Statisztikus fizikai modellek extrém nagy szimulációja

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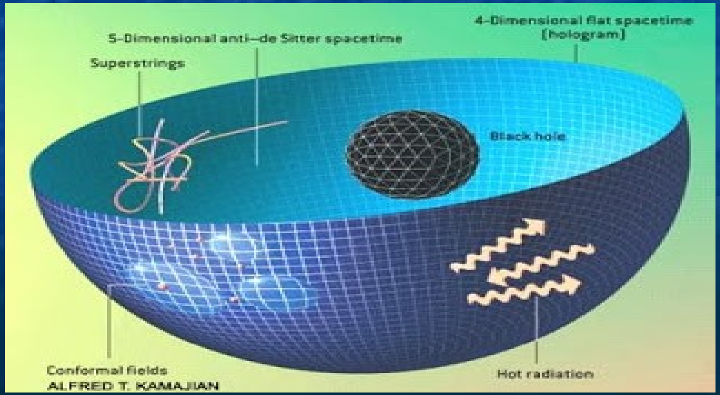
Grand challenges in science

- Understanding of physics far from equilibrium is recognized to be one of the ‘grand challenges’ of our time, by both the US National Academy of Sciences [1] and the US Department of Energy [2]
- [1] Committee on CMMP 2010 Condensed-Matter and Materials Physics:
  The Science of the World Around Us (Washington, DC: The National Academies Press)
  [2] BESAC Subcommittee on Grand Challenges for Basic Energy Sciences 2007 Directing Matter and Energy:
  Five Challenges for Science and the Imagination (Washington,DC: US Department of Energy)
- Furthermore, these studies point out the importance of non-equilibrium systems and their impact far beyond physics, including areas such as computer science, biology, public health, civil infrastructure, sociology, and finance
- Striking new example: string theory (quantum gravity) ↔ non-equilibrium physics



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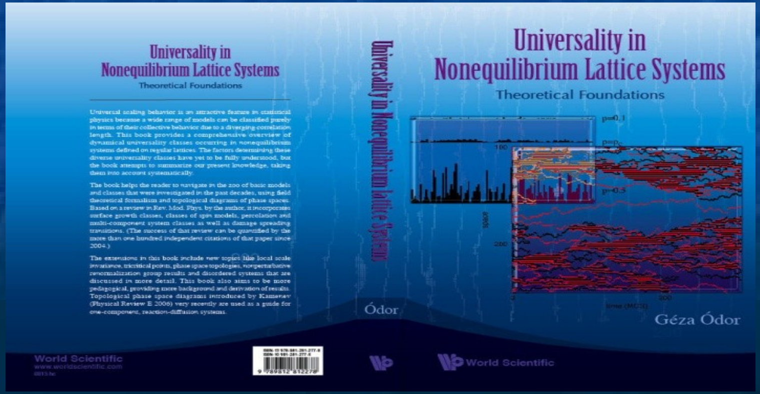
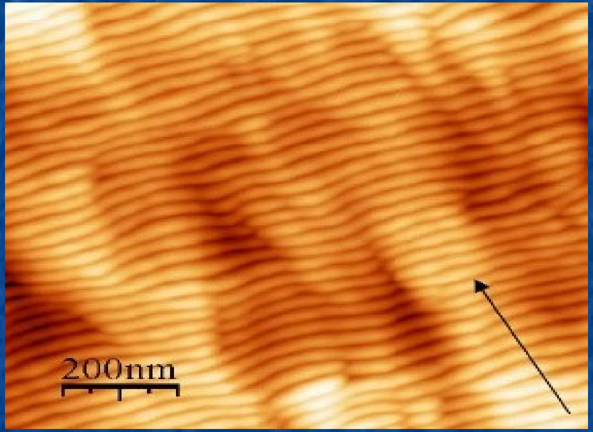
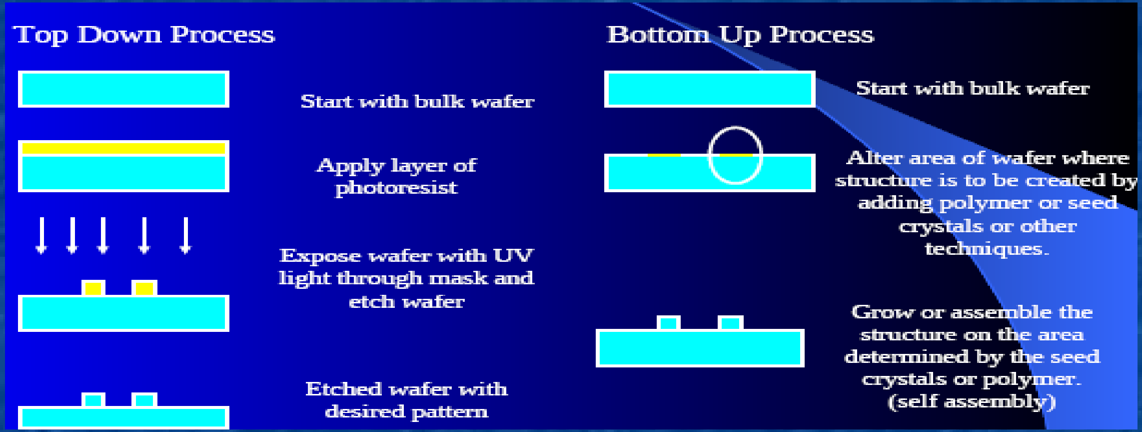

