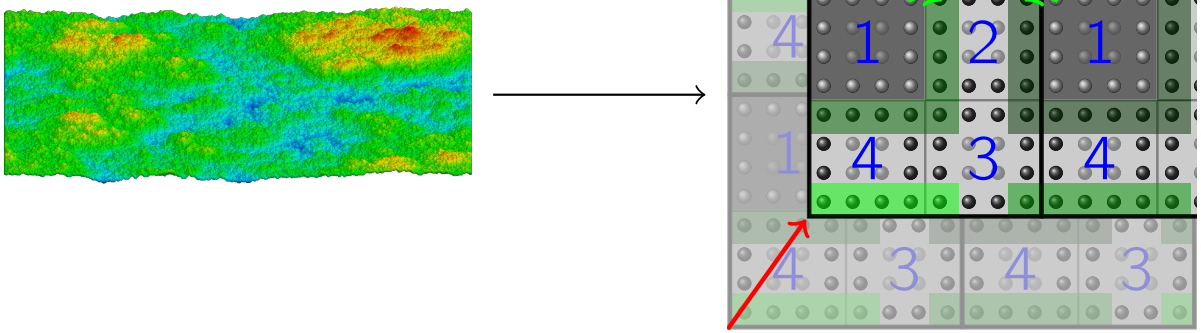
- device-layer domain boundaries break detailed balance:
  - move cannot be reversed at end of sweep
  - slower sweep at boundary

$$c(\varepsilon) = c_0 \cdot \mathrm{e}^{-B\varepsilon}$$

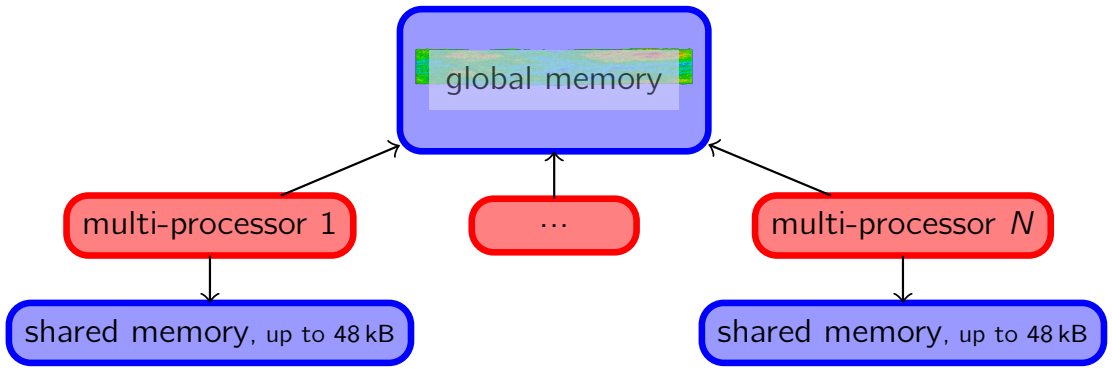
setup	c_0	B
aligned	1.08 ± 0.04	6.04 ± 0.03
random	1.00 ± 0.04	6.00 ± 0.03

$\Rightarrow$ solubility of particles at interface changed

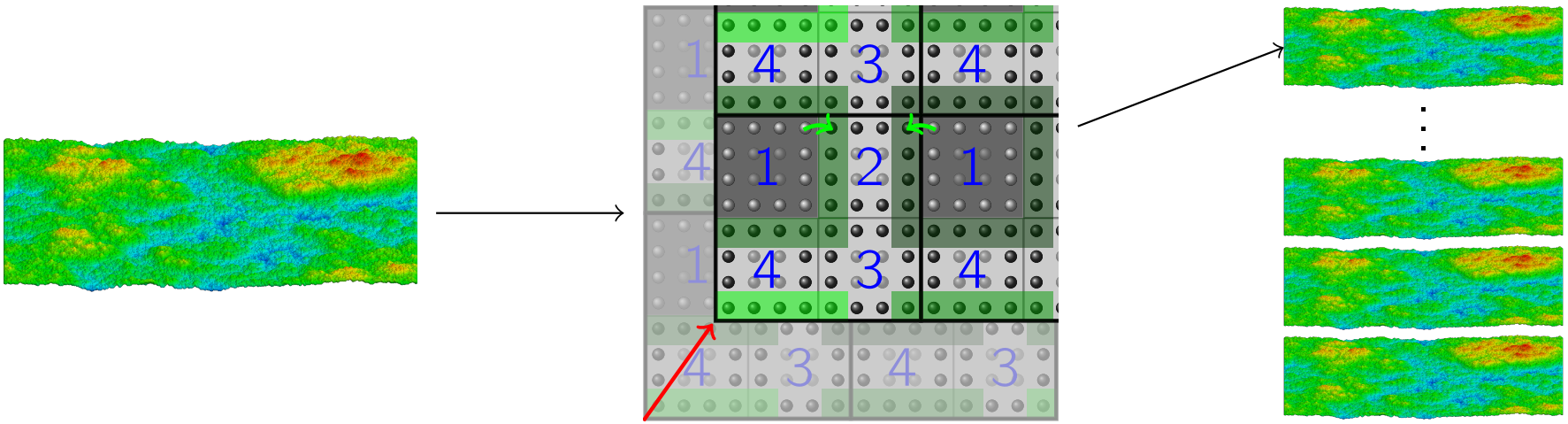
Multi-Surface Approach for GPUs



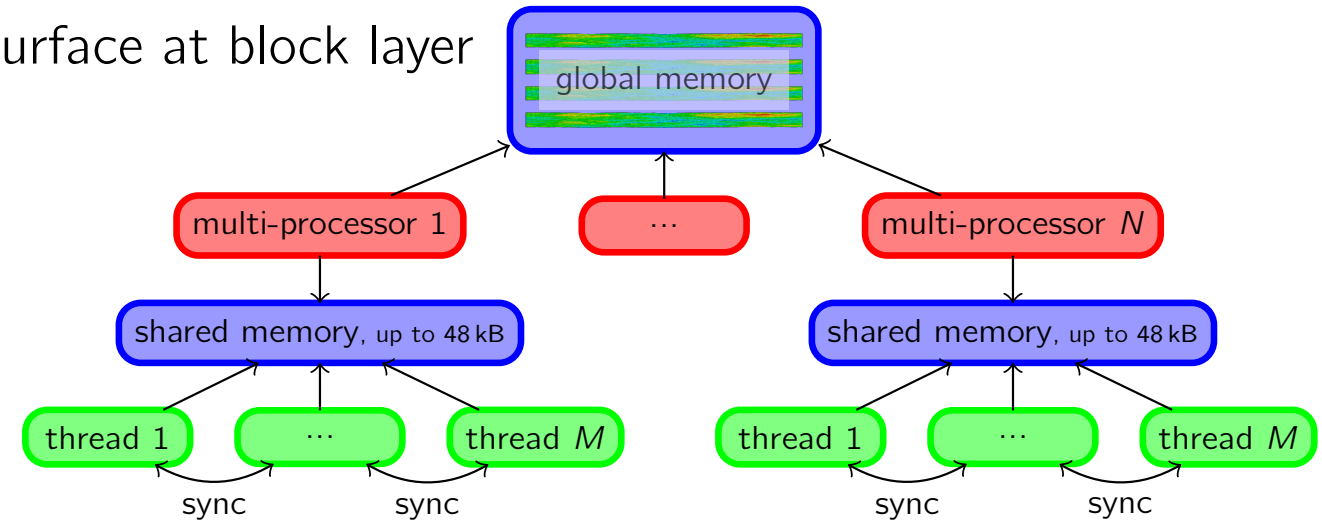
- double-tiling at device layer
  ... with random origin



