Statisztikus fizikai modellek szimulációja GPU-n

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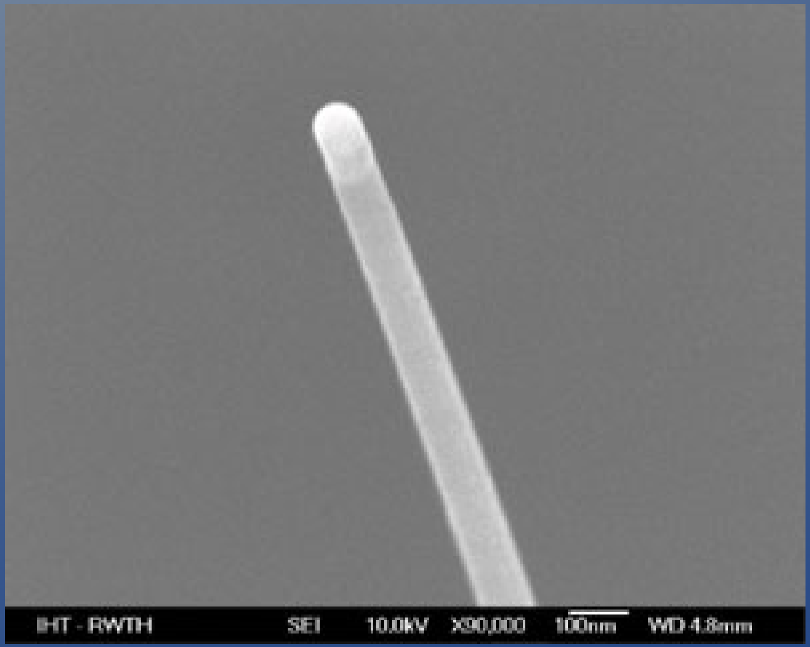
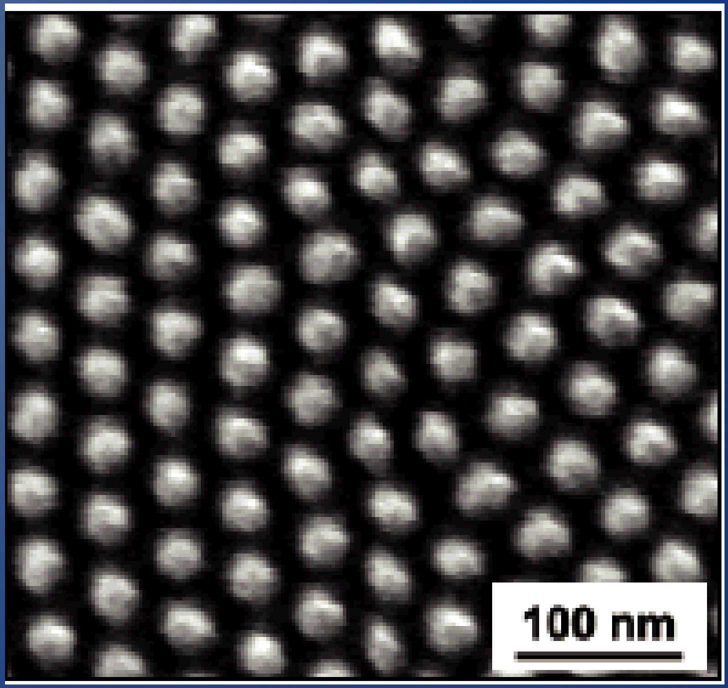
Motivations, common interest

Applied, Materials Science

In nanotechnologies large areas of **nanopatterns** are needed, which can be fabricated today only by expensive techniques, e.g. :
electron beam lithography or direct writing with electron and ion beams.