Universality in Nonequilibrium Lattice Systems
Theoretical Foundations
Géza Ódor
World Scientific

Our Motivation was

In nanotechnologies 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.





Top Down Process

Start with bulk wafer

Apply layer of photoresist

Expose wafer with UV light through mask and etch wafer

Etched wafer with desired pattern

Bottom Up Process

Start with bulk wafer

Alter area of wafer where structure is to be created by adding polymer or seed crystals or other techniques.

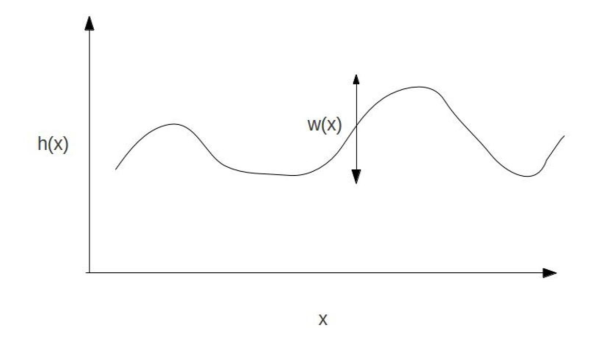
Grow or assemble the structure on the area determined by the seed crystals or polymer. (self assembly)

Similar phenomena: sand dunes, chemical reactions …
→ Universality & Nonequilibrium physics

Better understanding of basic surface growth phenomena is needed !

The Kardar-**P**arisi-**Z**hang (**KPZ**) equation

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



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:

$$<\eta(x,t)\ \eta(x',t')> = 2\,D\,\delta\,(x-x')(t-t')$$

Characterization of surface growth:

Interface Width:

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

Fundamental model of non-equilibrium surface physics

Surface growth power-laws:

$$W(L,t) \propto \begin{cases} t^{\beta} & \text{for } t_0 \ll t \ll t_s, \\ L^{\alpha} & \text{for } t \gg t_s. \end{cases}$$

Grand challenges in Statistical Physics and Surface Science

- Solution of KPZ equation in *d>1* dimensions
- Existence of the upper critical dimension, beyond which fluctuations are irrelevant (smooth surfaces) ?
  Most simulations predict: $d = \infty$
  ⇔ analytical studies
- Determination of universal scaling functions, ageing properties

Description of universal self-organized ripple/dot pattern formation

- Foundations of non-equilibrium statistical physics via understanding lattice gas models

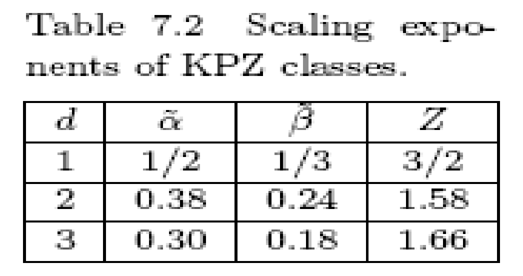
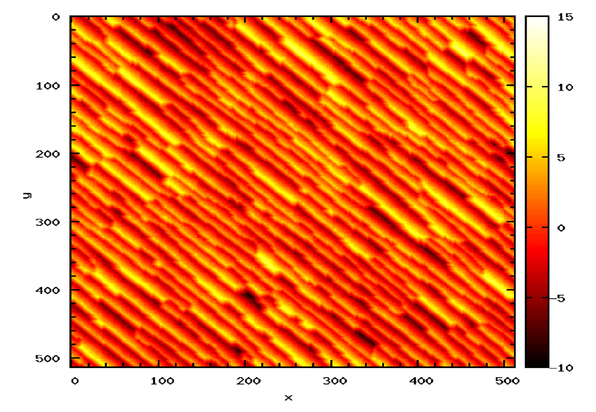
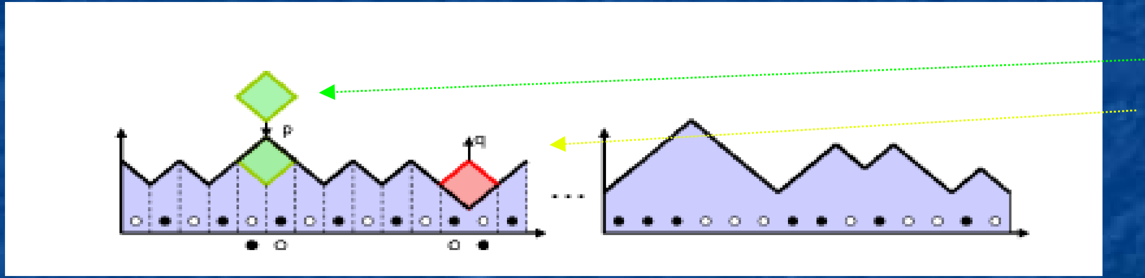


