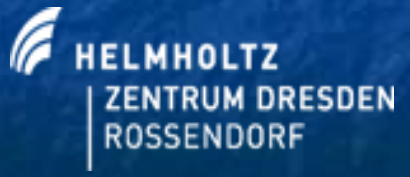
Extremely Large Scale Simulation of Surface Growth and Lattice Gases

Géza Ódor, Budapest (MTA-TTK-MFA), Gergely Ódor, (MIT Boston)
Jeffrey Kelling, Henrik Schulz, Karl-Heinz Heinig, Dresden (HZDR),
Ferenc Maté Nagy, Róbert Juhász Budapest (Wigner FKK)
German-Hungarian collaboration supported by
DAAD and MÖB: 2010-2011
NVIDIA Professor Partrnership 2010-

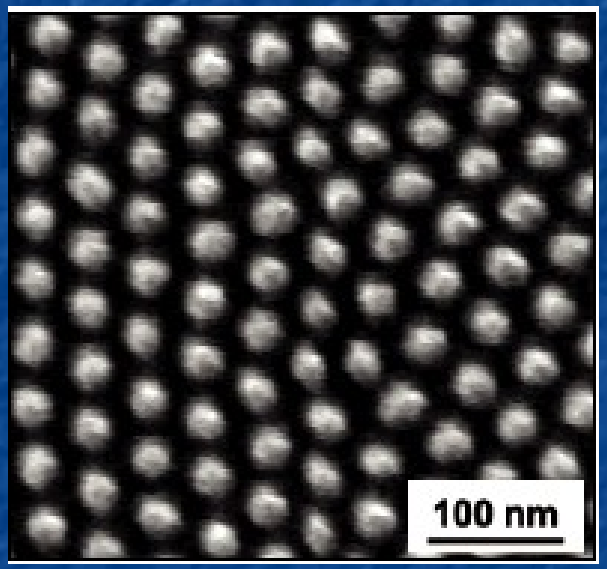
GTC2013 21/03/2013

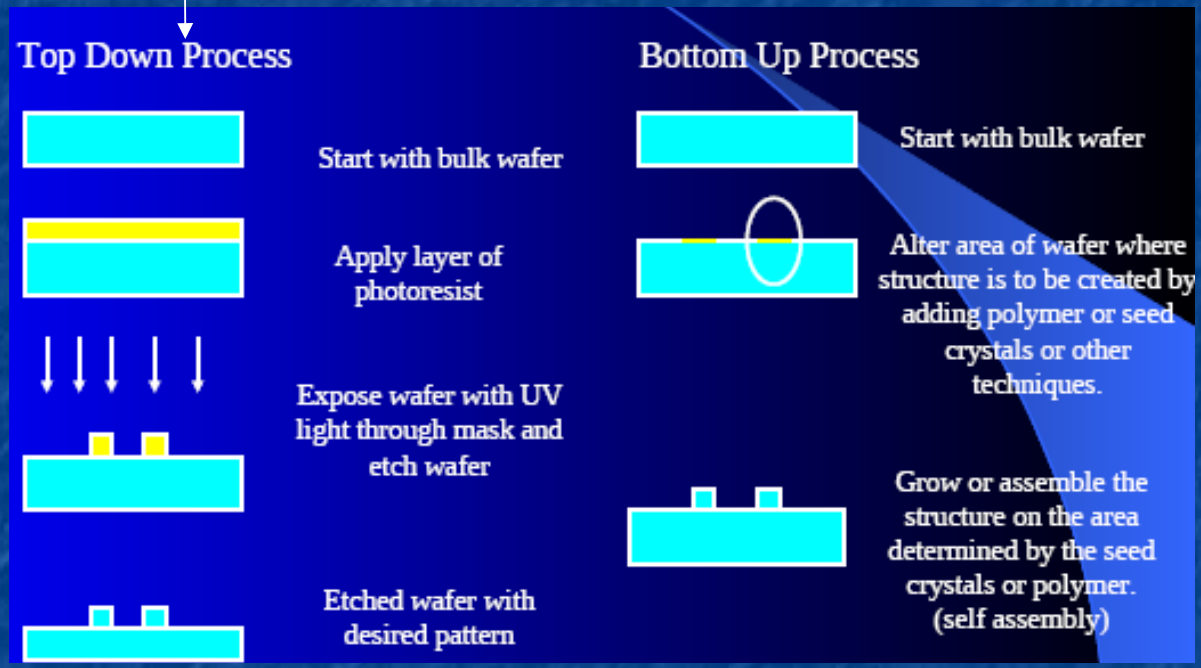


www.mfa.kfki.hu/~odor

Motivation

In nano-technologies large areas of **nano-patterns** are needed, fabricated today by expensive techniques, e.g. electron beam lithography or direct writing with electron and ion beams.





Similar phenomena: sand dunes, chemical reactions … → Universality

Better understanding of basic surface growth phenomena is needed !