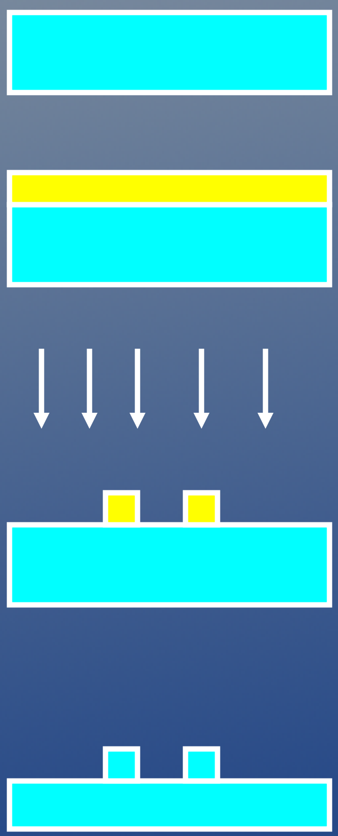
Silicon Nanowire Diameter <100nm



65 billion nanodots per square cm

Top-down versus Bottom-up technologies

Top Down Process



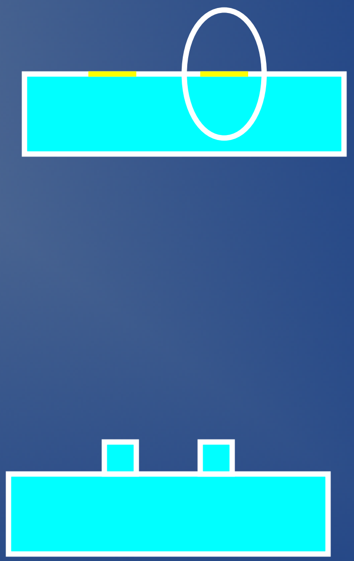
Start with bulk wafer

Apply layer of photoresist

Expose wafer with UV light through mask and etch wafer

Etched wafer with desired pattern

Bottom Up Process



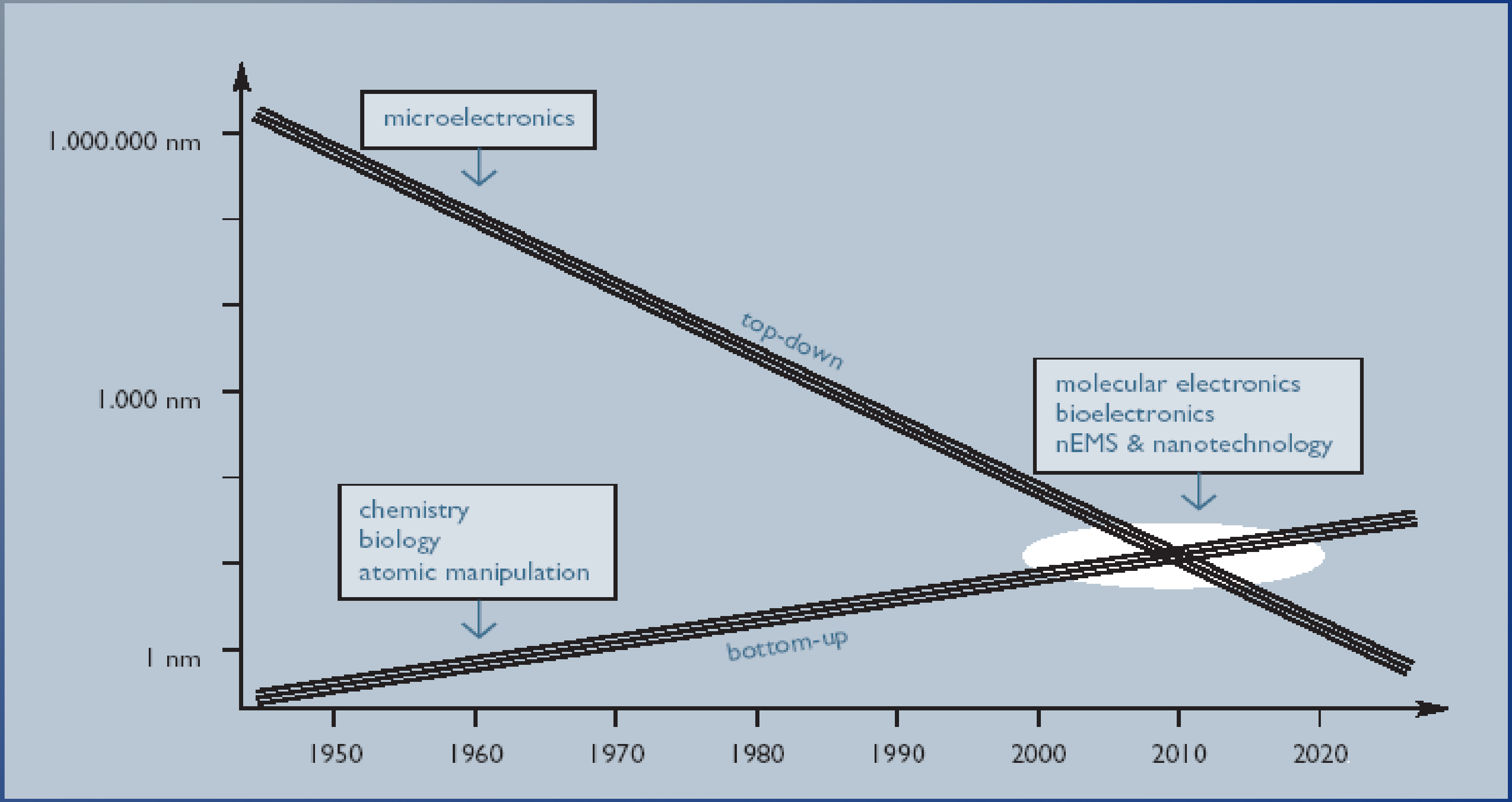
Start with bulk wafer

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 results can be obtained through bottom-up and top-down processes

Roadmap of Top-down and Bottom-Up Processing



http://www.imec.be/wwwinter/business/nanotechnology.pdf

Fundamental theoretical understanding of the ion-beam-induced surface patterning and scaling 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 : anisotropy, local growth velocity
η : roughens the surface by a zero-average Gaussian noise field:

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

Up-down symmetrical case: $\lambda = 0$: Edwards-Wilkinson (EW) equation

Characterization of surface growth:

Width:

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

Family-Vicsek scaling:

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

KPZ phase diagram, scaling classes

- Exactly solvable in *1+1 d*, but in higher dimensions theory fails being unable to access the strong coupling fixed point regime