Table 7.2 Scaling exponents of KPZ classes.

d	$\tilde{\alpha}$	$\tilde{\beta}$	Z
1	1/2	1/3	3/2
2	0.38	0.24	1.58
3	0.30	0.18	1.66



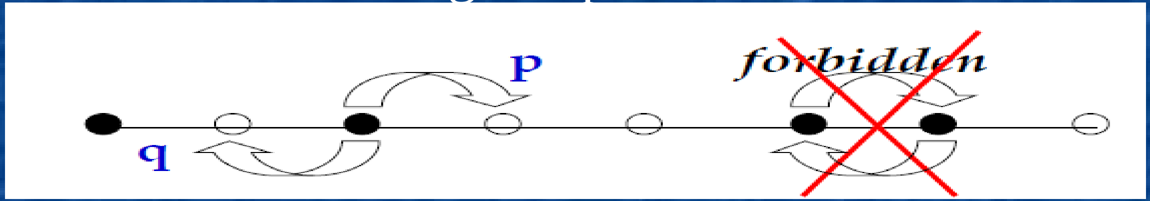
Mapping of KPZ onto ASEP in 1d

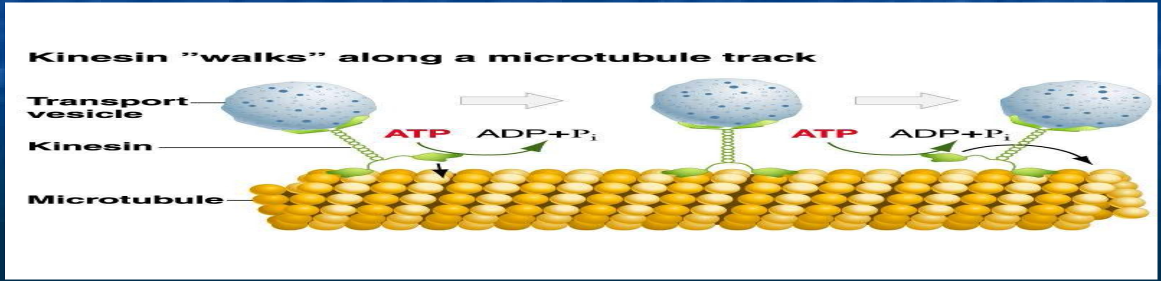


- Attachment (with probability ***p***) and
- Detachment (with probability ***q***)

- Corresponds to anisotropic diffusion of particles (bullets) along the *1d* base space (Racz et al 1987)

Kawasaki' exchange of particles



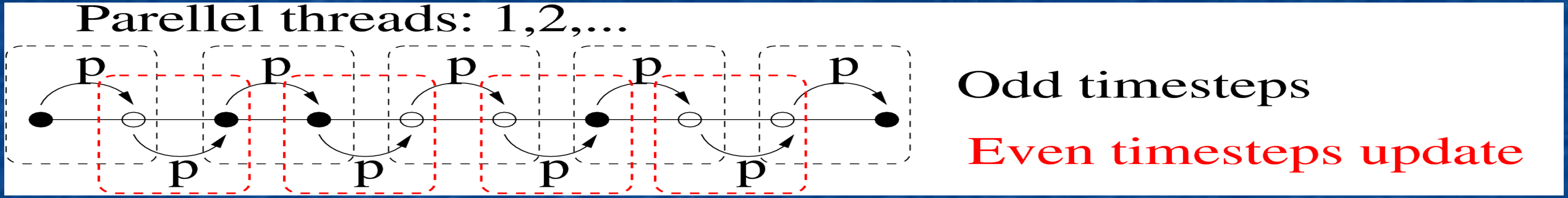


The simple **ASEP** (Ligget '95)
is an **exactly solved 1d lattice gas**

Widespread application in biology

Cellular automaton algorithm for 1d ASEP/KPZ

Parallel updates on a ring of size *L*:



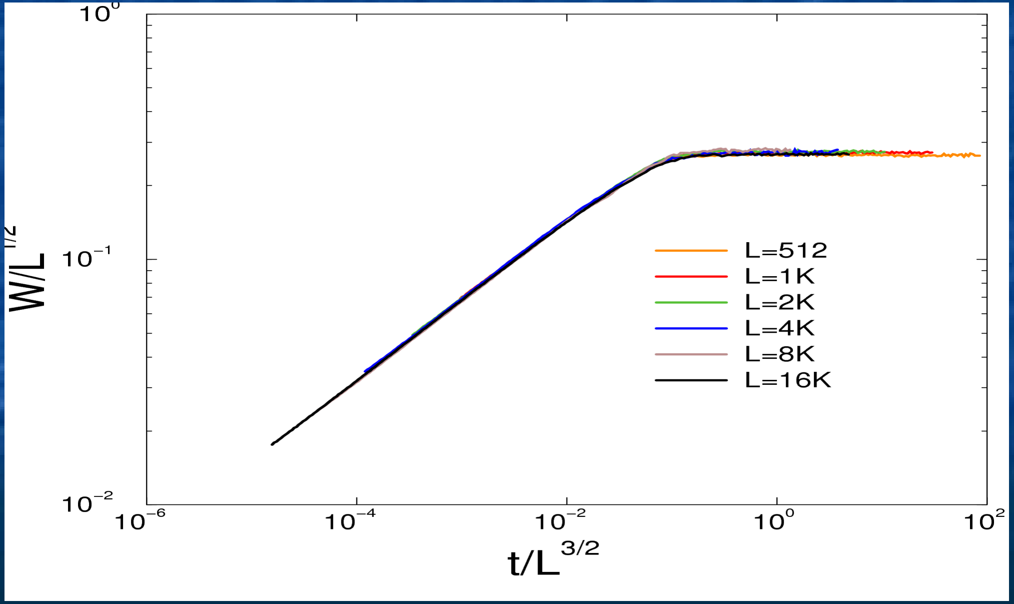
with probability *p* (**TASEP**)

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

L < 64K chains **fit** into the shared
memories of 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

No size limitation by shared memory

Uses vectorization of AMD

Portable for “any” parallel computers (in principle)

Tested by ASEP (KPZ) on ATI, NVIDIA, CPU clusters

Multi-GPU program using **M**essage **P**assing **I**nterface

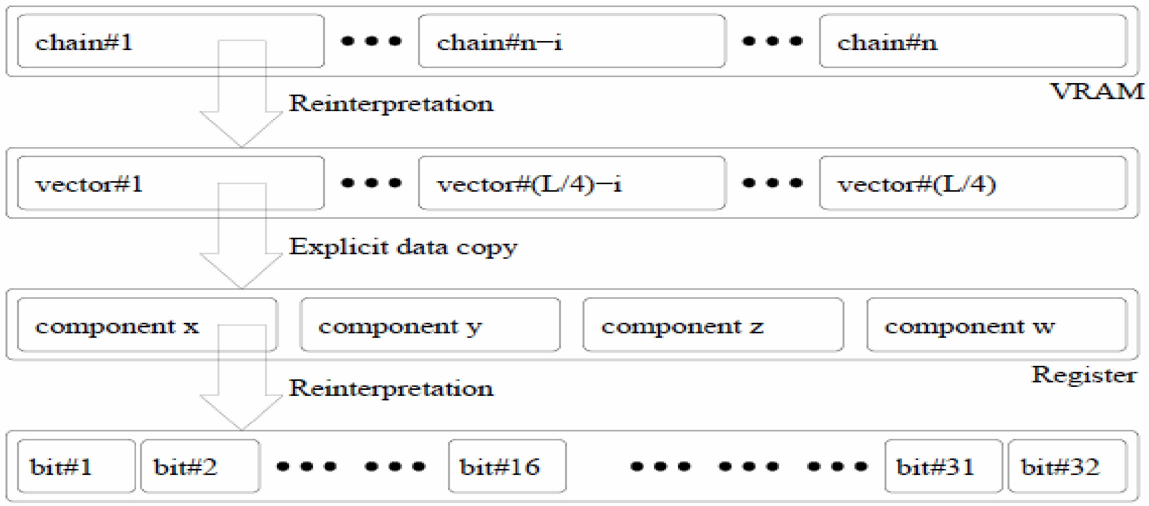
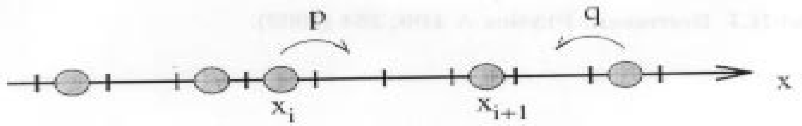


Figure 6: Memory map of data in the OpenCL algorithm.