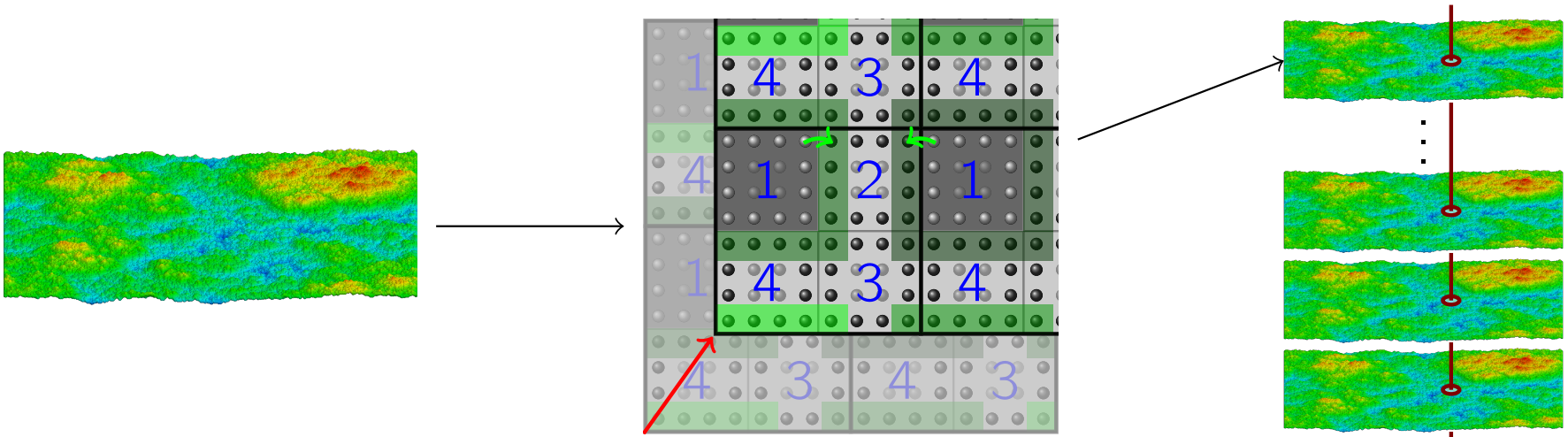
Multi-Surface Approach for GPUs



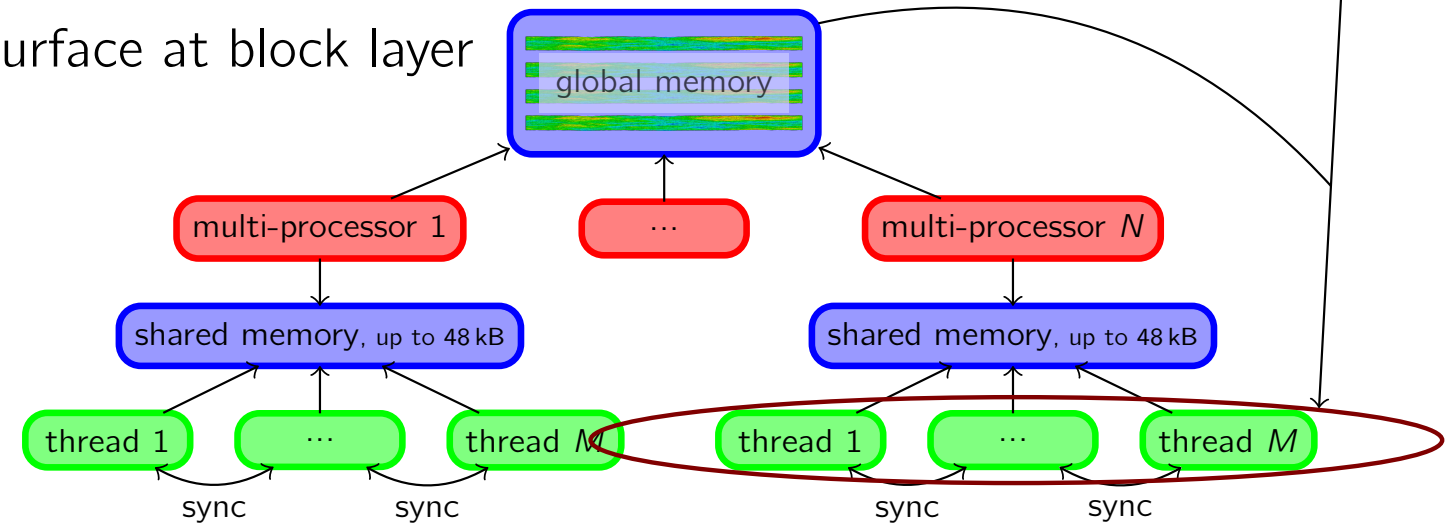
- double-tiling at device layer
  ... with random origin
- Multi-Surface at block layer



Multi-Surface Approach for GPUs



- double-tiling at device layer
  ... with random origin
- Multi-Surface at block layer



Example I: Phase separation in inhomogeneous systems

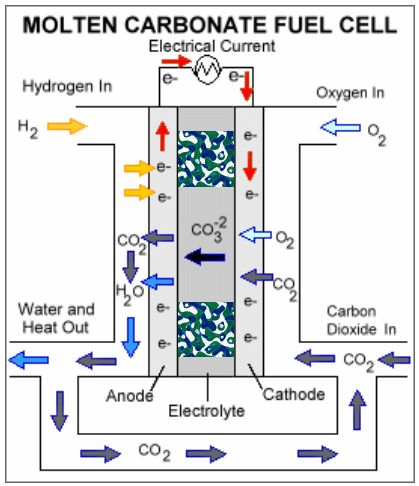
1 Kinetic Metropolis Lattice Monte Carlo (KMC)
- Multi-Surface Simulations

2 Example I: Phase separation in inhomogeneous systems

3 Example II: Structure formation under ion irradiation

4 Modeling in B2

Nano Sponge as Porous Matrix Material



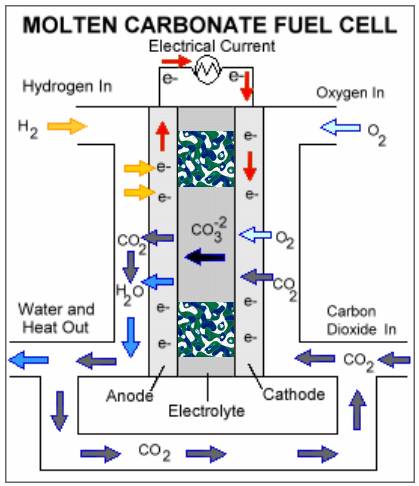
1

- porous matrix in Molten Carbonate Fuel Cells (MCFC)
- holding liquid electrolyte (Li_2CO_3) in nano-capillary matrix ($LiAlO_2$)

1MW MCFC2

[b] http://www.fuelcell.no/fuel_cell_types_mcfc_eng.htm

Nano Sponge as Porous Matrix Material



1

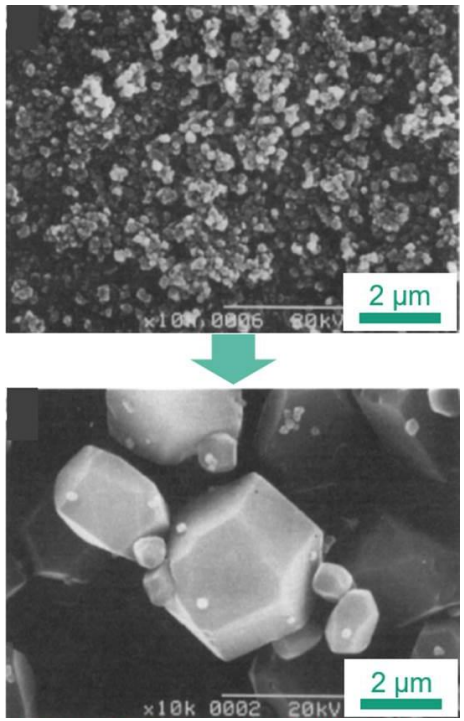
1MW MCFC2

- porous matrix in Molten Carbonate Fuel Cells (MCFC)
- holding liquid electrolyte (Li_2CO_3) in nano-capillary matrix ($LiAlO_2$)
- coarsening as degenerative process during operation—decreases capillarity

[b] http://www.fuelcell.no/fuel_cell_types_mcfc_eng.htm

Coarsening in the Presence of Inhomogeneities

- large clusters with depleted zones have been observed in porous matrix at end of lifetime



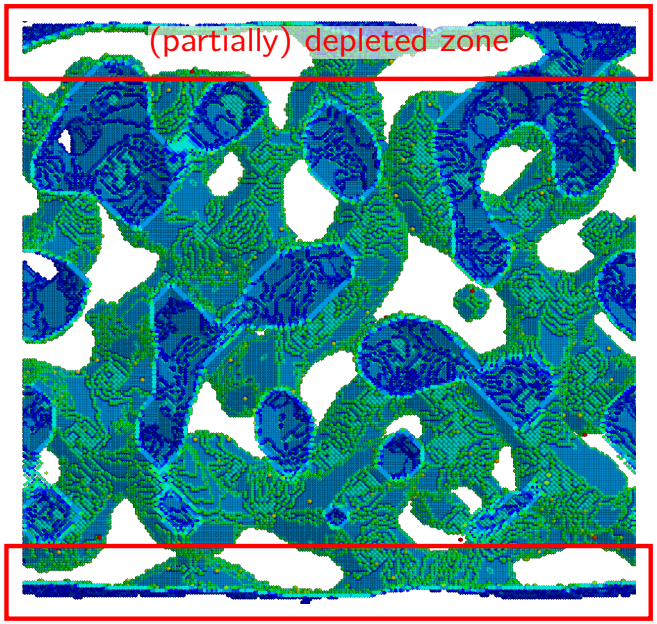
[1]