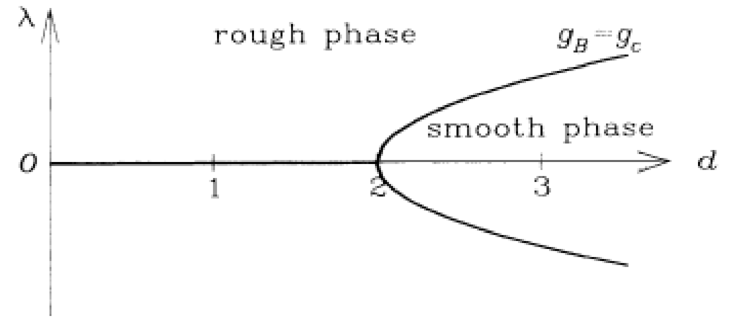


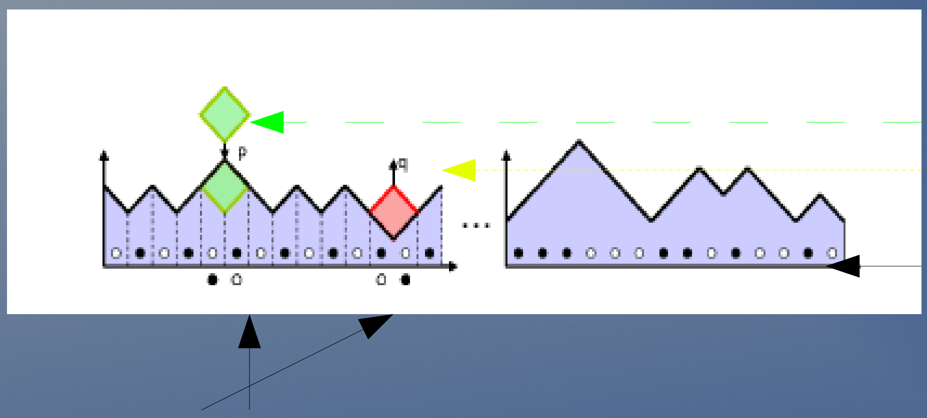
FIG. 1. Schematic phase diagram of the KPZ equation from the one-loop RG analysis. Transitions are marked by thick lines.

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

- The upper critical dimension is still debated: $d_c = 2, 4, \ldots \infty$?
- *2-dim exponent* estimates : $\alpha = 0.36 - 0.4$

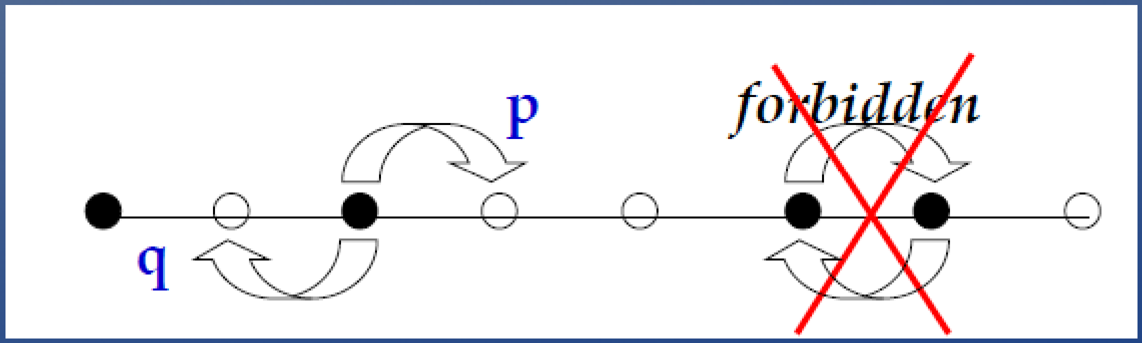
Mappings of KPZ onto lattice gas system in *1d*



'Kawasaki' exchange of particles

Mapping of the *1+1*d surface growth onto the 1d ***ASEP*** model

Attachment (with prob. ***p***) and Detachment (with prob. ***q***) -> Anisotropic diffusion of particles (**bullets**) along the *1d* base space (*M. Plischke, Rácz and Liu, PRB 35, 3485 (1987)*)



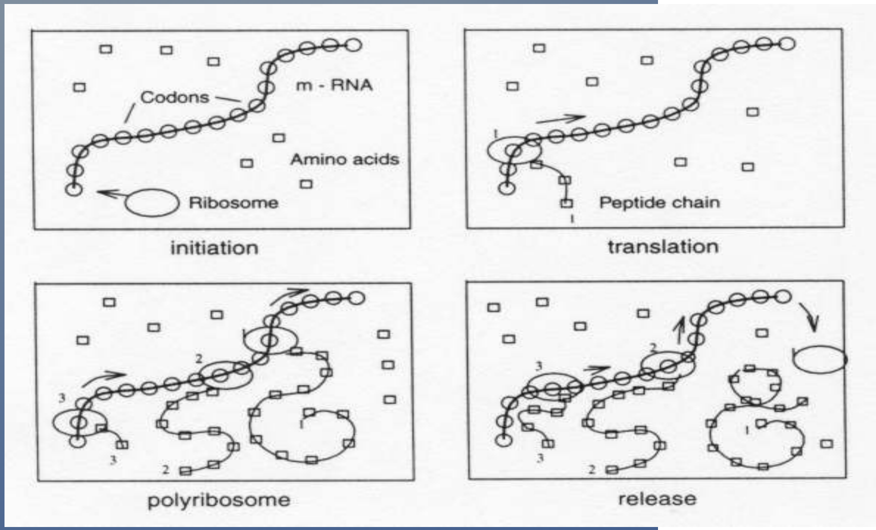
The simple ***ASEP*** (Ligget '95) is an exactly solved lattice gas

Many features (response to disorder, different boundary conditions ...) are known.