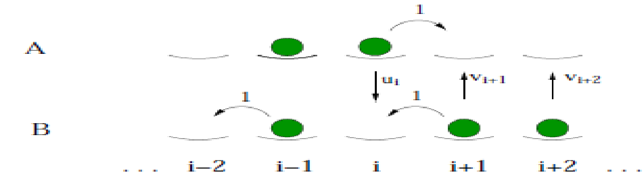
Disordered ASEP model simulations

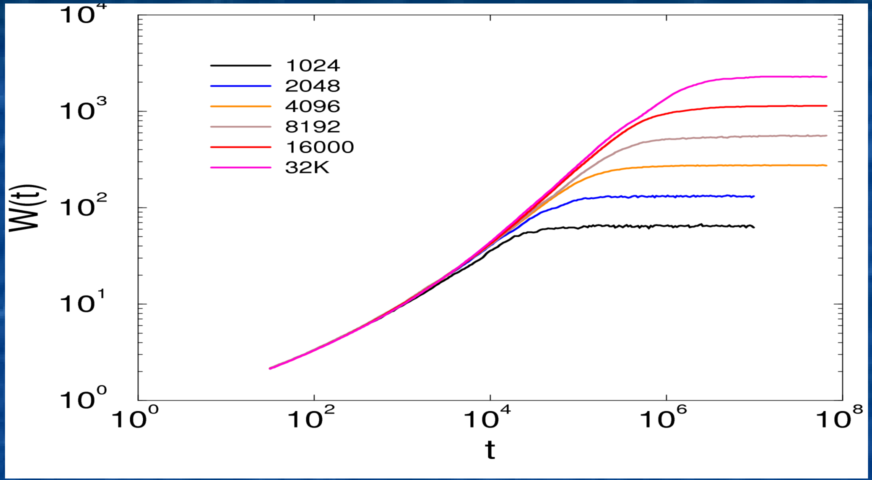
- Site-wise binary quenched disorder:

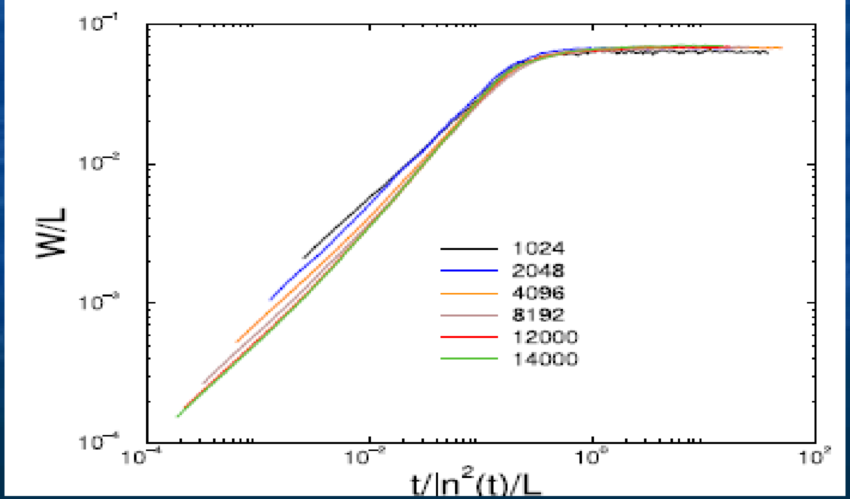


$$P(p_i) = (1-D)\delta(p_i - p) + D\delta(p_i - rp)$$

- Q-TASEP: *p_i=0.8 or 0.2, q_i=0*
  L=1024, 2048, ... 16000
  t_{max} = ***10^8* MCs**
- Studied by: *Krug 1999, Stinchcombe et al. 2008: $\beta<1$*
- ***Data collapse with $\alpha=\beta=z=1$***
  Precise form of log. corrections are confimed
- + *Q-PASEP and 2-lane TASEP:*

