Pushing the Limits of Lattice Monte-Carlo Simulations using GPUs

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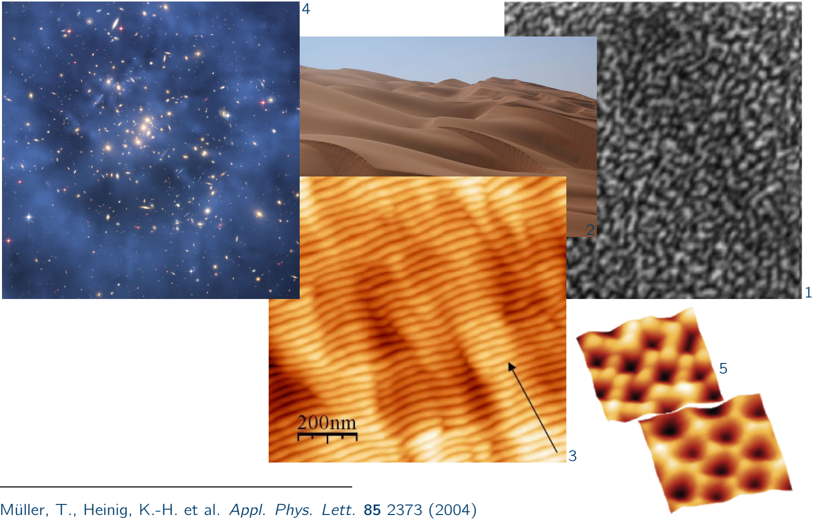
Stochastic Processes in Nature



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

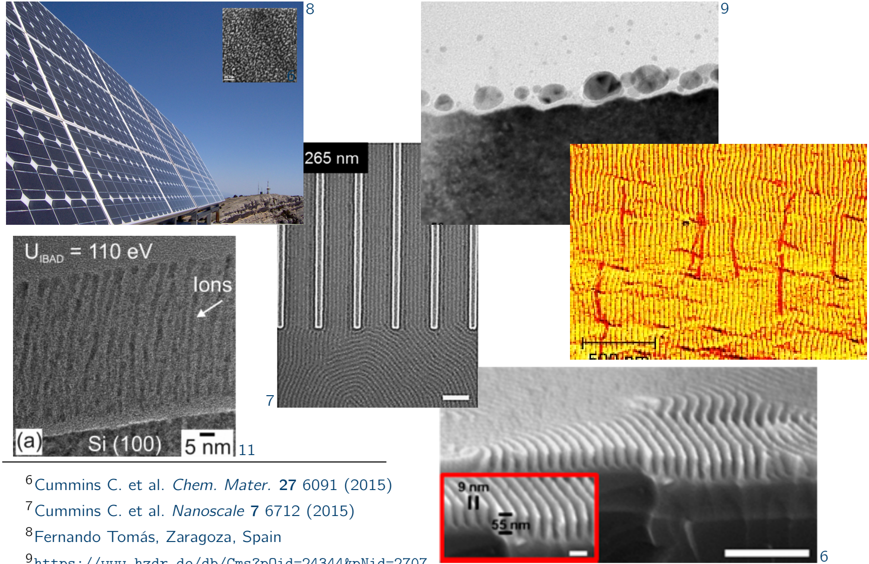
[2] `http://en.wikipedia.org/wiki/File:Rub_al_Khali_002.JPG`

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

[4] `http://hubblesite.org/newscenter/archive/releases/2007/17/image/a`

[5] Ou X., Keller A., Helm M., Fassbender J., Facsko S. *Phys. Rev. Lett.* **111** 016101 (2013)

Self-Organization in Technical Applications



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[6] Cummins C. et al. *Chem. Mater.* **27** 6091 (2015)

[7] Cummins C. et al. *Nanoscale* **7** 6712 (2015)

[8] Fernando Tomás, Zaragoza, Spain

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

[10] Teshome, B., Facsko, S., Keller, A. *Nanoscale* **6** 1790 (2014)

[11] Krause, M., Buljan, M. et al. *Phys. Rev. B* **89** 085418 (2014)