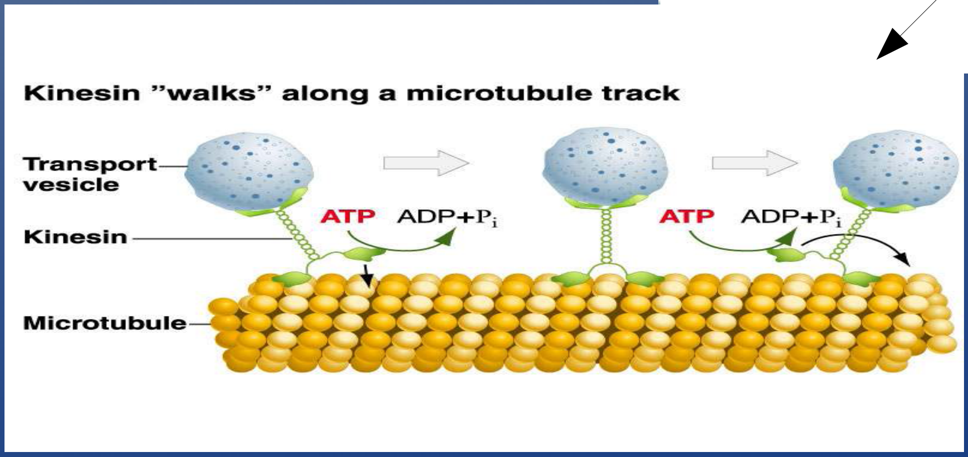
Applications of ASEP

ASEP = "Ising" model of nonequilibrium physics

since it is simple, exactly solvable, and has many applications as follows:

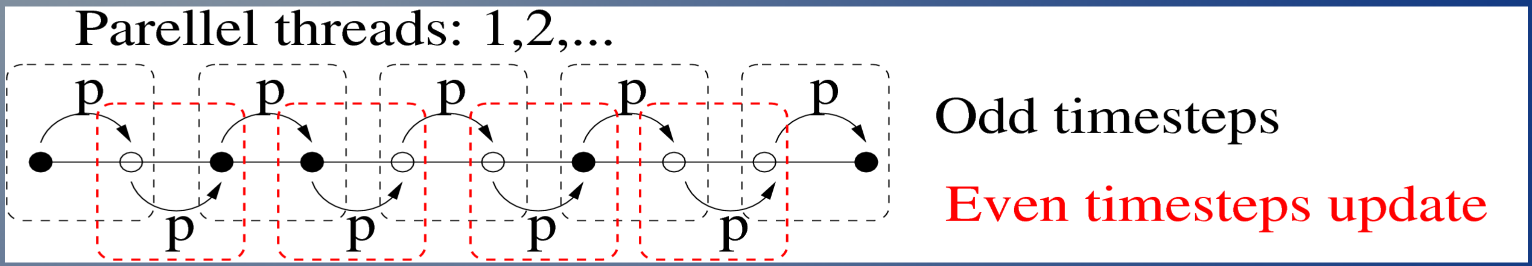


- Protein synthesis
- Surface growth
- Boundary induced phase transitions
- Real and/or Model Traffic
- Intracellular Transport
- Ant Trails



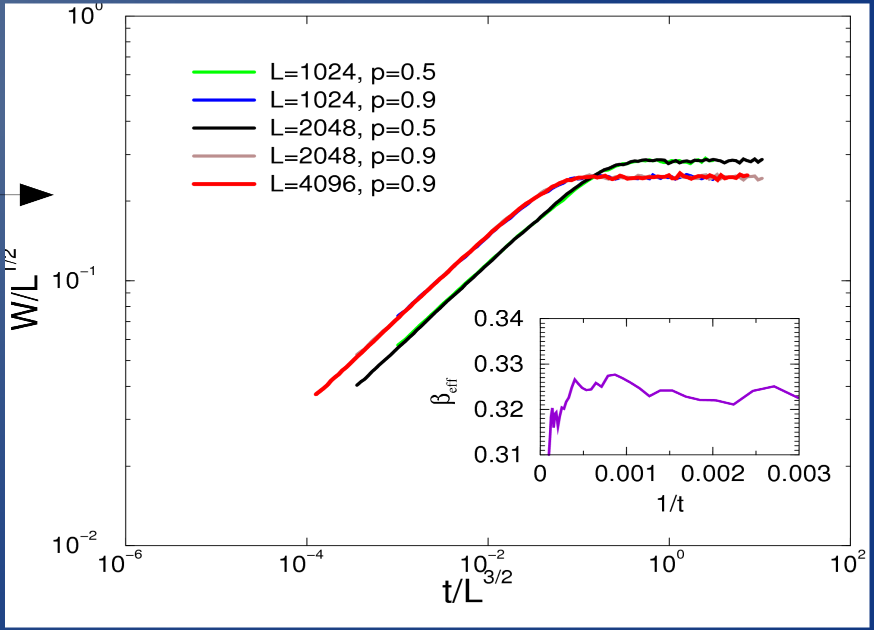
Test of parallel update algorithms for 1d ASEP/KPZ