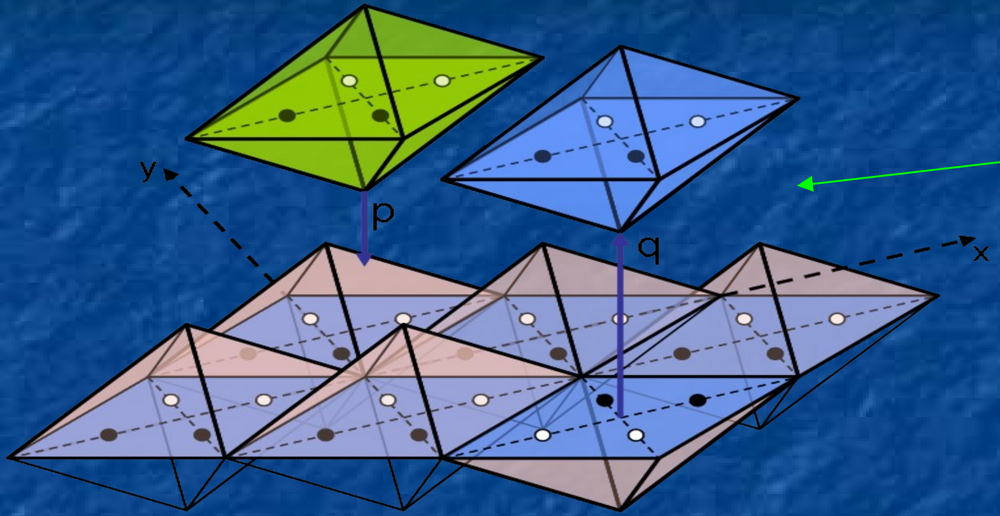






R. Juhász, G. Ódor, J. Stat. Mech. (2012) P08004

Mapping of KPZ growth in *2+1* dimensions

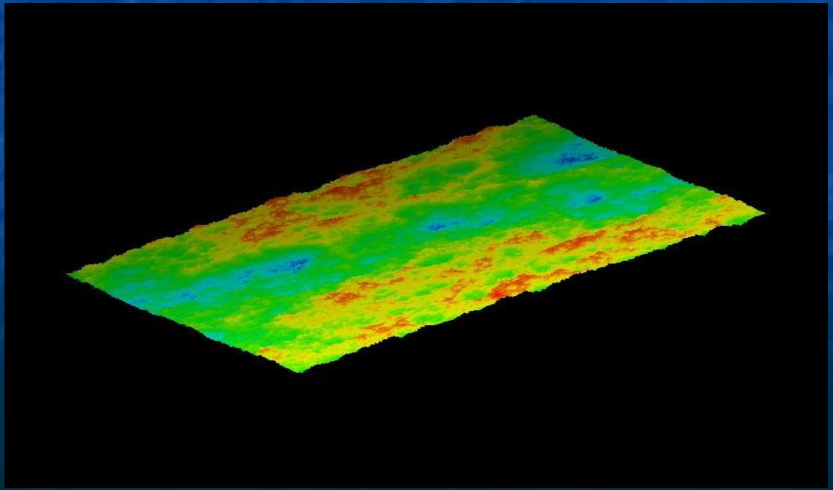


Octahedron model

- Cellular automaton update:

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

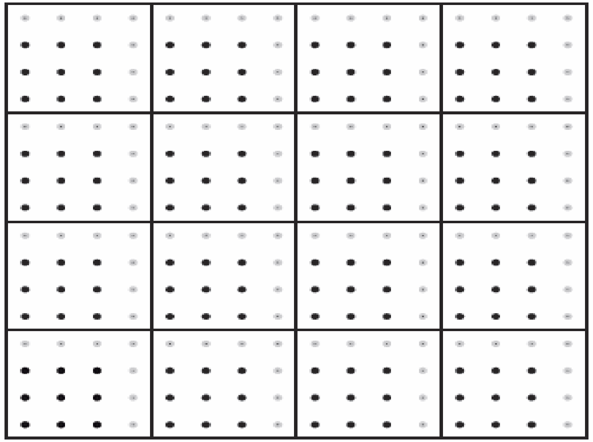
- **Driven diffusive gas of pairs (dimers)**
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 031112 (2010)*



Bit coded simulations on ***131072 x 131972*** sized systems provided high precision scaling exponent estimates and probability distributions

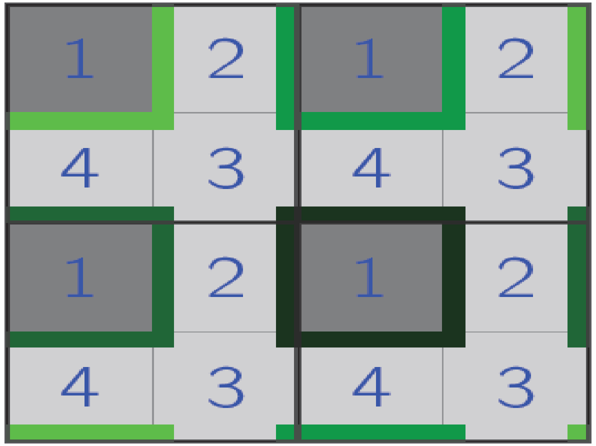
J. Kelling and G. Ódor *Phys. Rev. E* 84 (2011) 061150