Overview

Monte-Carlo Simulations Out-of-Equilibrium

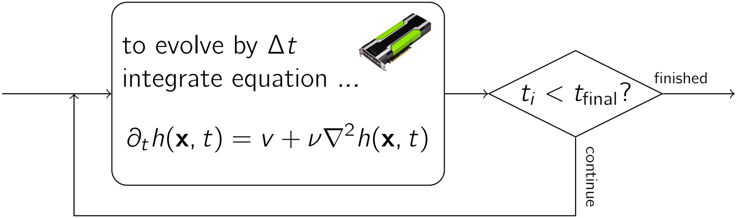
Simulation

t_i

advance time by integration or Monte Carlo sweep ...

t_{i+1}

Phase Field Methods



to evolve by Δt
integrate equation ...

$$\partial_t h(\mathbf{x}, t) = v + \nu \nabla^2 h(\mathbf{x}, t)$$

$t_i < t_{\text{final}}$?

finished

continue

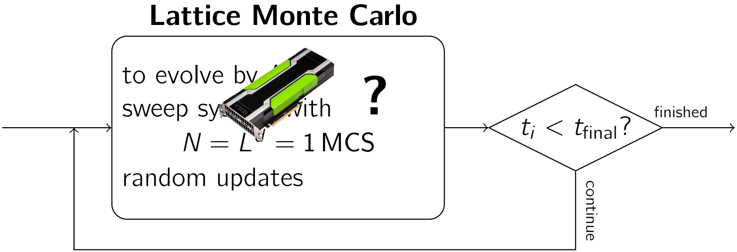
- simulated physical system evolves in discrete time steps Δt
- more accurate the smaller Δt and the larger the system

Simulation

t_i

advance time by
integration or Monte Carlo sweep ...

t_{i+1}



Lattice Monte Carlo

to evolve by
sweep sy with
$N = L^{d} = 1\,\mathrm{MCS}$
random updates

?

$t_i < t_{\text{final}}$?

finished

continue

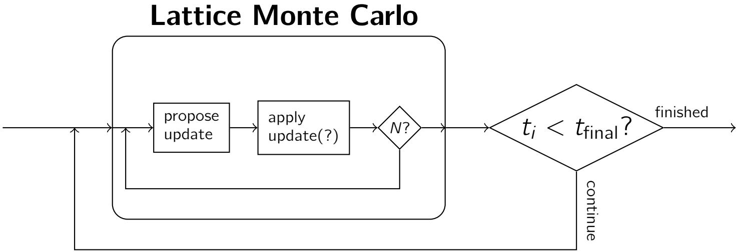
- simulated physical system evolves in discrete time steps Δt
- more accurate the larger the system
- updates are simple, but need to be applied in order
- uncorrelated updates—*We need those out-of-equilibrium.*

Simulation


t_i

advance time by
integration or Monte Carlo sweep ...

t_{i+1}


Lattice Monte Carlo

propose update

apply update(?)

$N?$

$t_i < t_{\text{final}}?$

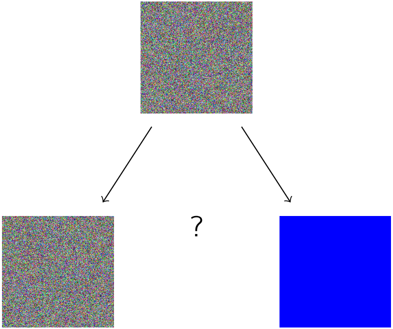
finished

continue

- 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.*

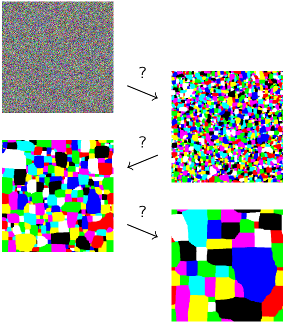
Equilibrium vs Non-Equilibrium

Equilibrium Properties:
only **final** state relevant



8-states Potts model

out-of-Equilibrium:
kinetics of interest



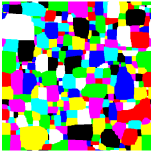
8-states Potts model, $\frac{J}{k_B T} = 5$

- optimal algorithm reaches equilibrium quickly
- optimal algorithm reproduces physical evolution