Kardar-Parisi-Zhang (KPZ) equation

$$\partial_t h(x,t) = \sigma \nabla^2 h(x,t) + \lambda (\nabla h(x,t))^2 + \eta(x,t)$$

σ : (smoothing) surface tension coefficient

λ : local growth velocity, up-down anisotropy

η : roughens the surface by a zero-average, Gaussian noise field with correlator:

$$\langle \eta(x,t)\, \eta(x',t') \rangle = 2\, D\, \delta^d (x-x')(t-t')$$

Characterization of surface growth:

Interface Width:

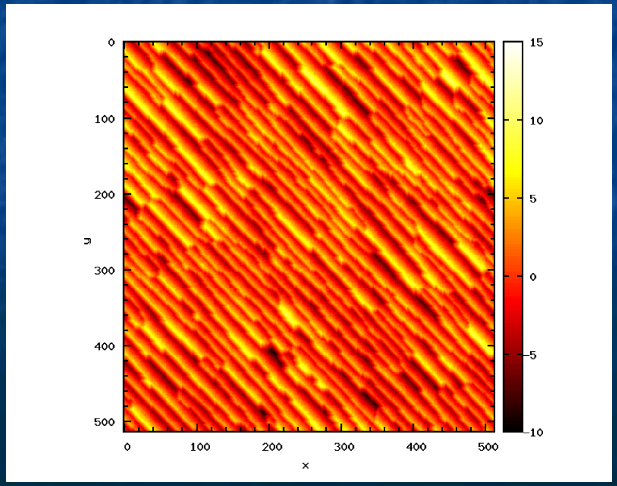
$$W(L,t) = \left[\frac{1}{L^2} \sum_{i,j}^{L} h_{i,j}^2(t) - \left(\frac{1}{L} \sum_{i,j}^{L} h_{i,j}(t) \right)^2 \right]^{1/2}$$

Family-Vicsek scaling:

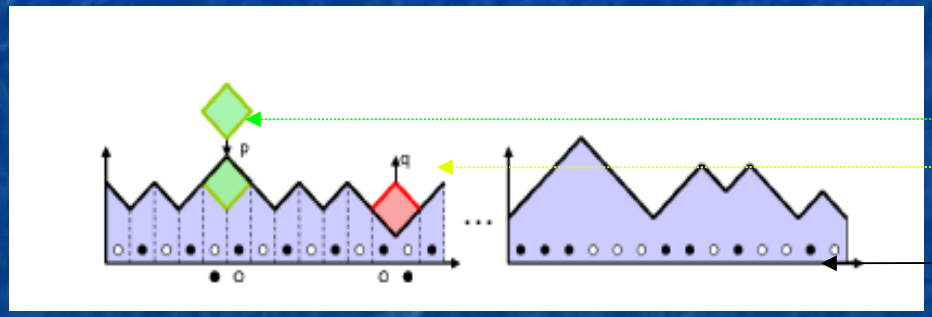
$$\begin{aligned} W(L,t) &\propto t^{\beta}, \quad \text{for} \quad t_0 << t << t_s \\ &\propto L^{\alpha}, \quad \text{for} \quad t >> t_s \ . \end{aligned}$$

Grand challanges in Statistical Physics and Surface Science

- Solution of KPZ equation in *d>1* dimensions: Even for 2d controversial results
- Existence of the upper critical dimension ? most simulations predict $d = \infty \Leftrightarrow$ analytical results
- Description of universal self-organized ripple/dot pattern formation
- Fondation of nonequilibrium statistical physics via understanding lattice gas models
- ...

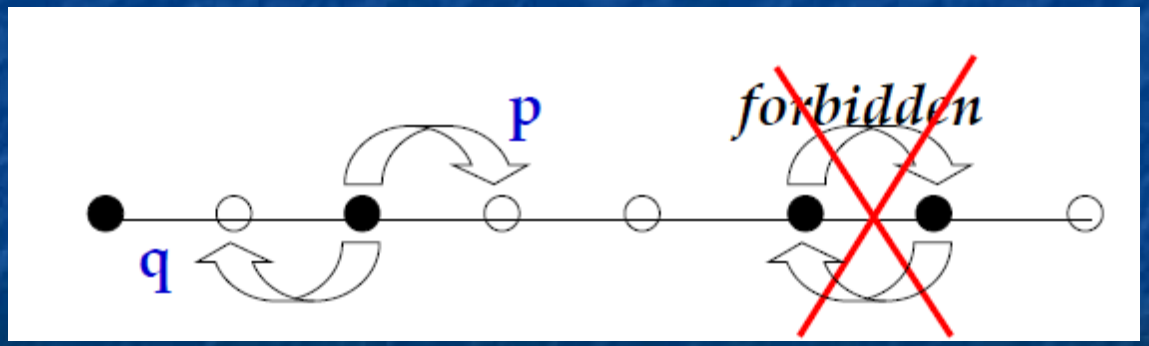


Mapping of KPZ onto ASEP in 1d



Kawasaki' exchange of particles

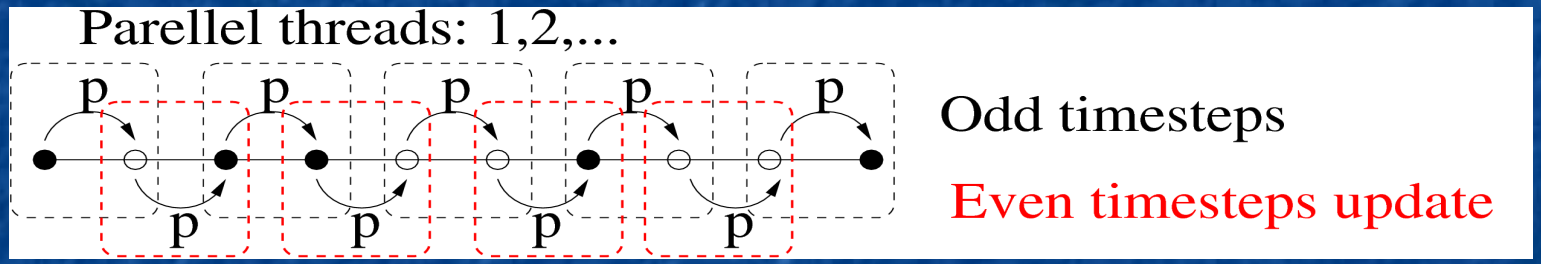
- Mapping of the *1+1* dimensional surface growth onto the 1d **ASEP** model:
- Attachment (with probability ***p***) and Detachment (with probability ***q***) corresponds to anisotropic diffusion of particles (bullets) along the *1d* base space (*M. Plischke, Rácz and Liu, PRB 35, 3485 (1987)*)