[1] Murai et al, *J. Electrochem. Soc.* **143** 2776 (1996)

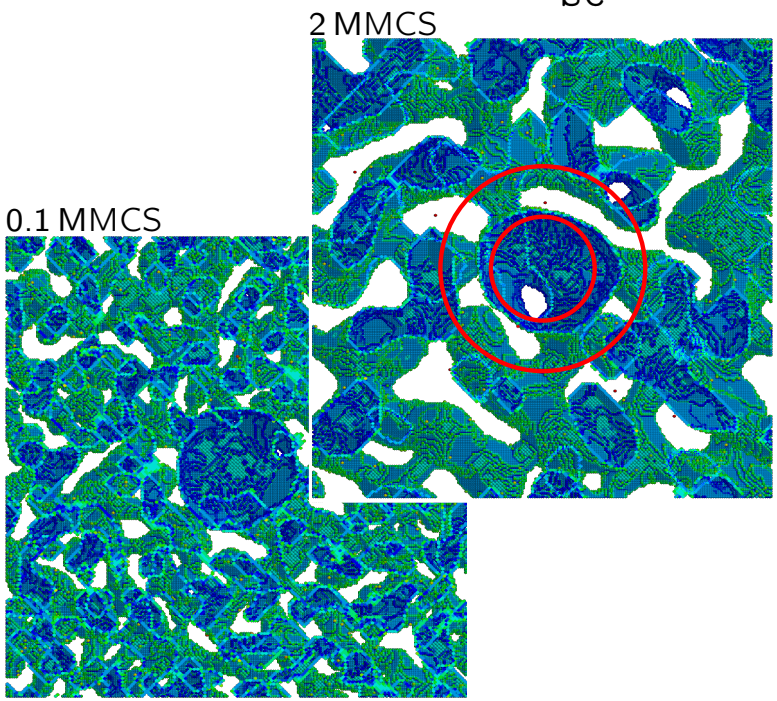
Coarsening in the Presence of Inhomogeneities

- large clusters with depleted zones have been observed in porous matrix at end of lifetime