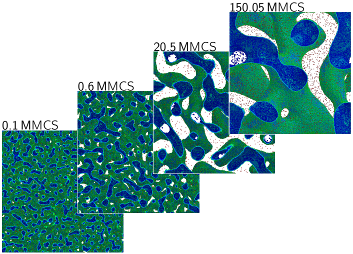
Types Monte-Carlo Dynamics/Algorithms

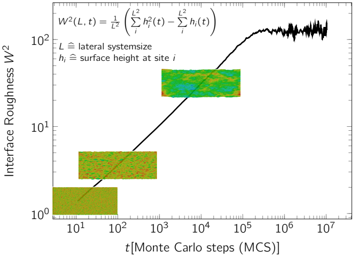
Dynamics	Equilibrium	Diffusion	Correlations
Random Sequential (RS)	slow	yes	no
Sequential	accelerated	biased	yes
Checkerboard SCA Stochastic Cellular Automaton	slow	yes	yes
Cluster	accelerated	no	—
…			

- Diffusion kinetics is mandatory.
- Correlations may leave some properties intact.
- SCA is computationally more efficient …



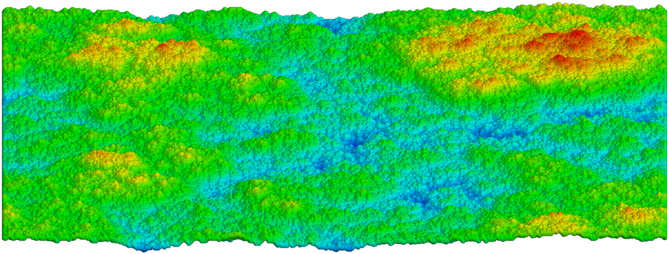
Dynamical Properties





- universal properties
  - growth exponents (surface roughness, structures)
  - autocorrelation and -response
    - fluctuation-dissipation relations
  - physical aging
- model-dependent properties
  - corrections
  - dependence on initial conditions
  - shape evolution (fabrication of nanostructures)

KPZ–Equation for Surface Growth



KPZ surface in the steady state

$$d_t h(\mathbf{x},t) = \underbrace{v}_{\text{mean growth vel.}} + \underbrace{\sigma_2 \nabla^2 h(\mathbf{x},t)}_{\text{surface tension}} + \underbrace{\lambda\,[\nabla h(\mathbf{x},t)]^2}_{\text{local growth vel.}} + \underbrace{\eta(\mathbf{x},t)}_{\text{noise}}$$

KPZ stochastic differential equation[1]

→ growth processes, randomly stirred fluids, directed polymers in random media, propagation of flame-fronts …

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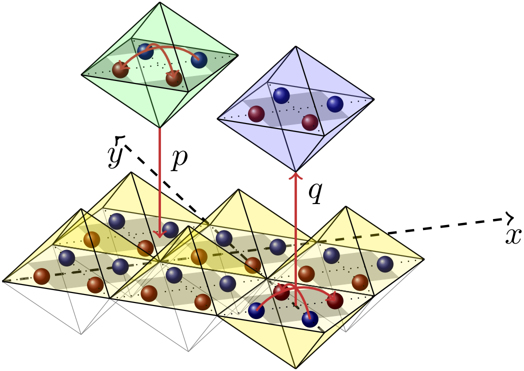
[1] Kardar, M., Parisi, G., Zhang, Y.-C. *Phys. Rev. Lett.* **56** 889 (1986)

Model—Octahedron-Model for KPZ Growth



$2+1$D roof-top model—octahedron model[2]

- lattice gas with directed dimer diffusion

↦ random deposition of octahedra

⇒ site-selection *only* source of noise for deposition prob. $p = 1$

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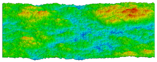
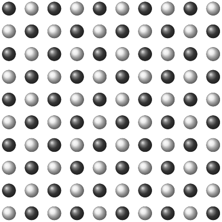
[2] Ódor, G., Liedke, B., Heinig, K.-H. *Phys. Rev. E* **79** 021125 (2009) (Plischke, M., Rácz, Z., Liu, D. *Phys. Rev. B* **35** 3485 (1987))

Domain Decomposition



lateral system size in aging simulations: $L = 2^{16}$

Stochastic Cellular Automaton (SCA)