The simple ***ASEP*** (Ligget '95) is an **exactly solved 1d lattice gas**
Many features: response to disorder, different boundary conditions ... are known.

Parallel update algorithms for 1d ASEP/KPZ

Parallel updates on a ring of size *L*:



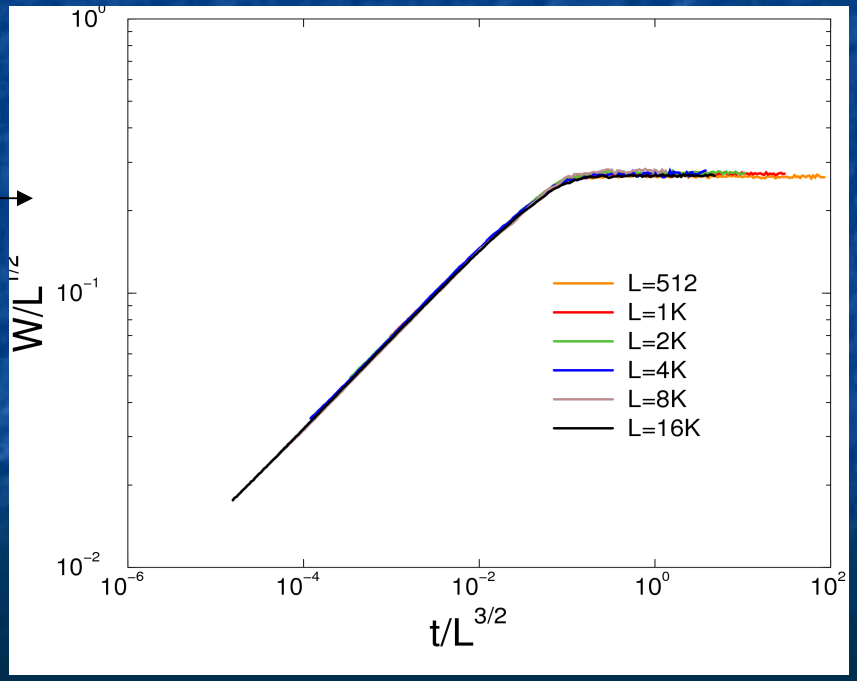
with probability *p* (**TASEP**)

Scaling by the serial **C** and **CUDA**:
Agreement with 1d KPZ scaling

L < 32K chains fit into shared memory of Tesla multiprocessor blocks

→ **no communication losses**

maximal speedup & scaling:
240 cores GPU Tesla:
100 x of a CPU (2.8 GHz)



H. Schulz, G. Ódor, G. Ódor, M. F. Nagy : Comp. Phys. Comm. 182 (2011) 1467

OpenCL Implementation

- Tested for TASEP (KPZ) on ATI, NVIDIA, CPU clusters
- Portable for “any” parallel Computers (in principle)
- Multi-GPU program using Message Passing Interface
- No size limitation by shared memory
- For larger system its speed is comparable to CUDA code

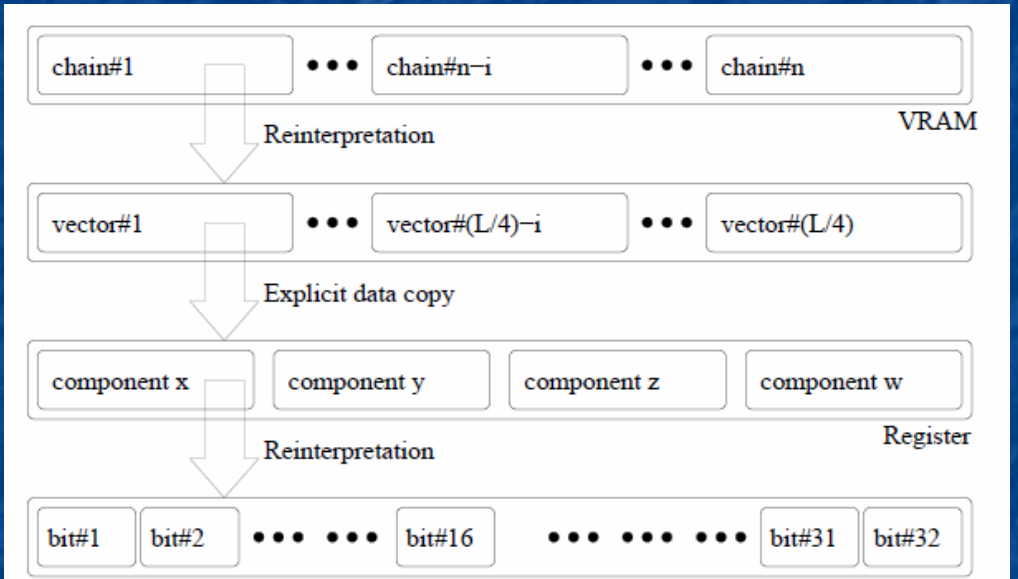
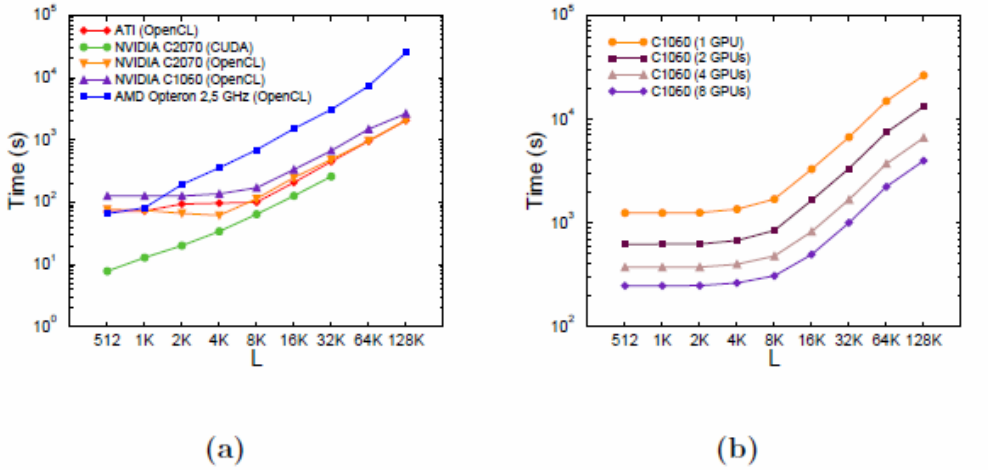