Domain decomposition methods



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

⇒ avoids accumulation of errors at borders



Double Tiling

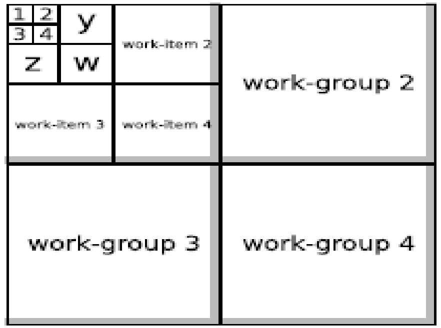
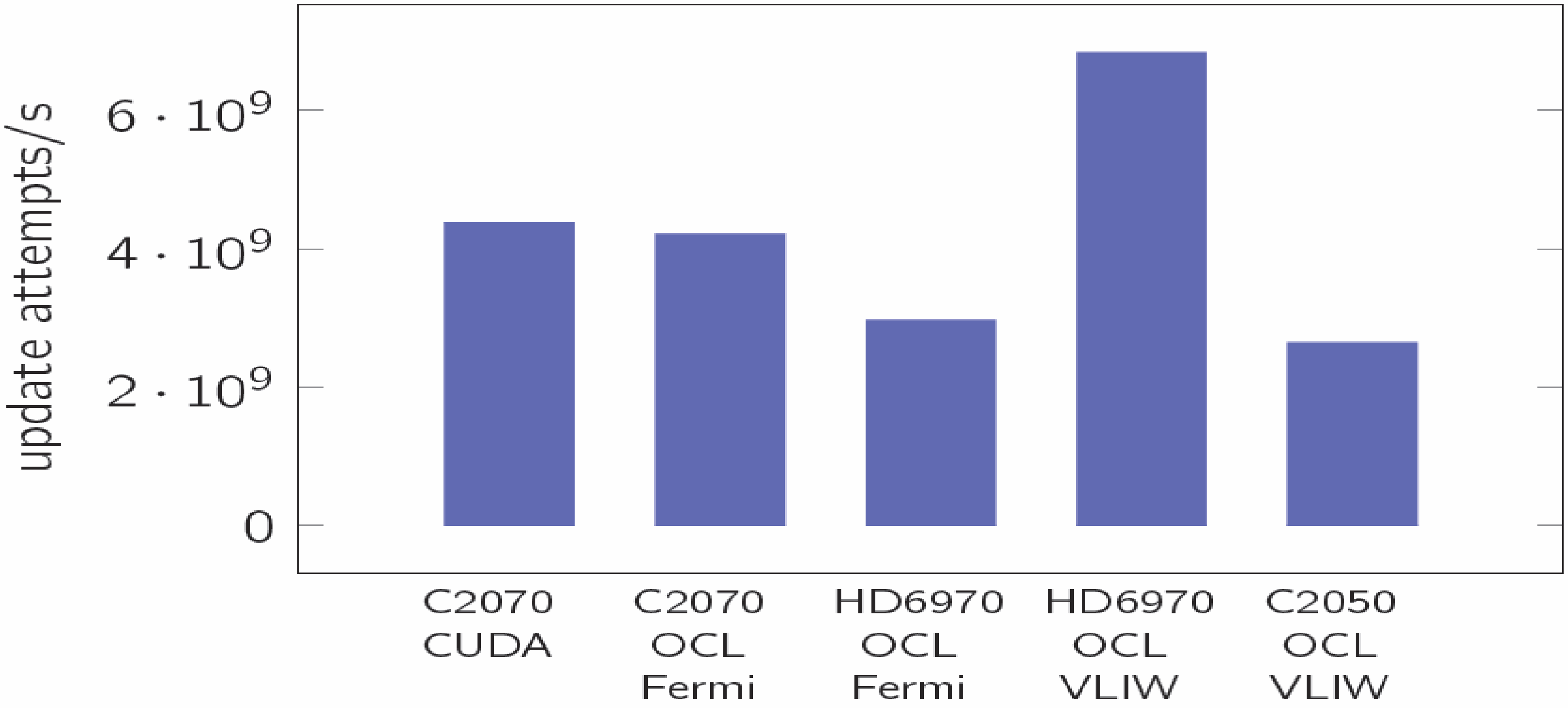