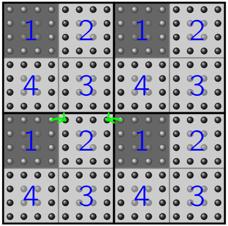


- update odd/even sublattice
  $p < 1$

+ linear memory access ⇒ fast

Random Sequential (RS)

on GPU: DTrDB



- update separate domains
  $p = 1$

+ uncorrelated updates

GPU implementation of Random Sequential Updates

1 Monte-Carlo Simulations Out-of-Equilibrium

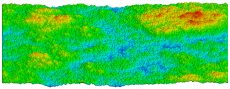
2 GPU implementation of Random Sequential Updates
- Performance: RS vs. SCA

3 Correlations: Random Sequential vs. SCA

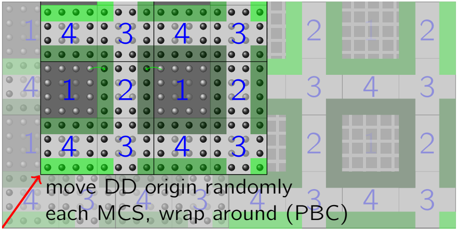
4 Beyond single Bits: Multi-Surface Approach on GPU
- Performance

5 Summary and Outlook

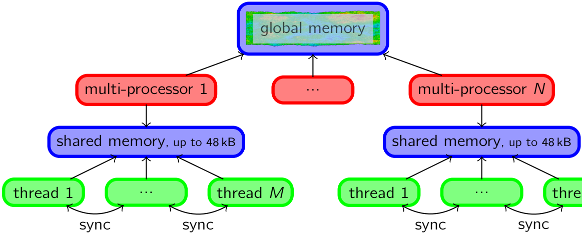
GPU Implementation of RS



- double-tiling at device layer
  ... with random origin
- single-hit delayed-border
  at block layer



move DD origin randomly
each MCS, wrap around (PBC)