flat interface

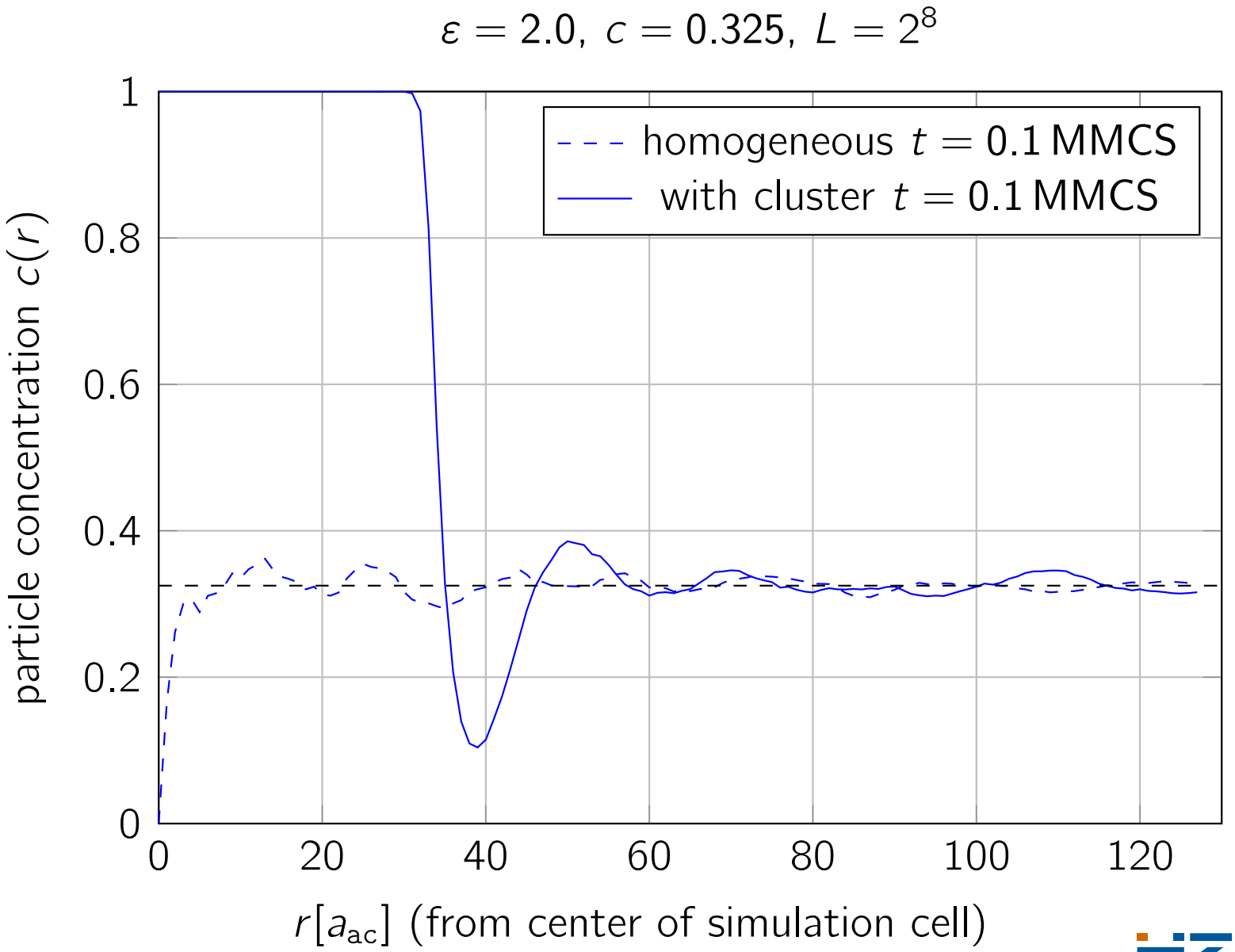


cluster $r = 32a_{sc}$

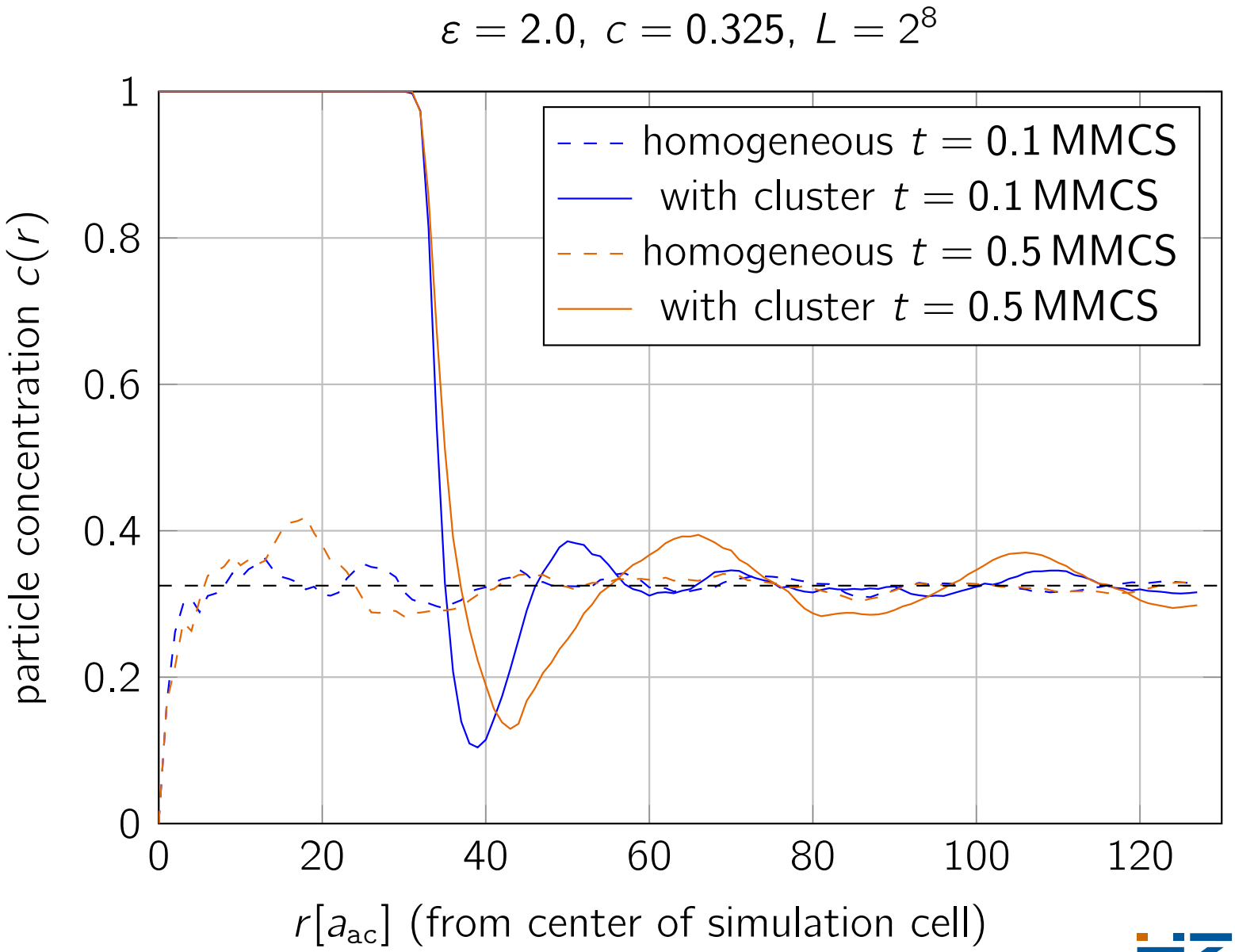


$$\varepsilon = 2.0,\ c = 0.325,\ L = 2^8$$

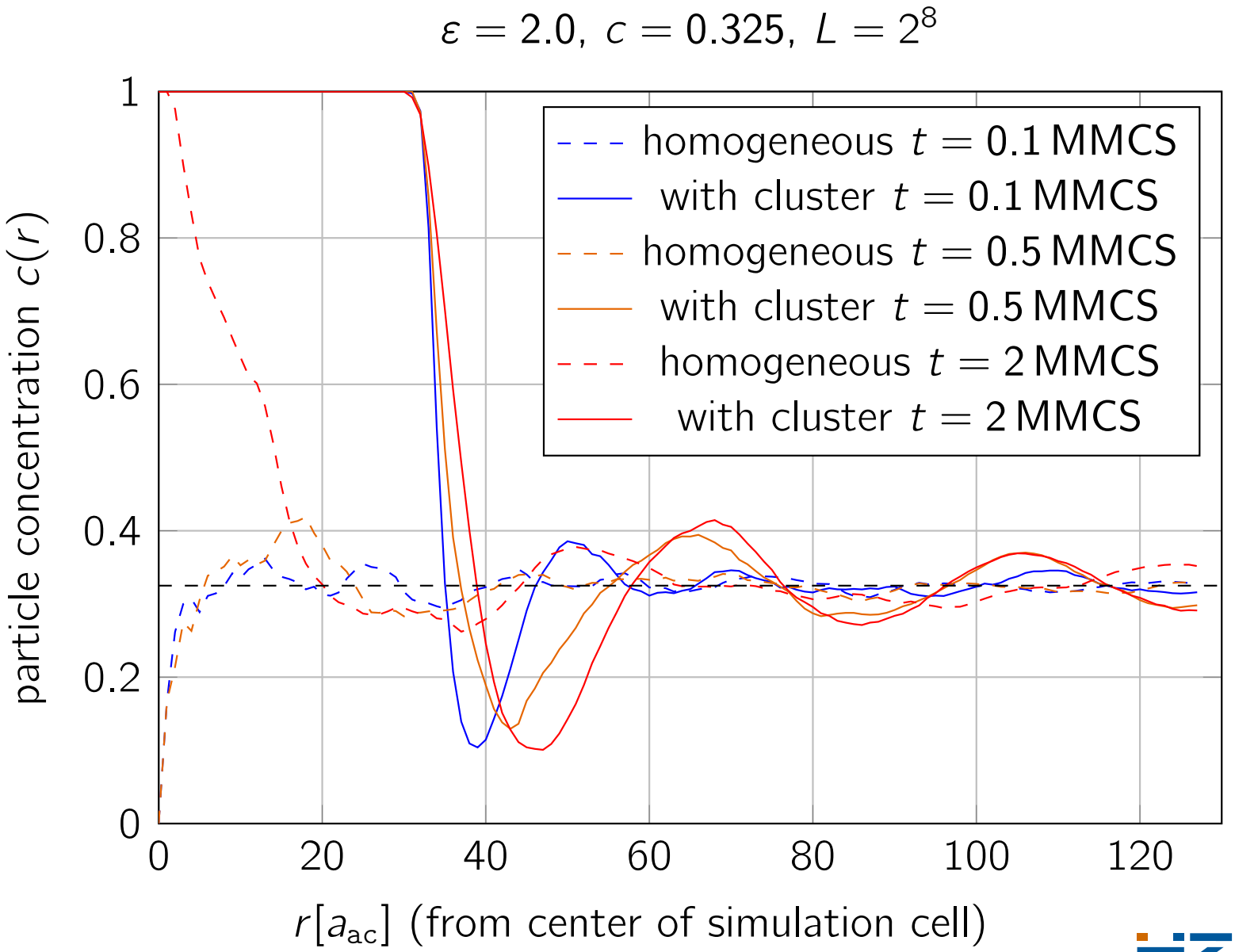
Sponge-Coarsening around Cluster



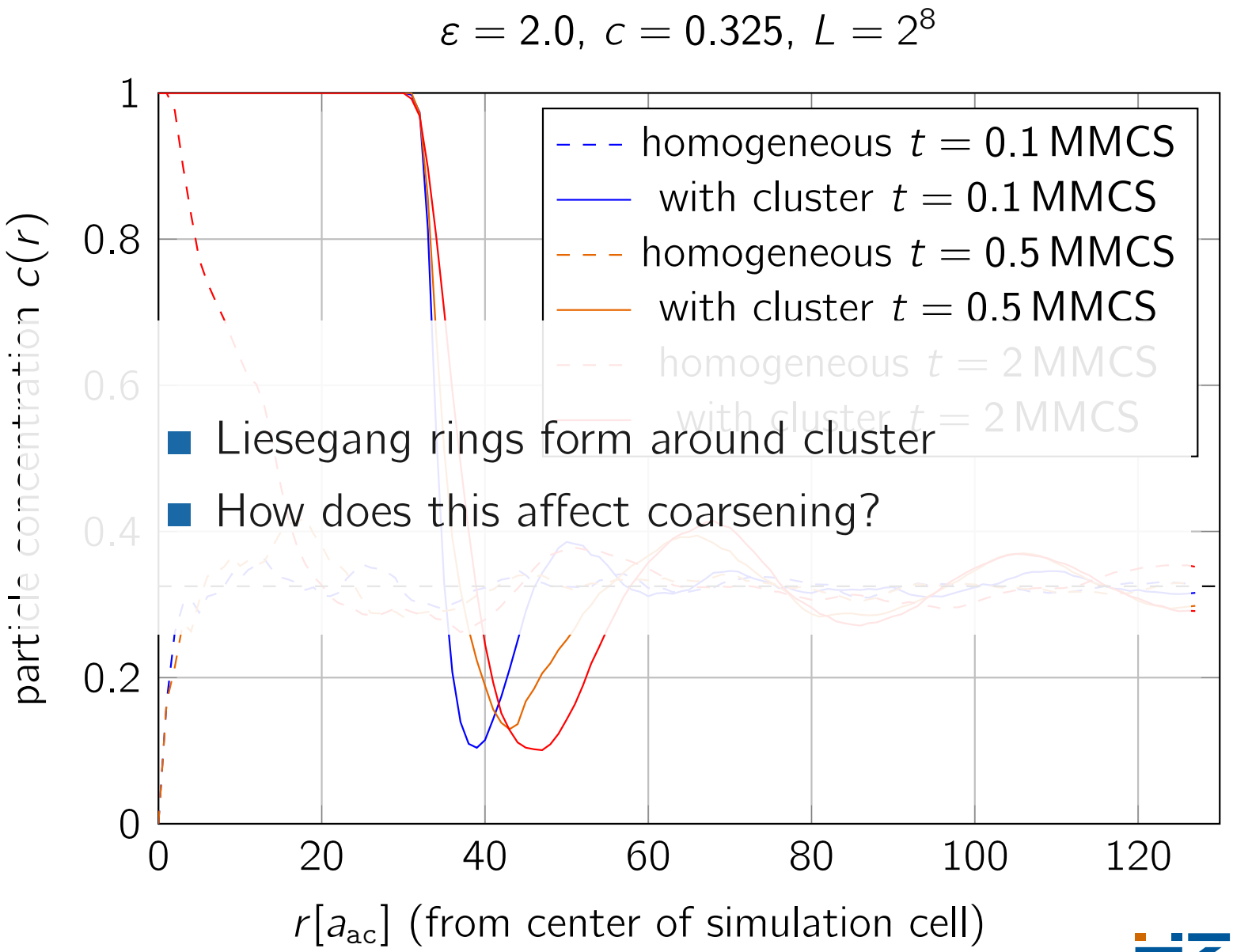
Sponge-Coarsening around Cluster



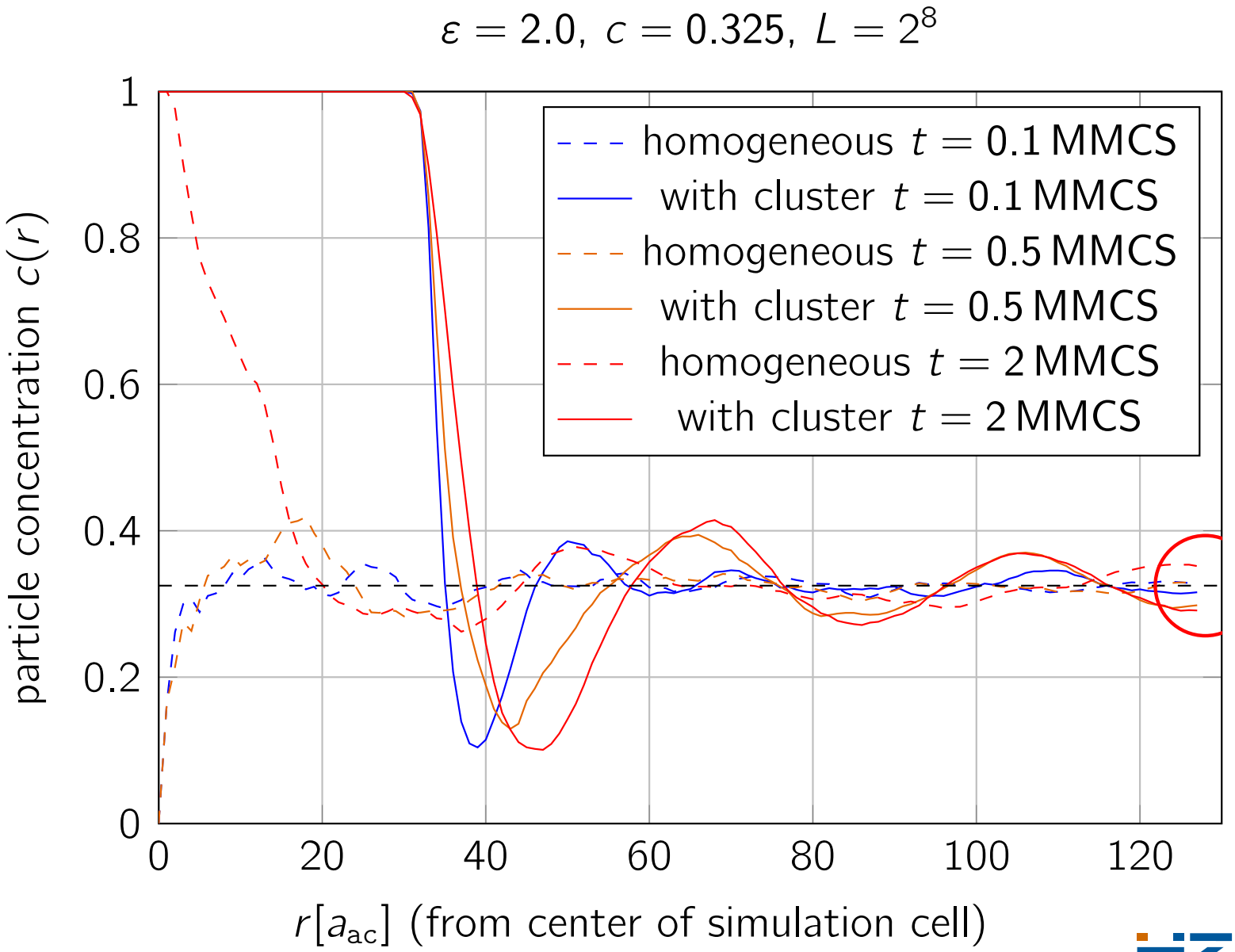