- Parallel updates on a ring of size *L*:



with probability *p* (reverse with *q*)

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



- L<16K programs fits into shared memory of multiprocessor blocks

→ no communication losses,

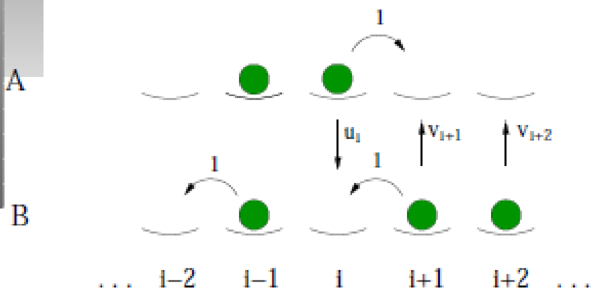
maximal speedup & scaling:

240 cores ~ 100x of a CPU (2GHz)

Further Motivations, non-trivial problem

Disordered ASEP

Bidirectional two-lane model



- single particle, homogeneous system: active diffusion (Klumpp & Lipowsky 2005)
- single particle in random environment
- many-particle system is qualitatively different from the disordered PASEP

Exploration of exremely slow (scaling) behavior: **Fits GPUs**

Mappings of KPZ growth in *2+1* dimensions

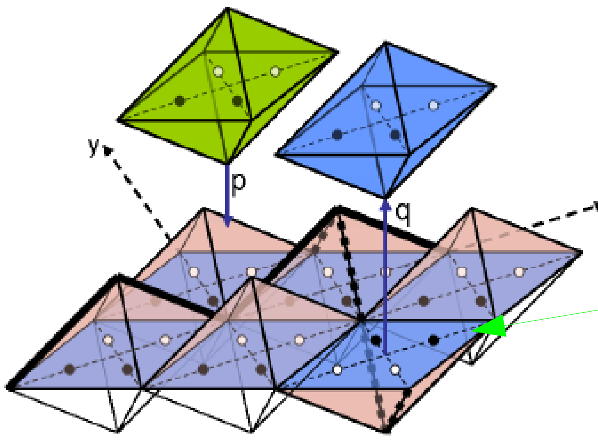


FIG. 2: (Color online) Mapping of the $2+1$ dimensional surface growth onto the $2d$ particle model (bullets). Surface attachment (with probability p) and detachment (with probability q) corresponds to Kawasaki exchanges of particles, or to anisotropic diffusion of dimers in the bisectrix direction of the x and y axes. The crossing points of dashed lines show the base sub-lattice to be updated. Thick solid/dashed lines on the surface show the x/y cross-sections, corresponding to the $1d$ model (Fig. 1.)

Generalized Kawasaki update:

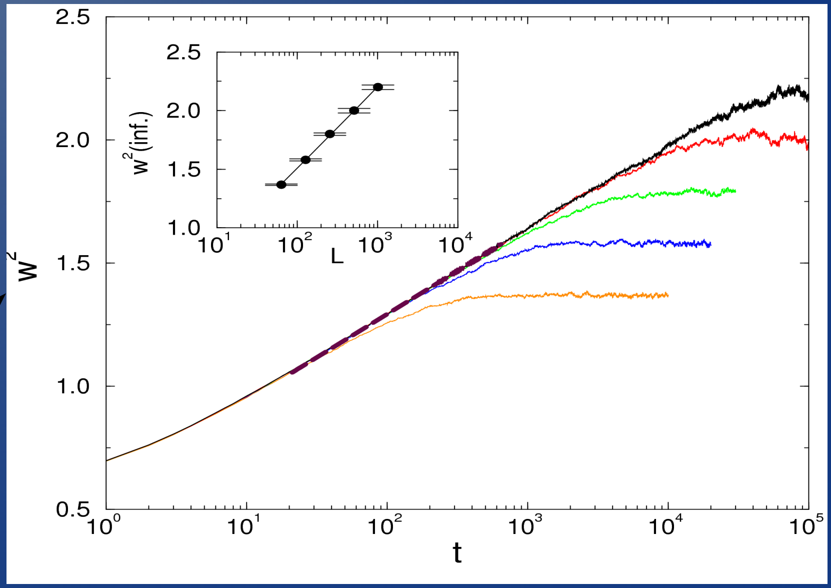
$$\begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \rightleftharpoons \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}$$

Octahedron model

Driven diffusive gas of pairs (dimers)

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

For *p = q =1* Edwards-Wilkinson scaling:



$W^2(t) = 0.152\ ln(t) + b$ for $t < t_{sat}$

$W^2(L) = 0.304\ ln(L) + d$ for $t > t_{sat}$

First 2-dim KPZ CUDA implementation on byte-fields (dimers)

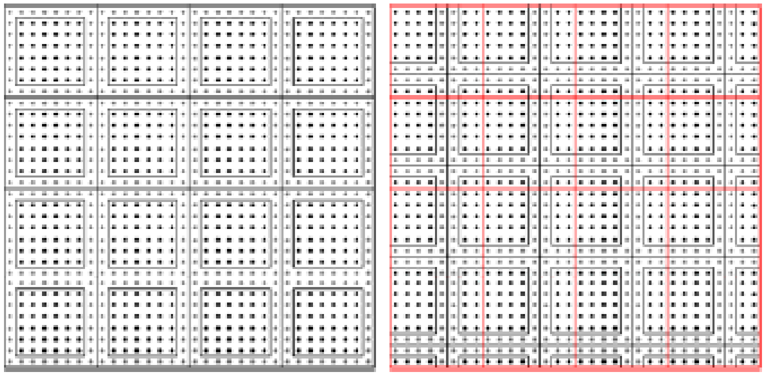


Figure 4: Initial decomposition of the domain (left) and decomposition of the domain after moving the origin (right). Red lines illustrate the new decomposition on the old but moved system.

Table 1: Summary of the experimentally discovered speed-up values on different architectures

System	Number of cores used	Processor clock rate	Speed-up
AMD Opteron 2346	1	1,8 GHz	1
Nvidia Quadro FX 3700	112	500 MHz	24
Nvidia Tesla S1070	240	602 MHz	41

H. Schulz, G.Ó, Jeffrey Kelling, Karl-Heinz Heinig, Bartosz Liedke, Nils Schmeißer

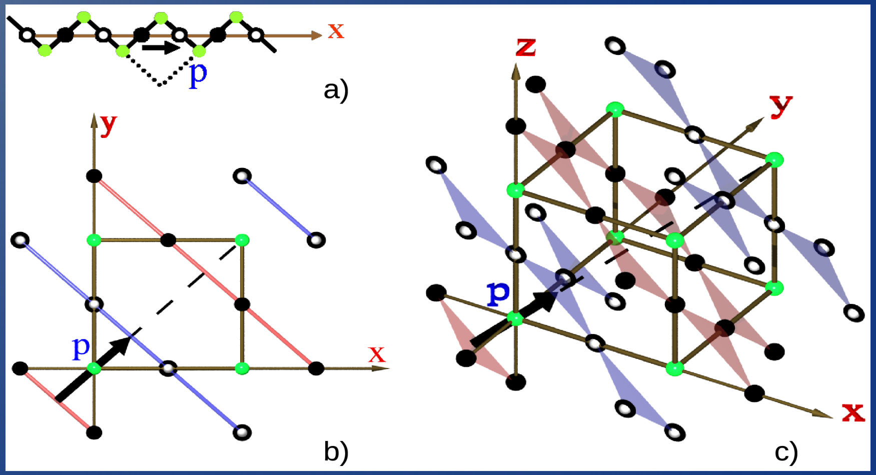
Proceedings of the 3rd International Workshop "Innovation in Information Technologies - Theory and Practice", September 6th-10th, Dresden, Germany, 2010

Prospects: KPZ in higher dimensions

- Generalization of the rooftop (octahedron) model in higher (d=*3,4,5*) dimensions (*64*^{5} sized lattices!)

  In *d* dimensions: *KPZ* ~ spatially anisotropic, driven random walk of oriented *d-mers* ⇒ Topological exclusion effects make them nontrivial

- **Upper-critical dimension: Irrelevancy of topological constraints above a finite d_c ?**



G.Ó, B.L, K.H: PRE81 (2010) 031112

Pattern formation with the octahedron model

Competing KPZ and surface diffusion :

Noisy **Kuramoto-Sivashinsky** equation (KPZ + Mullins Diffusion):

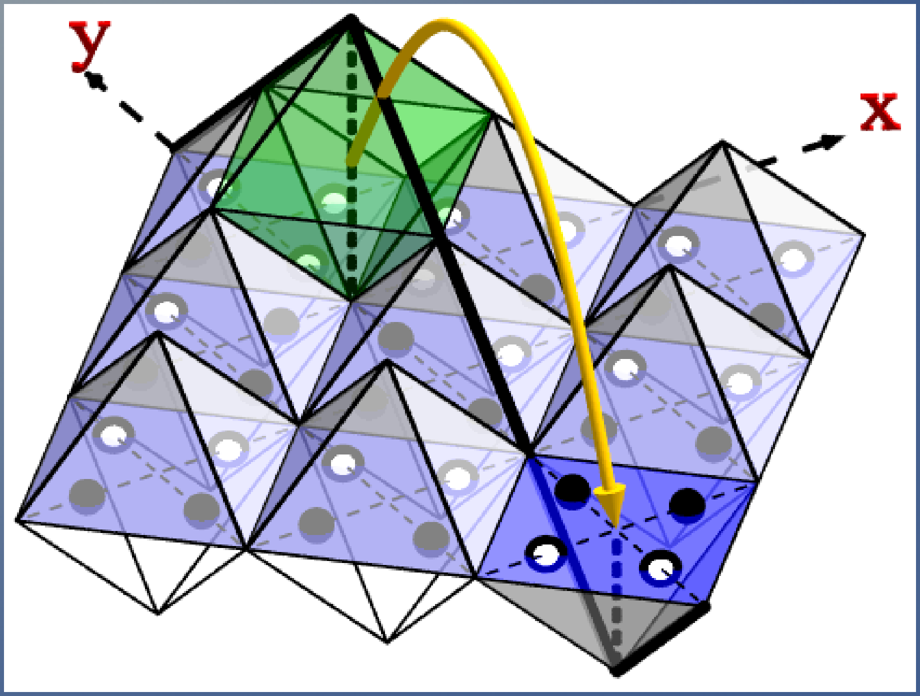
$$\partial_t h(x,t) = \sigma \nabla^2 h(x,t) + \lambda (\nabla h(x,t))^2 + \eta(x,t) + \kappa \nabla^4 h(x,t)$$