global memory

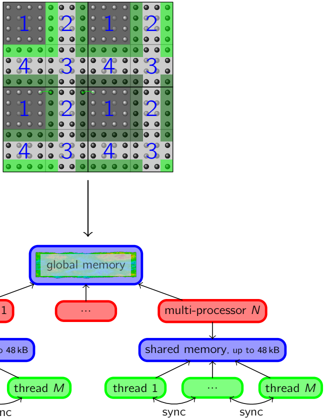
multi-processor 1
···
multi-processor N

shared memory, up to 48 kB
shared memory, up to 48 kB

thread 1
···
thread M
sync
sync

thread 1
···
thre
sync
sync

Bit-Coded KMC on GPUs—Limitations

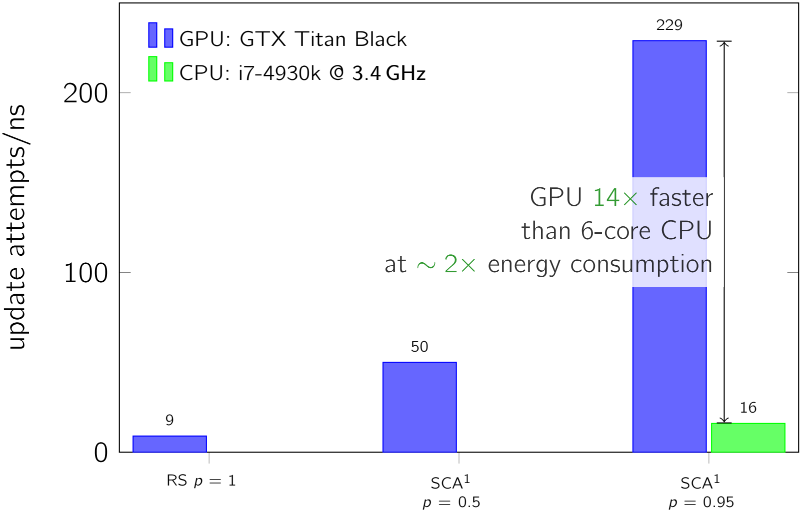


- domain decomposition tiles need to fit into shared memory

⇒ max. 2 - 4 states per lattice sites

- algorithm should better not lead threads to diverge

Performance of Bit-Coded RS vs. SCA



GPU 14× faster
than 6-core CPU
at ∼ 2× energy consumption

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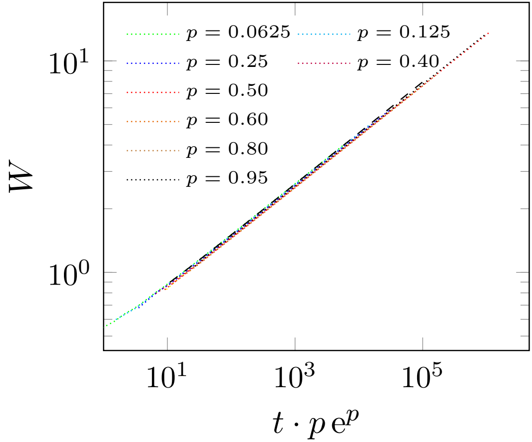
[1] Kelling, J., Ódor, G., Gemming, S.:
IEEE International Conference on Intelligent Engineering Systems (2016) `arXiv:1606.00310`

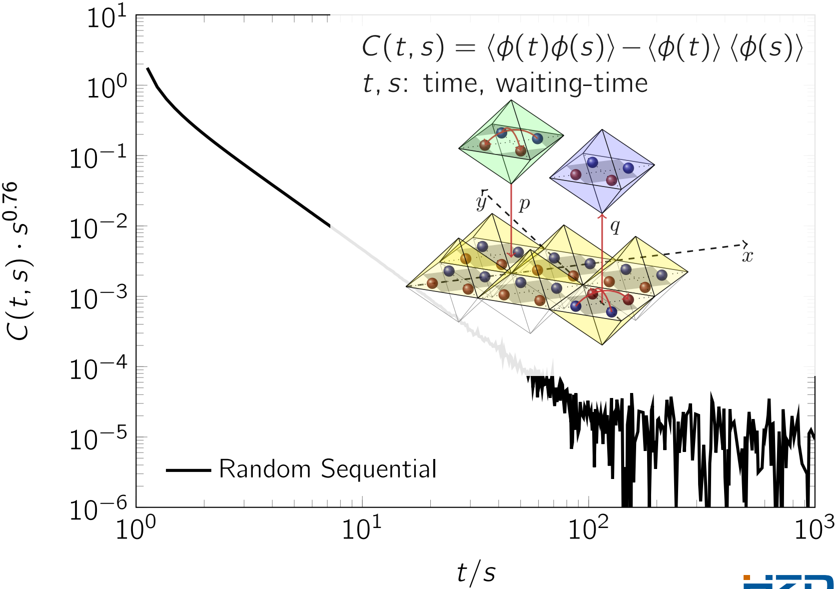
Correlations: Random Sequential vs. SCA

Growth of Surface Roughness

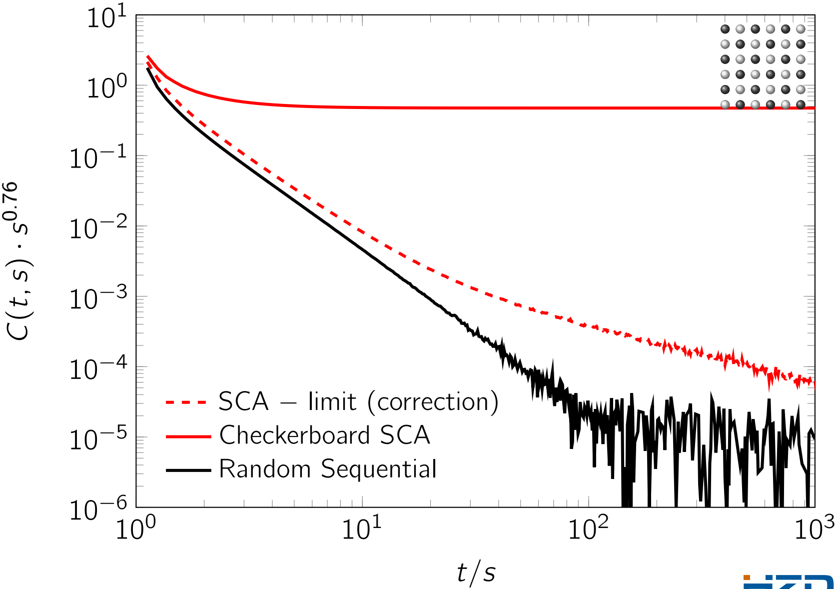
$$W(L,t) = \frac{1}{L}\sqrt{\sum_i^{L^2} h_i^2(t) - \sum_i^{L^2} h_i(t)}$$