Sponge-Coarsening around Cluster



Sponge-Coarsening around Cluster



Sponge-Coarsening around Cluster



Example II: Structure formation under ion irradiation

1 Kinetic Metropolis Lattice Monte Carlo (KMC)
- Multi-Surface Simulations

2 Example I: Phase separation in inhomogeneous systems

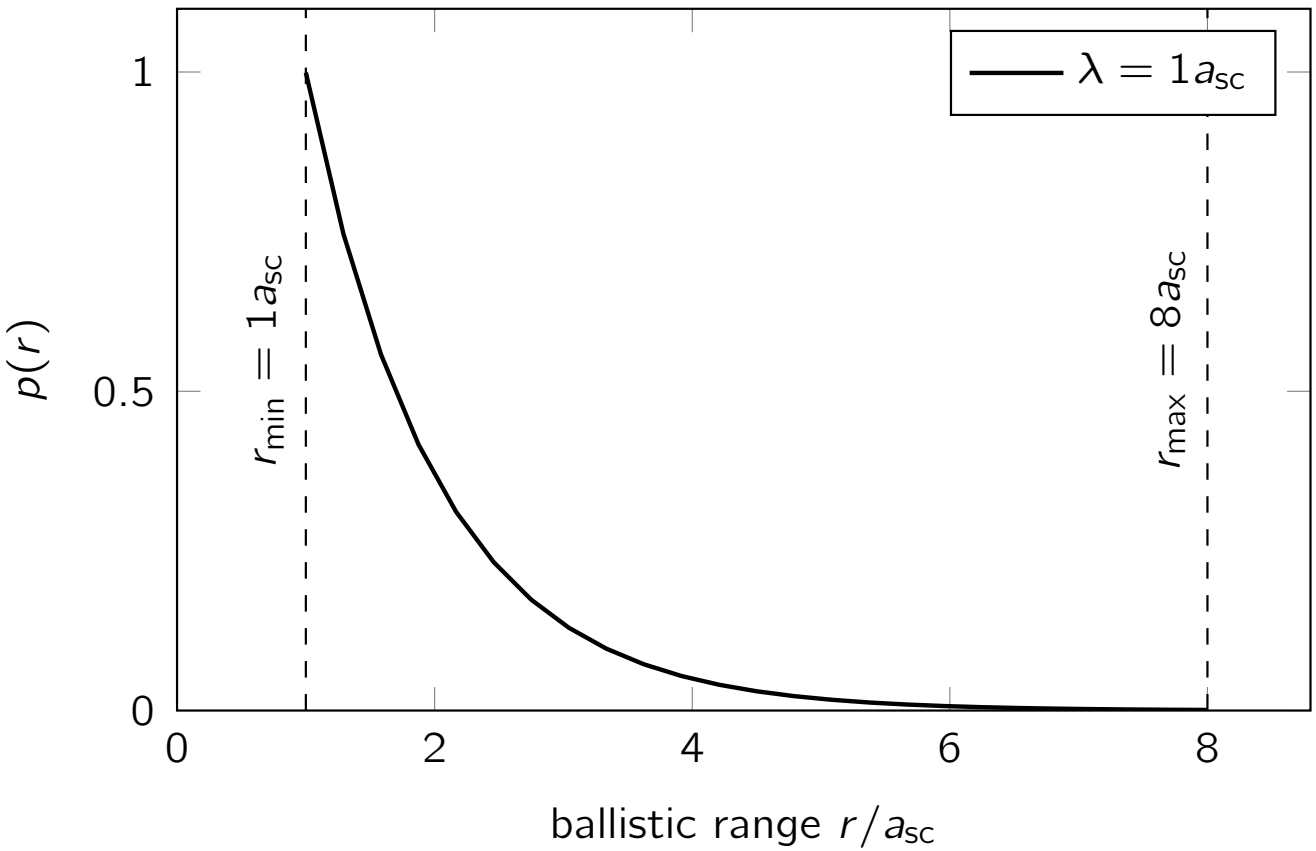
3 Example II: Structure formation under ion irradiation