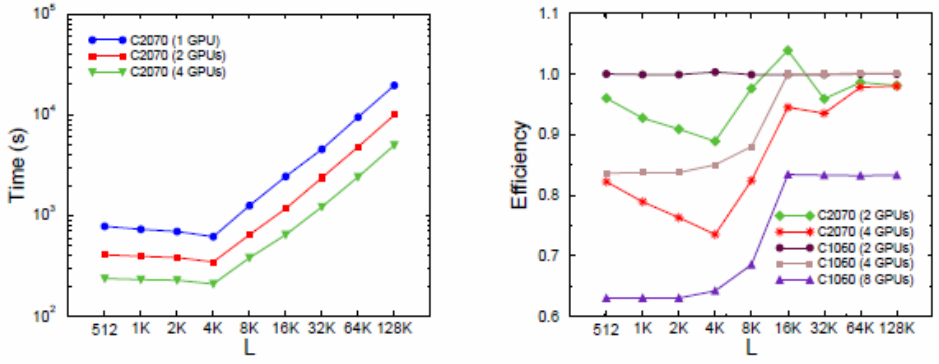
Figure 6: Memory map of data in the OpenCL algorithm.

Run-time analysis



(a) (b)

Figure 8: Run-time comparisons for different implementations (CUDA, OpenCL) of TASEP on different platforms (single ATI GPU, single NVIDIA GPU, single cluster node containing 16 CPU cores) (a) and for the OpenCL implementation using 1, 2, 4 and 8 NVIDIA C1060 (b).



(a) (b)

Figure 9: (a) Run-time comparisons for the OpenCL implementation using 1, 2 and 4 NVIDIA C2020. (b) Efficiency on 2, 4 and 8 NVIDIA C1060 and 2 and 4 NVIDIA C2070. The peak for $L = 16K$ on NVIDIA C2070 comes from a small delay on the server in the referenced 1-GPU simulation.

Disordered ASEP model simulations

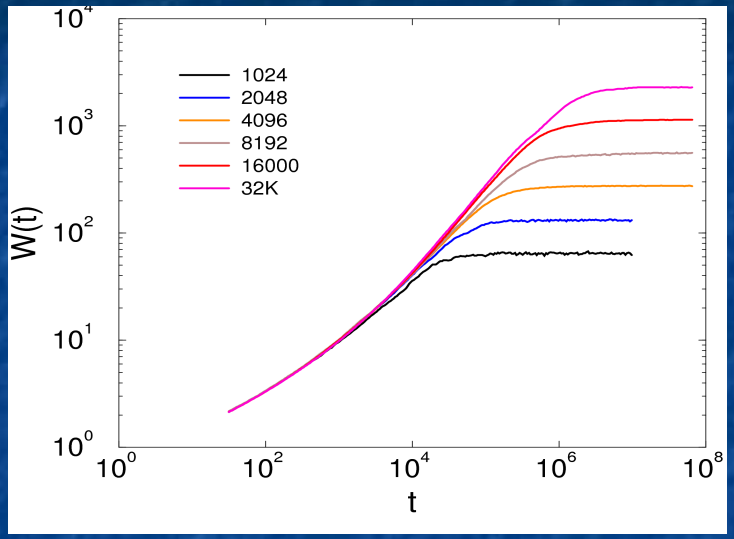
- Site-wise binary Quenched disorder:

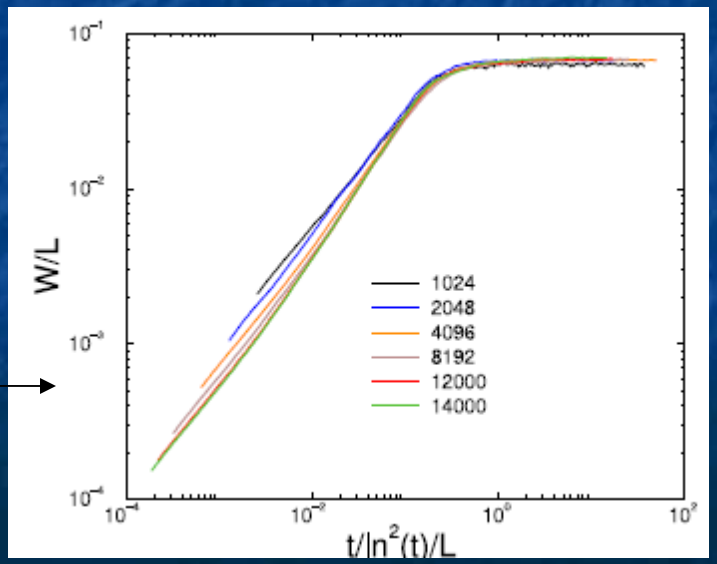
$$P(p_i) = (1-D)\delta(p_i - p) + D\delta(p_i - rp)$$

- Corresponds to KPZ growth with columnar disorder:

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

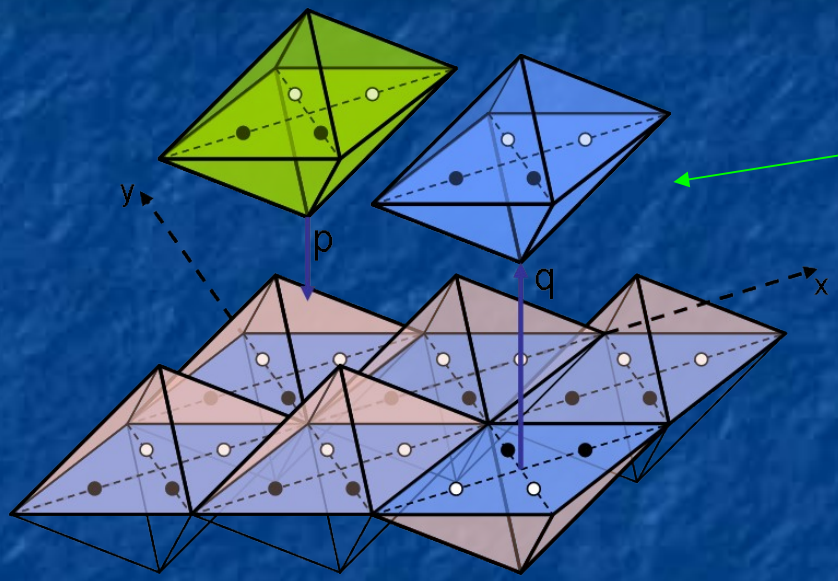
- Q-TASEP: *p_i=0.8 or 0.2, q_i=0*
  L=1024, 2048, ... 14000
  *t_{max} = **10^8 MCs***
- Studied by: *Krug 1999, Stinchcombe et al. 2008: β <1*
- *Data collapse with **α=β=z=1** faster than KPZ growth !*
- *Precise form of log. corrections are derived*
- *+ Q-PASEP and 2-lane TASEP:*





R. Juhász, G. Ódor, G. Ódor, J. Stat. Mech. (2012) P08004

Mapping of KPZ growth in *2+1* dimensions



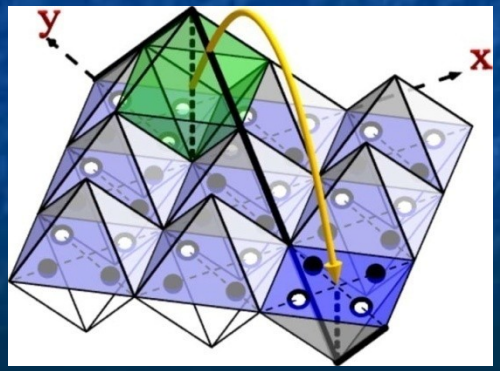
- Generalized Kawasaki update:

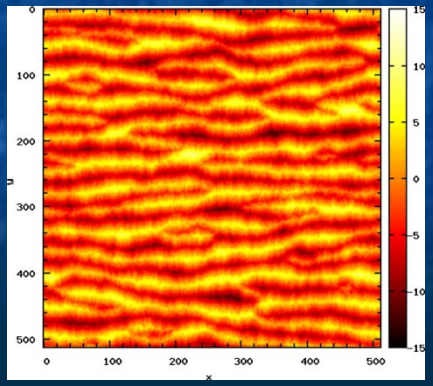
$$\begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \rightleftharpoons \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}$$

- **Octahedron model**

  Driven diffusive gas of pairs (dimers)

- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 031112 (2010)*



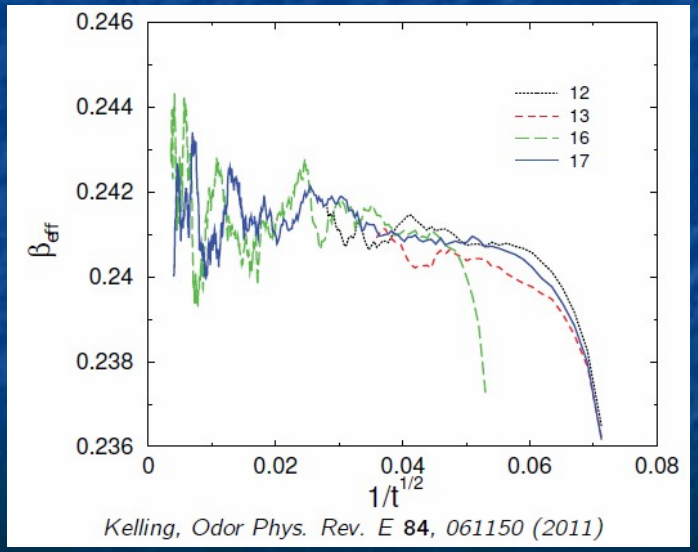


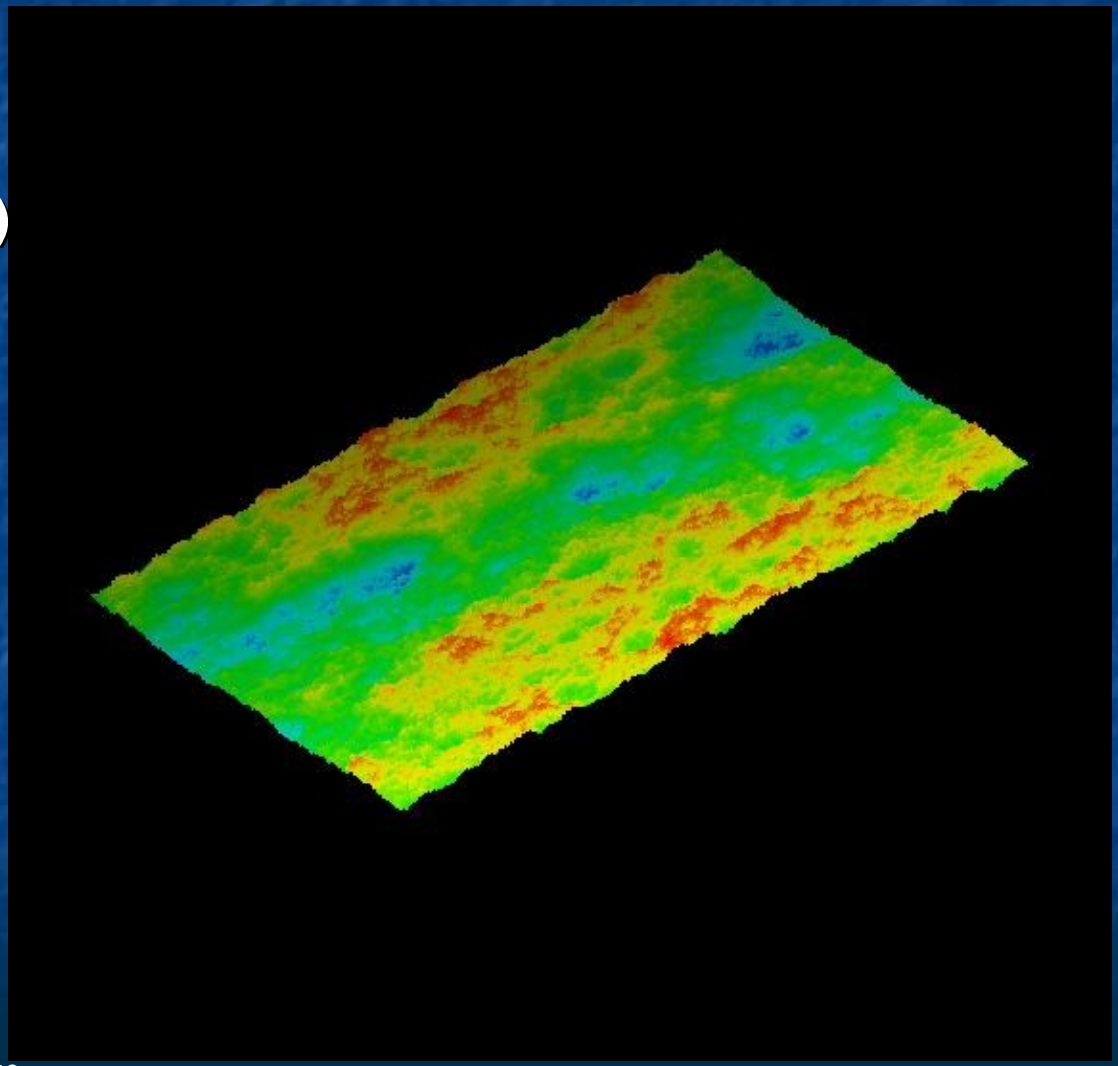
- **Surface pattern formation via dimer model**

- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 051114 (2010)*

CUDA code for 2d KPZ

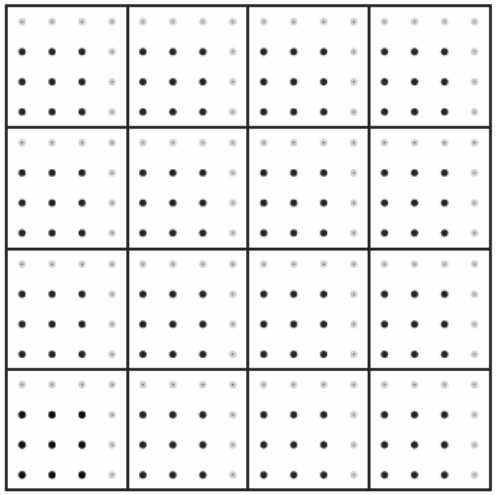
- Each 32-bit word stores the slopes of 4x4 sites
- **Speedup 430 x (Fermi) with respect a CPU core of 2.8 GHz on: 131072 x 131972 size**