To generate patterns inverse (uphill) diffusion is needed !

Alternating deposition/removal (prob. *p,q*) and surface diffusion (prob. *D*)

Scaling behavior of the 2d **Kuramoto-Sivashinsky ~ KPZ** ???
debated Field Theoretical hypothesis *1995 (Howard & Cuerno)*

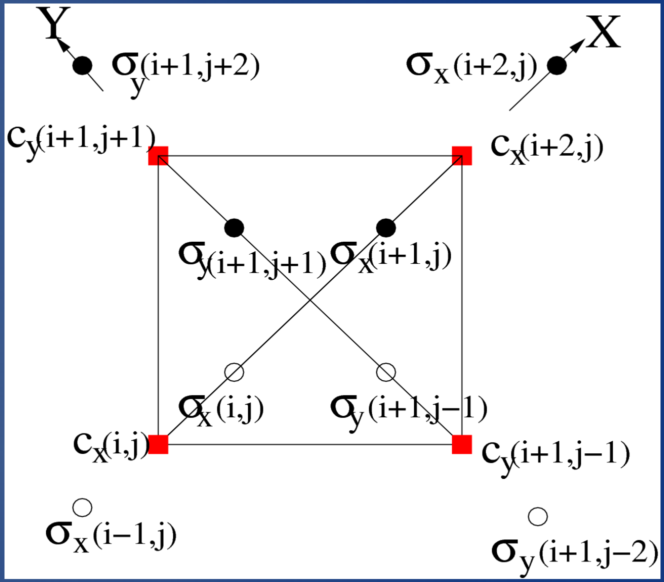
Surface diffusion (Molecular Beam Epitaxy classes)



dimer attraction

Simultaneous octahedron deposition/removal: attracting or repelling dimers

G.Ó, et al. PRE81 (2010) 051114



$$c_\chi(i,j) = \sigma_\chi(i,j)\sigma_\chi(i+1,j)$$

Curvature driven octahedron model

$$\Delta H = \Delta \sum_{\chi=x,y} \sum_{\langle i,j \rangle} c_\chi(i,j) + \Delta \sum_{\chi=x,y} \sum_{\langle i',j' \rangle} c_\chi(i',j')$$

/\

\/\/\/ → \/   \/

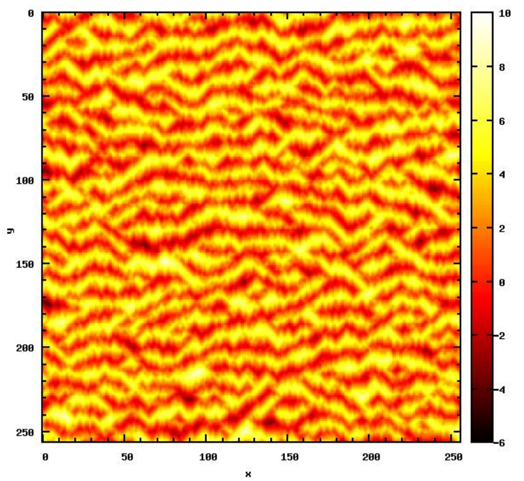
Arrhenious type update probability →

$$w_{i \to i'} = 1/2[1 - a \tanh(-\Delta H^2)]$$

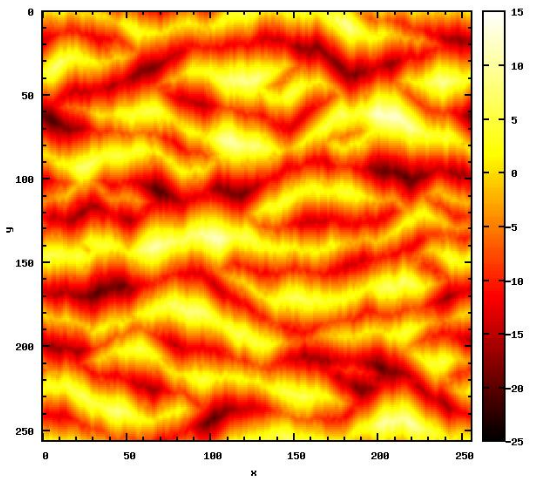
Surface hight patterns generated by the dimers