4 Modeling in B2

Recoil Mixing: Model

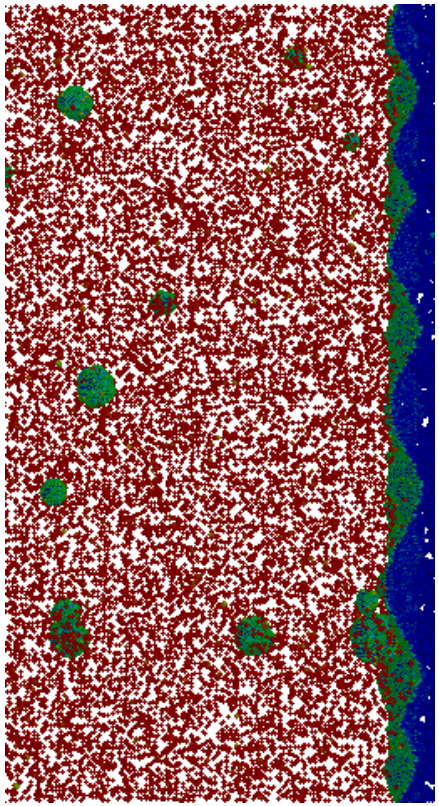
- incident ion hits lattice atoms creating a cascade of displacements
- energy gets divided among displaced atoms $\Rightarrow$ exponentially distributed range

$$p(r) \sim \mathrm{e}^{-r/\lambda}$$

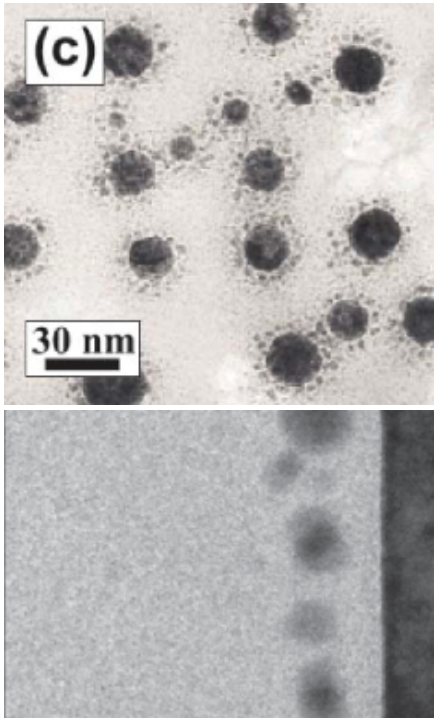


Inverse Ostwald Ripening

Inverse Ostwald Ripening



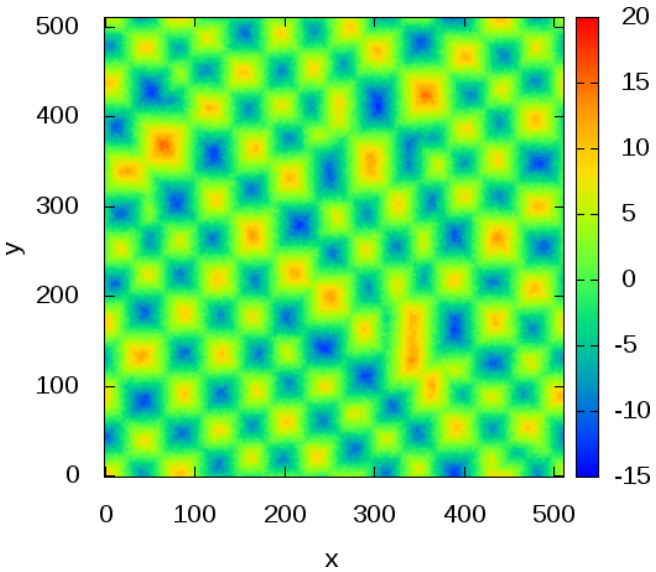
Simulation of a (100)–interface
$\varrho = 1 \times 10^{-3}$



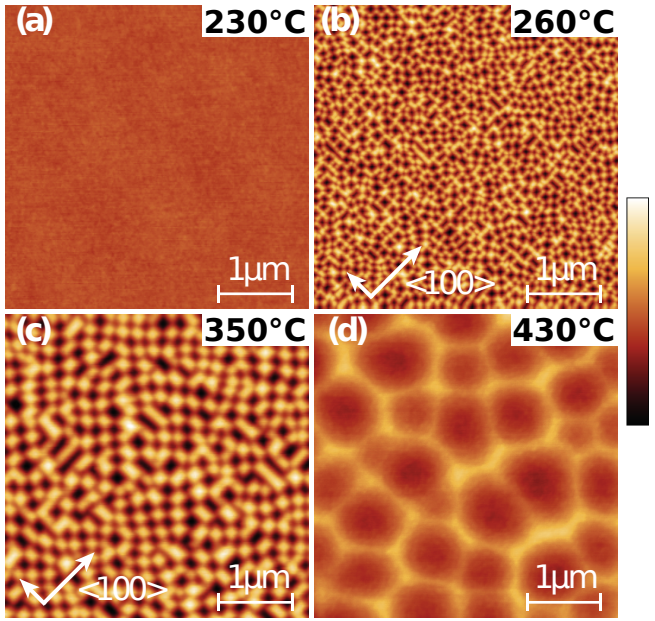
TEM pictures of Au nano clusters in SiO_2 matrix after irradiation with Au ions.
Heinig et al. Appl. Phys. A **77**, *17 (2003)*

Irradiation of Interfaces

Instability of buried Interfaces or Surfaces



Simulation of a (100)–interface
$\varrho = 1 \times 10^{-3}$



AFM picture of a Ge (100)–surface after irradiation with Ge ions.

Ou et al. (2013) submitted (arXiv 1303.5133)

Modeling in B2

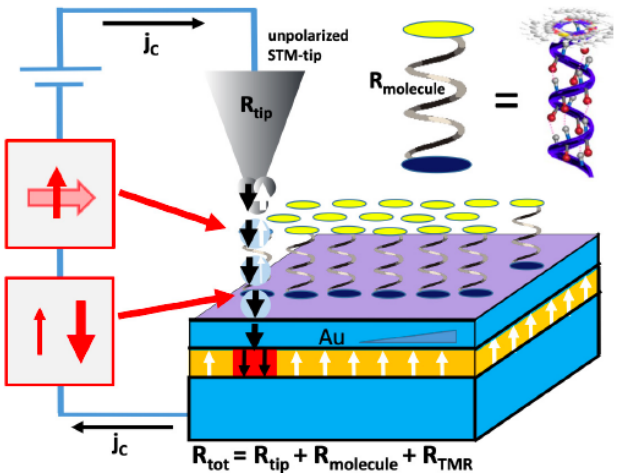
1 Kinetic Metropolis Lattice Monte Carlo (KMC)
- Multi-Surface Simulations

2 Example I: Phase separation in inhomogeneous systems

3 Example II: Structure formation under ion irradiation

4 Modeling in B2

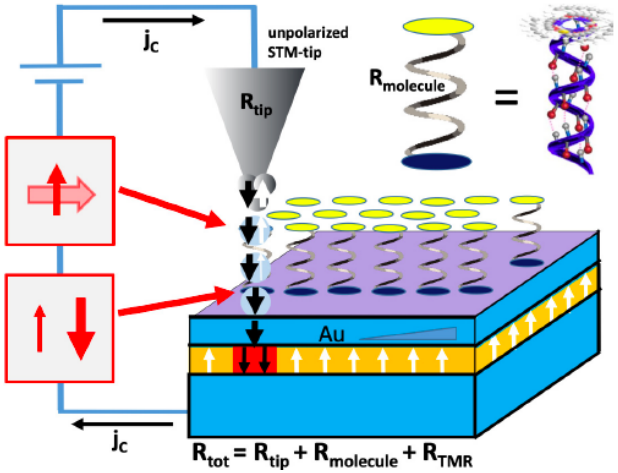
Modeling within SFB Subproject B2

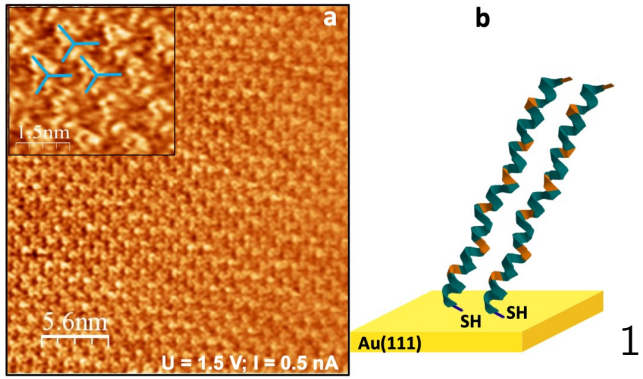


[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

Modeling within SFB Subproject B2

Modeling of structure formation of molecules using KMC





[1]