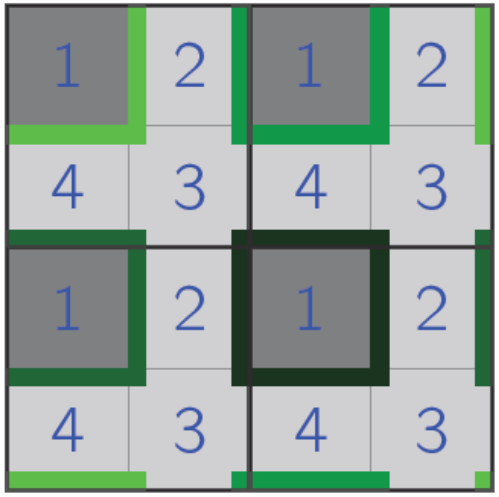
J. Kelling and G. Ódor Phys. Rev. E 84 (2011) 061150

Domain decomposition



- dead border decomposition at device level (active sites $(n-1) \times (n-1)$)
- randomly moving origin (word-wise)
- every MCS at device layer

$\Rightarrow$ avoids accumulation of errors at borders



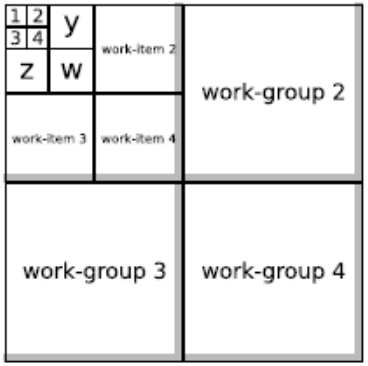


Fig. 3: Decomposition of the whole system into work-groups at device layer, with gray areas indicating dead borders. Further decomposition at work-group layer using double tiling is indicated for work-group 1: Each work-item executes four virtual threads using VLIW vector operations. The virtual threads are denoted by their corresponding vector components (x, y, z, w). A single–hit double tiling scheme is employed to distribute the work-group among all virtual threads. The cells of the four sets of domains are indicated for virtual thread 1.x.

J. Kelling, G. Ódor, M. F. Nagy, H. Schulz and K. -H. Heinig, EPJST 210 (2012) 175-187

Runtime Analysis

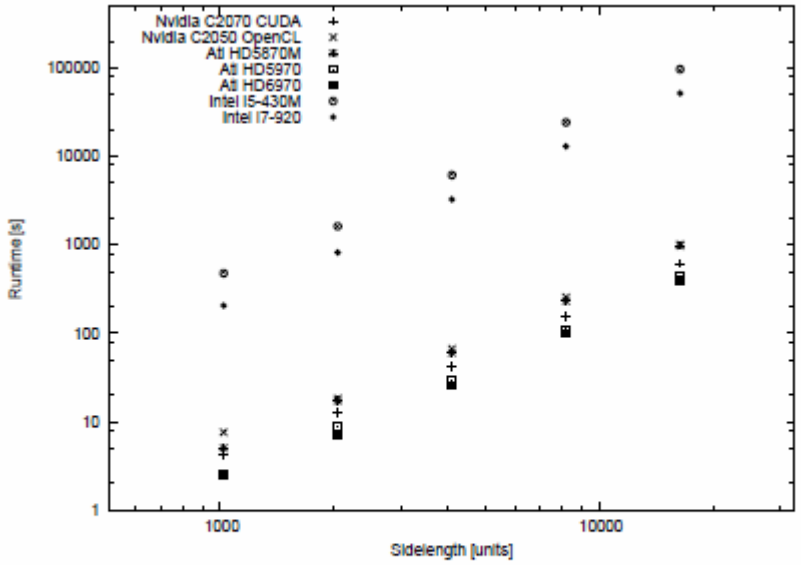


Fig. 4: Run-time comparison of the different architectures and programming models. For the KPZ model. The Run-time scales with the lateral system dimension as $\sim L^{1.855}$.