Anisotropic surface diffusion

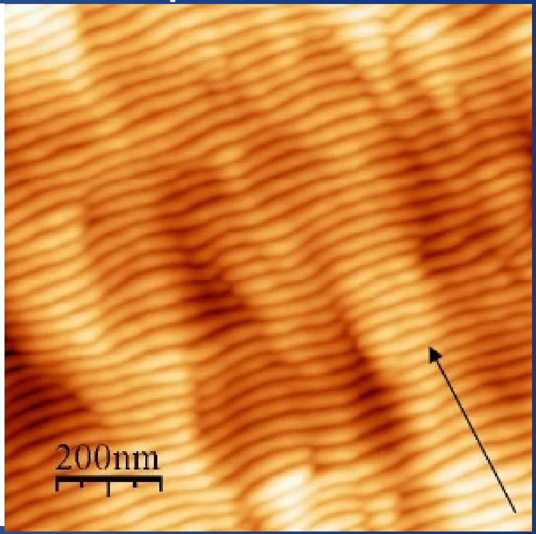
10KMCS



30KMCS



Experiment



Silicon surface after 500 eV Ar+ sputtering under 67°. The ripples have a periodicity of 35 nm and a height of 2nm.

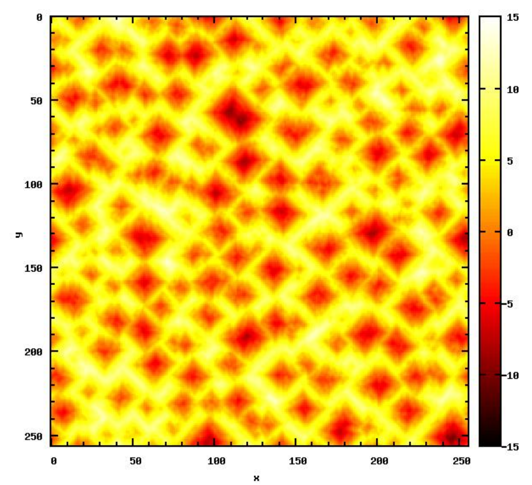
Coarsening ripples

Wavelength growth (scaling) ?

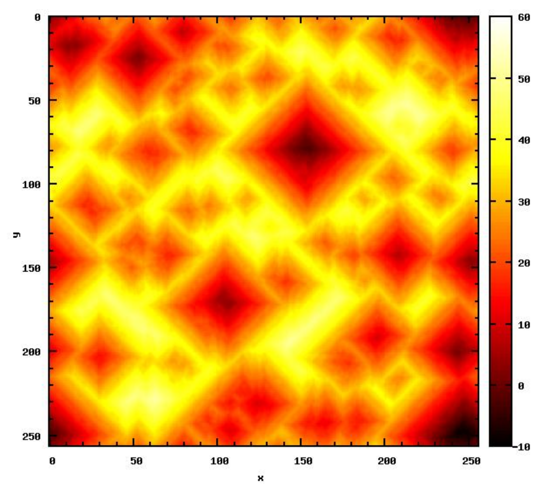
Patterns generated

Isotropic surface diffusion

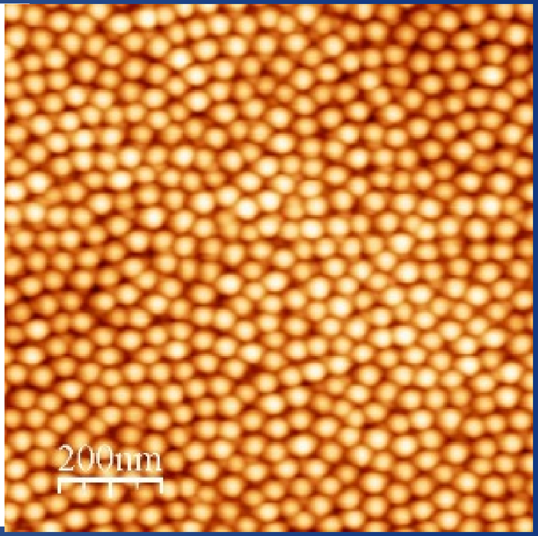
1KMCS



10KMCS



Experiment



GaSb surface after normal 500 eV Ar+ sputtering. The periodicity and the height of the dots are both 30 nm.

Coarsening dots

CUDA code implementation

Important issues:

- CUDA code runs faster than C by a factor $\Leftrightarrow$ programming effort ?
- Fit into shared GPU memory to reduce communication losses
- Bit coding
- Smaller sizes, Finite Size Scaling (FSS) studies
- Good/fast random number generator selection

Project works for 2010-2011

- *Local Supercomputer thanks to NVIDIA professor partnership:*

  4 x Quadro FX5800 GPUs 960 cores, 16GB dev. mem.

- *d=1,2*... ASEP KPZ codes, test, benchmarking
- Disordered model studies, publications
- Multi-GPU: Extension of single GPU/CPU codes to multi-nodes with MPI with FZD people

  → Larger sized systems
- **DAAD student scholarship : 2x1 months should be spent soon !**