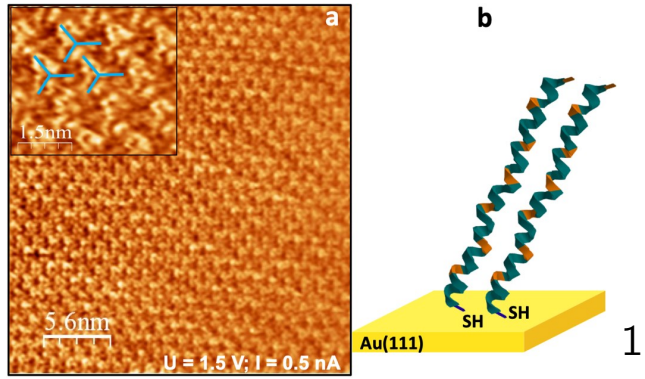
[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

Modeling within SFB Subproject B2

Modeling of structure formation of molecules using KMC

1. modelling/prediction of long range order in dependence on:
   - substrate facet
   - binding group
   - helix–helix interaction

(based on parameters from subproject B1)



[1]

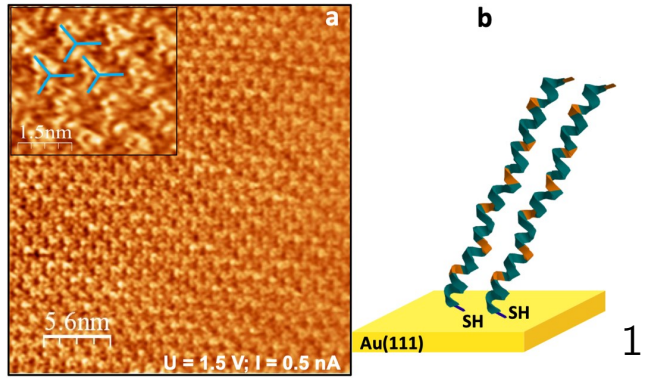
[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

Modeling within SFB Subproject B2

Modeling of structure formation of molecules using KMC

1. modelling/prediction of long range order in dependence on:
   - substrate facet
   - binding group
   - helix–helix interaction

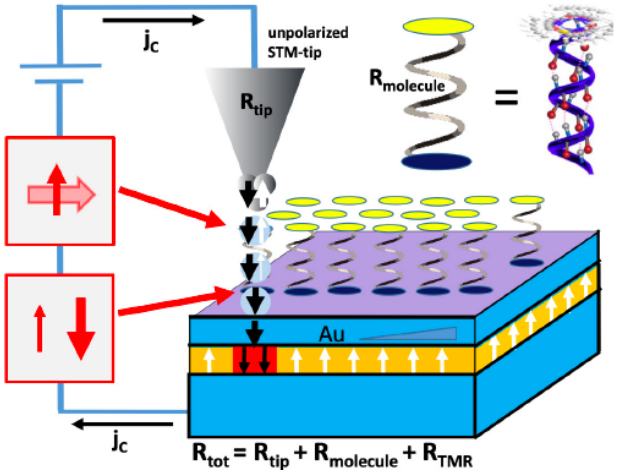
   (based on parameters from subproject B1)
2. prediction of structure formation with multiple species

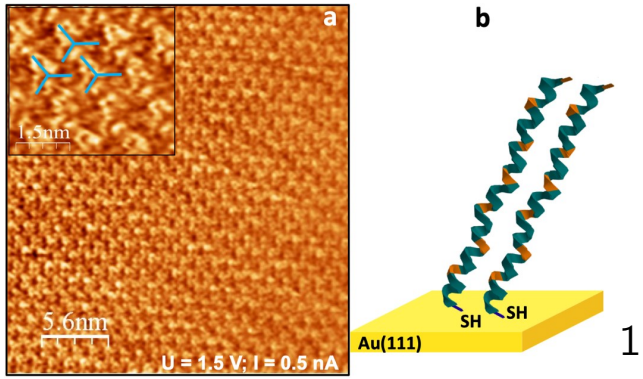


[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

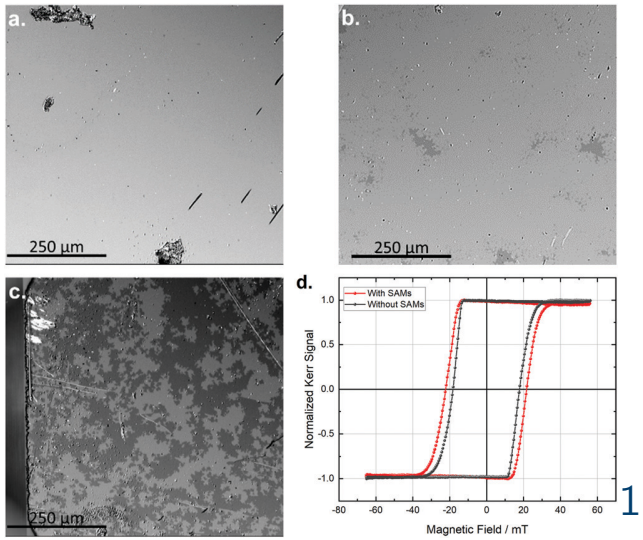
Modeling within SFB Subproject B2

Modeling of structure formation of molecules using KMC





1



1

Modeling of magnetic ordering of buried layer

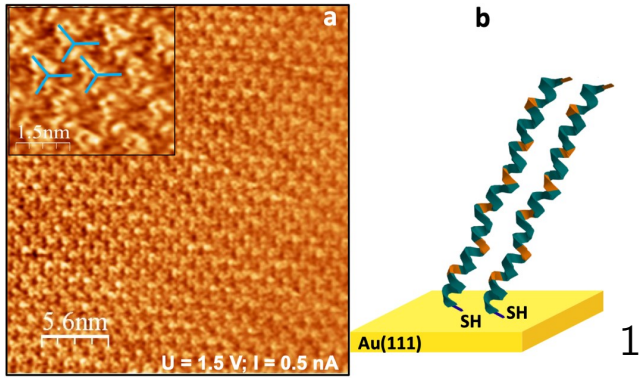
[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

Modeling within SFB Subproject B2

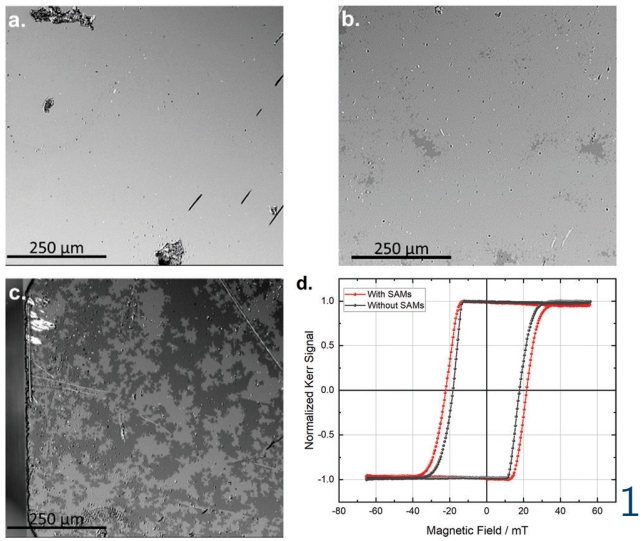
Modeling of structure formation of molecules using KMC

Modeling of magnetic ordering of buried layer

1. prediction of phase diagrams of magnetization, taking into account
   - posssibly periodic file from helical molecules
   - disorder in molecular monolayer
2. gauge magnetic interaction parameters against experimental measurements