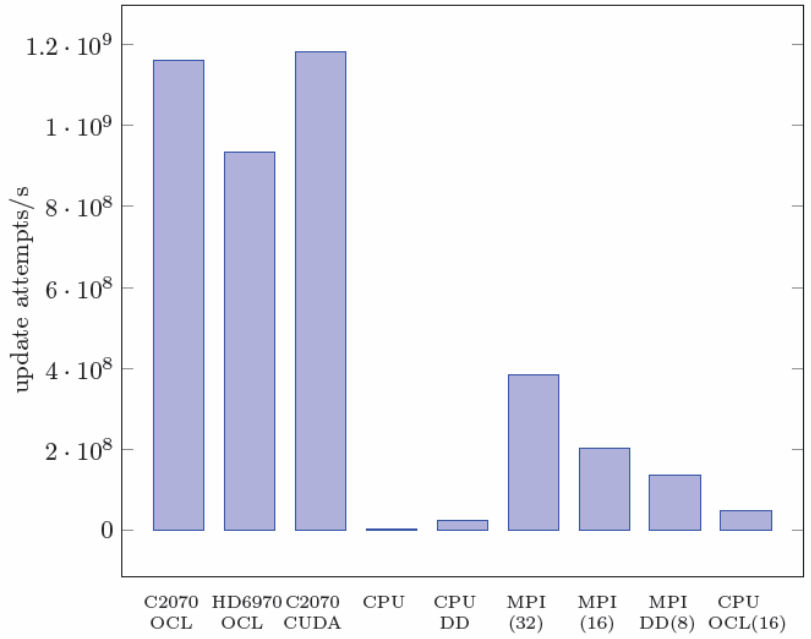
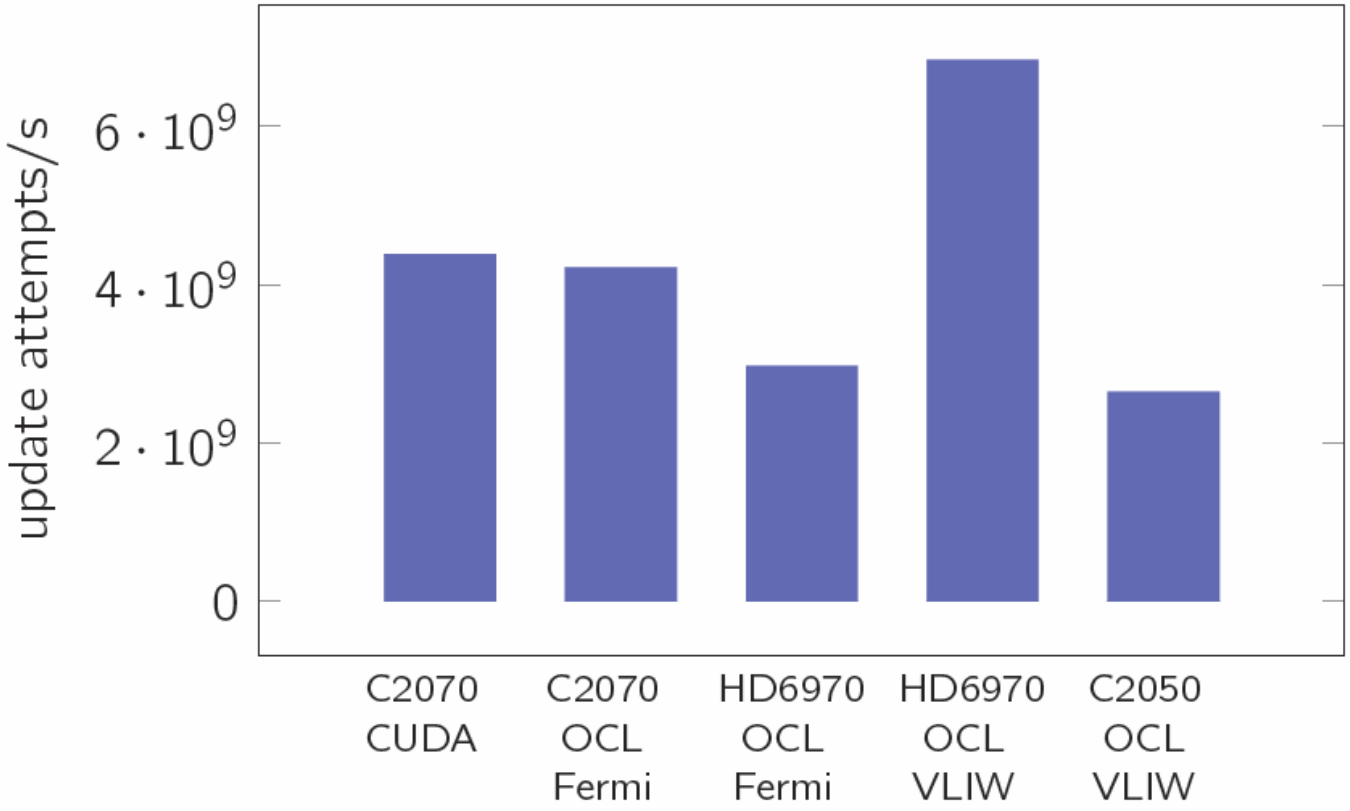


Fig. 6: Performance comparison of KMC implementations on GPUs and AMD Opteron CPUs using MPI or pure CPU code. The suffix 'DD' denotes L1 cache optimized CPU code. The numbers in parenthesis give the number of CPU cores used for multi CPU implementations. The values are in the order of $\sim 10^9$ for GPUs and $\sim 10^7$ for CPUs.

OpenCL and Optimizations



Kelling, Odor, Nagy, et al. Eur. Phys. J. Special Topics **210**, *175 (2012)*

- HD6970 provides 128-bit registers (Very Long Instruction Word)

$\Rightarrow$ Even with OpenCL different architectures require different code

Conclusions & outlook

- Fast parallel simulations due to mapping onto stochastic cellular automata (lattice gases)
- Important scaling results in 1d disordered ASEP models with **ultra-slow dynamics**
- **Extremely large scale** (2^{17}x2^{17}) **results** in 2d KPZ clarified long lasting debate: ruling out simple (¼, 4/10) scaling exponents
  + determination of **Universal Scaling Functions**

Double Tiling is more efficient than Dead Border domain decomposition

OpenCl performs almost as good as CUDA on NVIDIA devices,
but it could not fulfill it's promise on platform independence

Extension for studying Surface pattern formation would be very efficient

- **Acknowledgements**: DAAD-MOB, OTKA, OSIRIS FP7, NVIDIA
- Publications:

H. Schulz, G. Ódor, G. Ódor, M. F. Nagy, Computer Physics Communications 182 (2011) 1467.
J. Kelling and G. Ódor, Phys. Rev. E 84, 061150 (2011),
G. Ódor, B. Liedke, K.-H. Heinig J. Kelling, Appl. Surf. Sci. 258 (2012) 4186
J. Kelling, G. Ódor, M. F. Nagy, H. Schulz and K. -H. Heinig, EPJST 210 (2012) 175-187