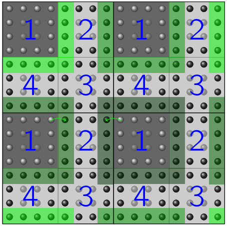
Auto-Correlation of Slopes (Lattice Gas)



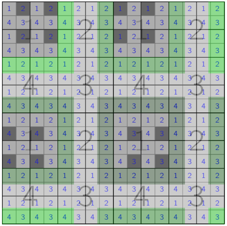
Auto-Correlation of Slopes (Lattice Gas)



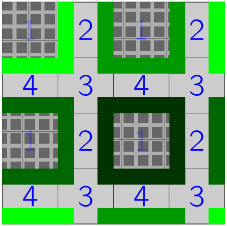
Domain Decomposition for RS



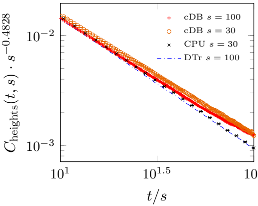
DT...

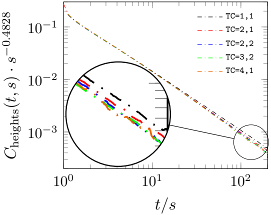


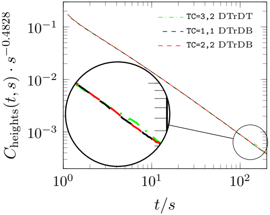
DTrDT



DTrDB



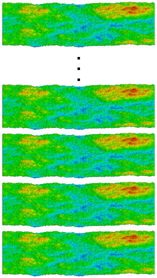




Beyond single Bits: Multi-Surface Approach on GPU

Multi-Surface Coded Simulations on GPU

- efficient simulation of independent copies



vector of $32, \ldots, 128, 256, \ldots$ layers depending on application

⇒ very efficient use of GPUs

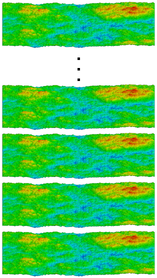
(vector processors/data parallelism)

⇒ high energy efficiency

⇒ projected good parallel scaling (multi-GPU)