1

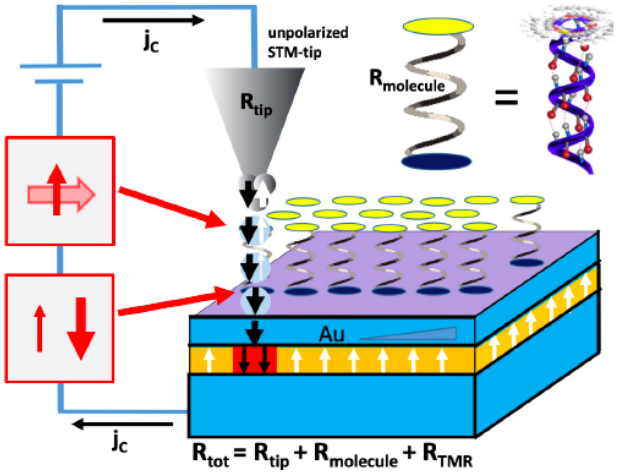


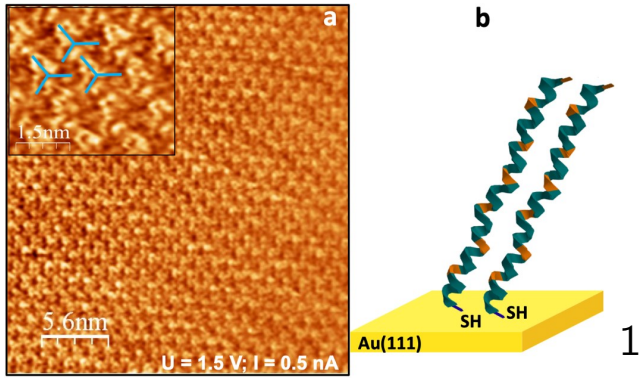
1

[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

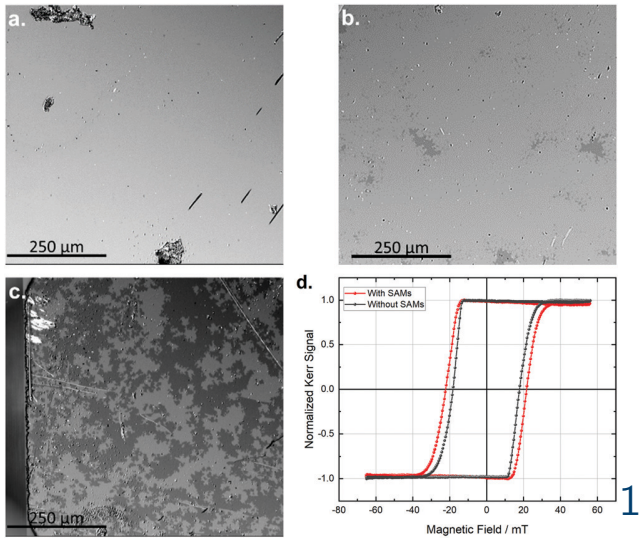
Modeling within SFB Subproject B2

Modeling of structure formation of molecules using KMC





1



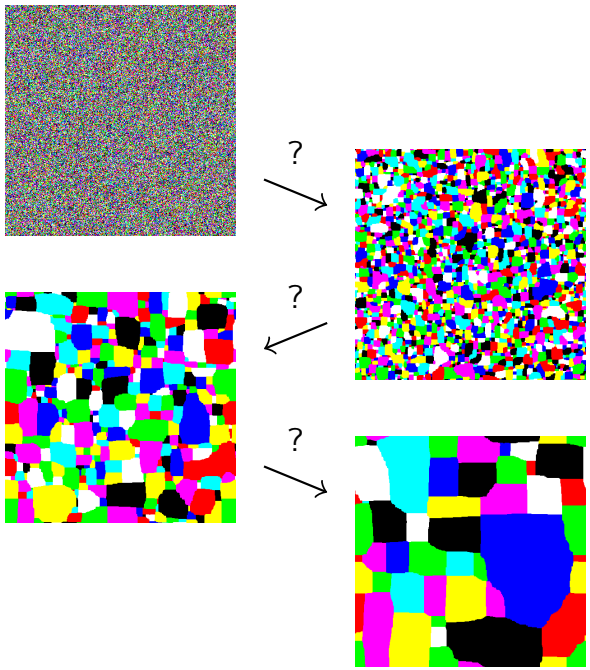
1

Modeling of magnetic ordering of buried layer

[1] Sharma, A., et al. *J. Mater. Chem. C* **8** 11822 (2020)

Dynamics vs Steady-State

if **kinetics** of interest
system out-of-equilibrium:

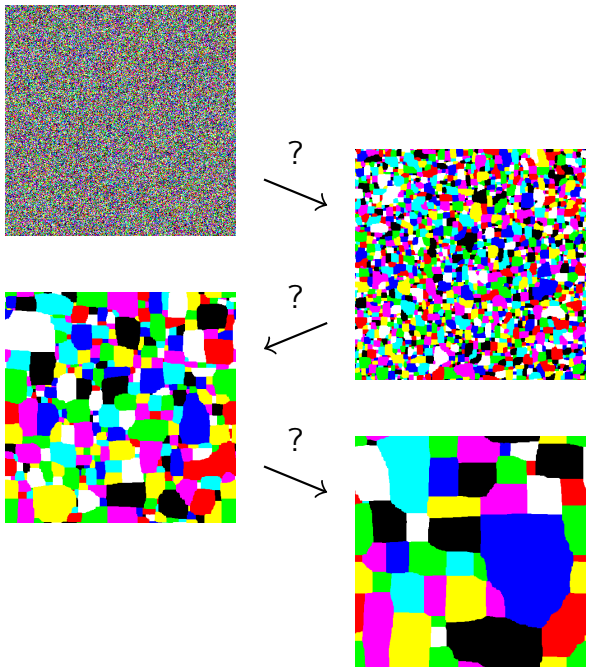


8-states Potts model, $\frac{J}{k_B T} = 5$

- optimal algorithm reproduces physical evolution

Dynamics vs Steady-State

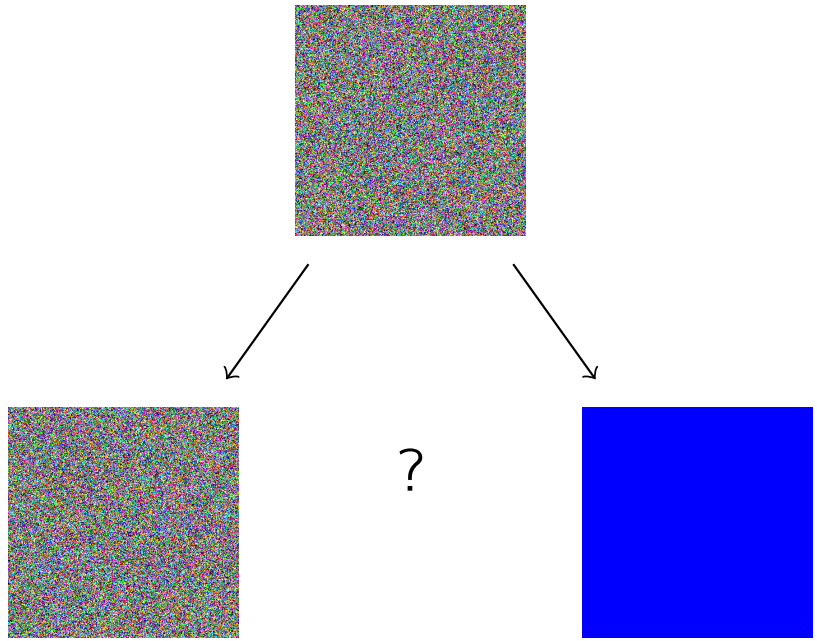
if **kinetics** of interest
system out-of-equilibrium:



8-states Potts model, $\frac{J}{k_B T} = 5$

- optimal algorithm reproduces physical evolution

if only **final** state relevant
system (equilibrium) steady-state:



8-states Potts model

- optimal algorithm reaches equilibrium quickly

Acknowledgements

- Sibylle Gemming
- Géza Ódor
- Martin Weigel
- Guido Juckeland

- Artur Erbe
- Jörg Schuster
- Peter Zahn
- Karl-Heinz Heinig
- Henrik Schulz
- Nils Schmeißer
- Michael Bussmann

- my other colleagues

Thank You.

J.Kelling@HZDR.de

This work has received funding from the Erasmus+ program via the Leonardo-Büro Sachsen and Coventry University.

Computing time was provided by ZIH Dresden, NIIF Hungary and the HZDR computing center.

Selected Publications

- Kelling, J., Ódor, G.:
  Extremely large-scale simulation of a Kardar-Parisi-Zhang model using graphics cards
  Phys. Rev. E **84** 061150 (2011)
- Kelling, J., Ódor, G., Nagy, M. F., Schulz, H., Heinig, K.-H.:
  Comparison of different parallel implementations of the 2+1-dimensional KPZ model and the 3-dimensional KMC model
  Eur. Phys. J. ST **210** 175 (2012)
- Kelling, J., Ódor, G., Gemming, S.:
  Bit-Vectorized GPU Implementation of a Stochastic Cellular Automaton Model for Surface Growth
  IEEE International Conference on Intelligent Engineering Systems (2016)
- Kelling, J., Ódor, G., Gemming, S.:
  Universality of 2+1 dimensional RSOS models
  Phys. Rev. E **94** 022107 (2016)
- Kelling, J., Ódor, G., Gemming, S.:
  Local scale-invariance of the 2 + 1 dimensional Kardar–Parisi–Zhang model
  J. Phys. A **50** 12LT01 (2017)
- Kelling, J., Ódor, G., Gemming, S.:
  Suppressing correlations in massively parallel simulations of lattice models
  Comp. Phys. Commun. **220** 205 (2017)
- Ódor, G., Kelling, J.: Critical synchronization dynamics of the Kuramoto model on connectome and small world graphs, *Sci. Rep.* **9**, 19621, (2019)