Fig. 3: Decomposition of the whole system into work-groups at device layer, with gray areas indicating dead borders. Further decomposition at work-group layer using double tiling is indicated for work-group 1: Each work-item executes four virtual threads using VLIW vector operations. The virtual threads 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

OpenCL and Optimizations



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

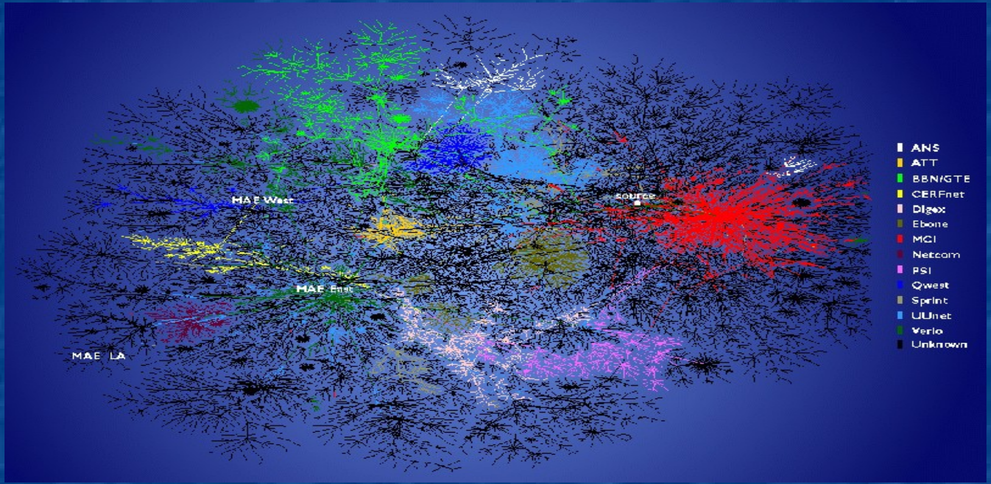
- HD6970 provides 128-bit registers (Very Long Instruction Word)

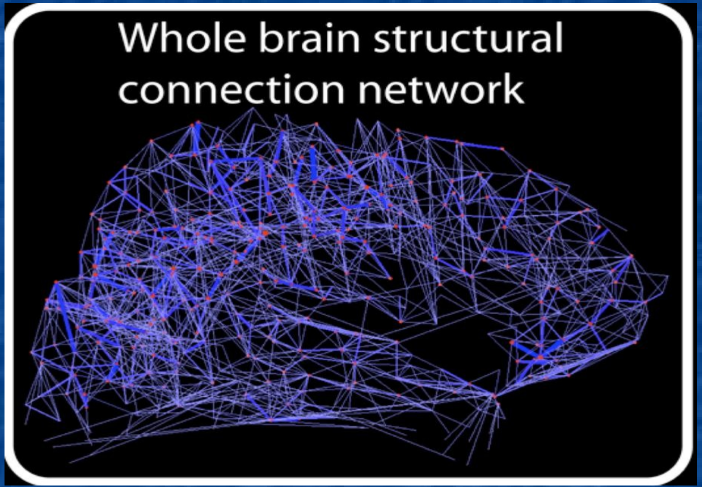
⇒ Even with OpenCL different architectures require different code

Novel research Interest
in collaboration with spanish research groups

Understanding generic slow dynamics of information spreading in networks

M. A. Munoz, R. Juhasz, C. Castellano, and G, Ódor, Phys. Rev. Lett. 105, 128701 (2010)





Spectral decomposition analysis of the Adjacency Matrices

Requires efficient network generation and sparse matrix eigenvalue solvers

See: G Ódor : Rare regions of the susceptible-infected-susceptible model on Barabasi-Albert networks,
Phys. Rev. E 87, 042132 (2013) or : arXiv:1306.3401

Supported by the project FuturICT.hu

Conclusions & outlook

- Fast parallel simulations due to mapping onto stochastic cellular automaton (lattice gases)
- Important scaling results in 1d disordered ASEP models with **ultra-slow dynamics**
- **Extremely large scale** (2^{17} **x** 2^{17}) **results** in 2d KPZ clarified long lasting debate: ruling out rational (¼, ...) scaling exponents of a field theory
  + 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 could not fulfill it's promise on platform independence

  Extension for studying Surface pattern formation would be very efficient

  Application to Network studies is under way
- **Acknowledgements**: DAAD-MÖB, OTKA, OSIRIS FP7, NVIDIA, FuturICT.hu

  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
  R. Juhász, G. Ódor, J. Stat. Mech. (2012) P08004
  J. Kelling, G. Ódor, M. F. Nagy, H. Schulz and K. -H. Heinig, EPJST 210 (2012) 175-187