Multi-Surface Coded Simulations on GPU

- efficient simulation of independent copies



Trivially parallel → **Multi-Surface**

↦ large samples ⇒ good statistics

↦ large parameter studies

↦ large sets of initial conditions

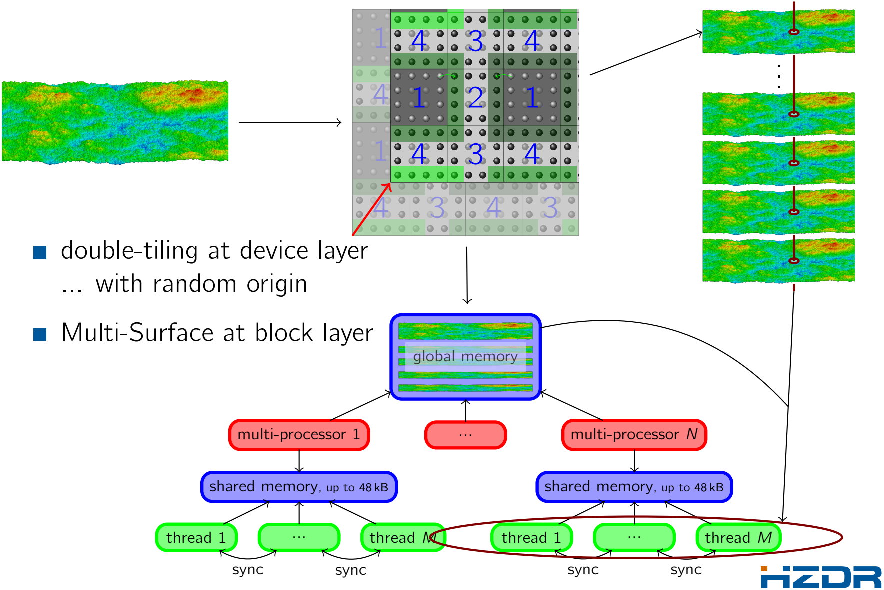
+ random site-selection

Multi-Surface Approach for GPUs

- double-tiling at device layer

  … with random origin

- Multi-Surface at block layer



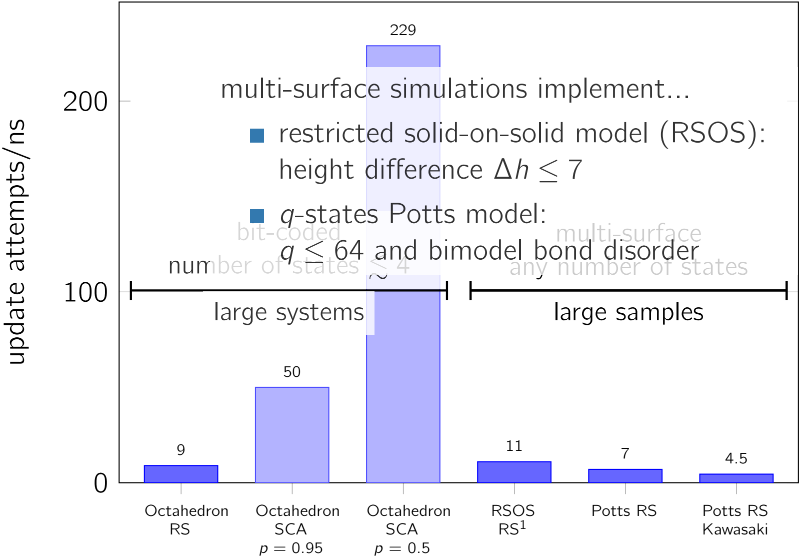
multi-processor 1
…
multi-processor N

shared memory, up to 48 kB
shared memory, up to 48 kB

thread 1
…
thread M
thread 1
…
thread M

sync
sync
sync
sync

Performance of Lattice Monte-Carlo Codes



multi-surface simulations implement...

- restricted solid-on-solid model (RSOS): height difference $\Delta h \leq 7$
- q-states Potts model: $q \leq 64$ and bimodel bond disorder

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[1] Kelling, J., Ódor, G., Gemming, S.: *Phys. Rev. E* **94** 022107 (2016)

Summary and Outlook

Summary and Outlook

- many physical systems are governed or can be described by stochastic processes
    - computing dynamical properties (e.g. in KPZ)
    - nanostructure evolution, aging
- type of dynamics can matter
- different GPU algorithms to choose from:
    - SCA: good enough for most scaling properties
    - Bit-coded RS: (virtually) uncorrelated noise
      up to $\sim 16 \times 10^9$ lattice sites on single GPU
    - Multi-Surface: flexible (many states, disorder), still efficient
      system size limited by GPU memory
      to do: multi-GPU implementation (straight-forward)

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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)
- Ódor, G., Kelling, J., Gemming, S.:
  Aging of the (2+1)-dimensional Kardar-Parisi-Zhang model
  Phys. Rev. E **89** 032146 (2014)
- 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)
  `arXiv:1606.00310`
- Kelling, J., Ódor, G., Gemming, S.:
  Universality of 2+1 dimensional RSOS models
  Phys. Rev. E **94** 022107 (2016)

Image Sources

1. Müller, T., Heinig, K.-H. et al. *Appl. Phys. Lett.* **85** 2373 (2004) *As referenced in RainbowEnergy project.*
2. `http://en.wikipedia.org/wiki/File:Rub_al_Khali_002.JPG`
3. `https://www.hzdr.de/db/Cms?pOid=24344&pNid=2707`
4. `http://hubblesite.org/newscenter/archive/releases/2007/17/image/a`
5. Ou X., Keller A., Helm M., Fassbender J., Facsko S. *Phys. Rev. Lett.* **111** 016101 (2013)
6. Cummins C. et al. *Chem. Mater.* **27** 6091 (2015)
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