# GPU szimulációk a statisztikus fizikában

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MŰSZAKI FIZIKAI ÉS ANYAGTUDOMÁNYI INTÉZET

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Budapest 2/7/2012

Supported by: DAAD-MÖB 2010/2011,
OTKA 77629,
NVIDIA Professor Partnership,
OSIRIS FP7

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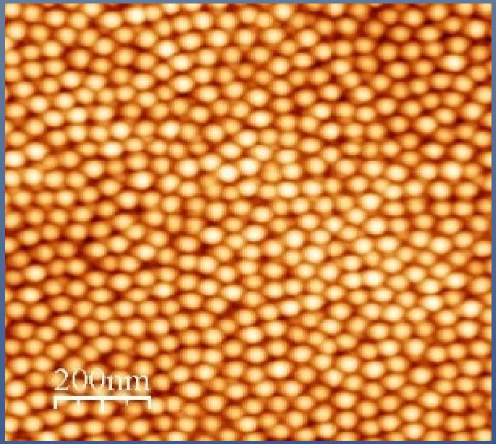
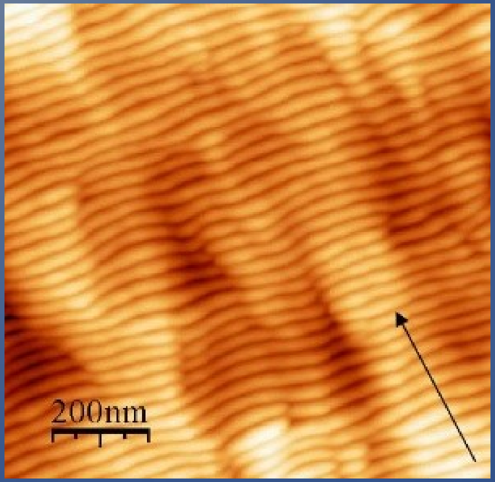
# Motivations, common interest
## Materials Science, Statistical Physics

In nanotechnologies large areas of **nanopatterns** are needed, which can be fabricated today by ion-beam induced self-organized ripple and dot pattern growth




Similar phenomena: sand dunes, chemical reactions … → **Universality**
Better understanding of **basic surface** growth phenomena is needed !

# Kardar-Parisi-Zhang (KPZ) equation

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

$\sigma$ : (smoothing) surface tension coefficient
$\lambda$ : local growth velocity, up-down anisotropy
$\eta$ : roughens the surface by a zero-average, Gaussian noise field with correlator:

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

## 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:

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

$$z = \alpha/\beta$$

# KPZ scaling problems

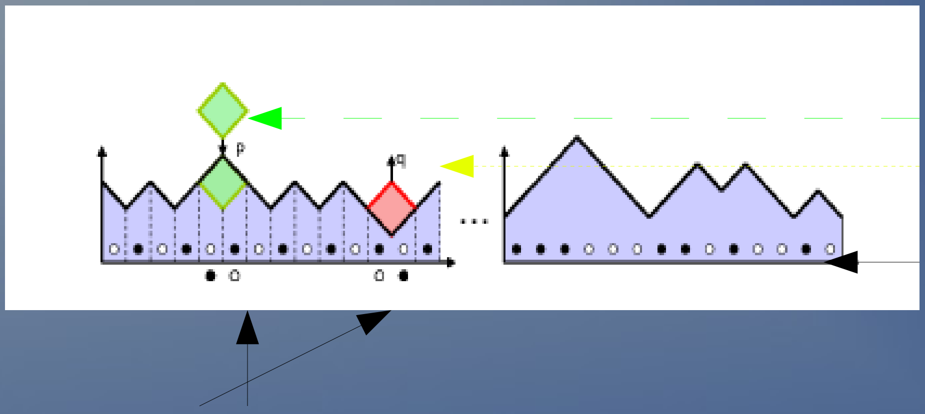
- Exactly solvable in *1+1 d*, but in higher dimensions theory fails
  being unable to access the strong coupling fixed point regime

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 |

- *2-dim exponent* estimates : $\alpha$ *= 0.36 – 0.4,* $\beta$ *= 1/4 ?*
- *The upper critical dimension is still debated:* $d_c = 2, 4, \ldots \infty$ *?*

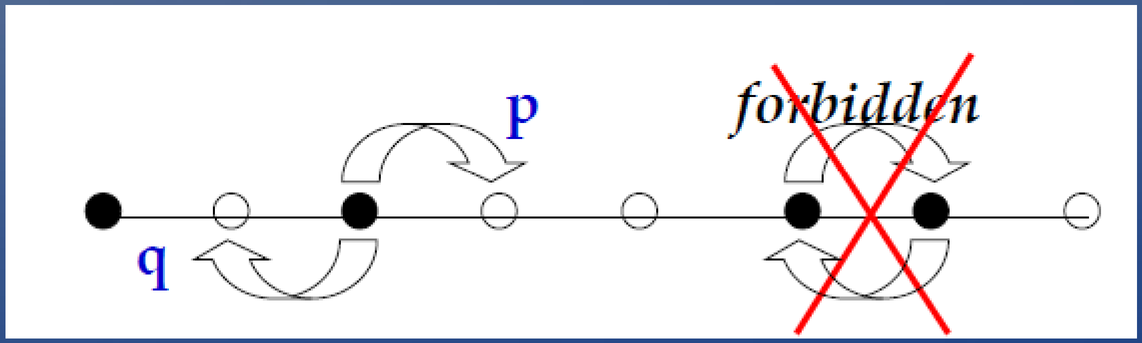
# Mappings of KPZ onto lattice gas system in *1d*




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)*)



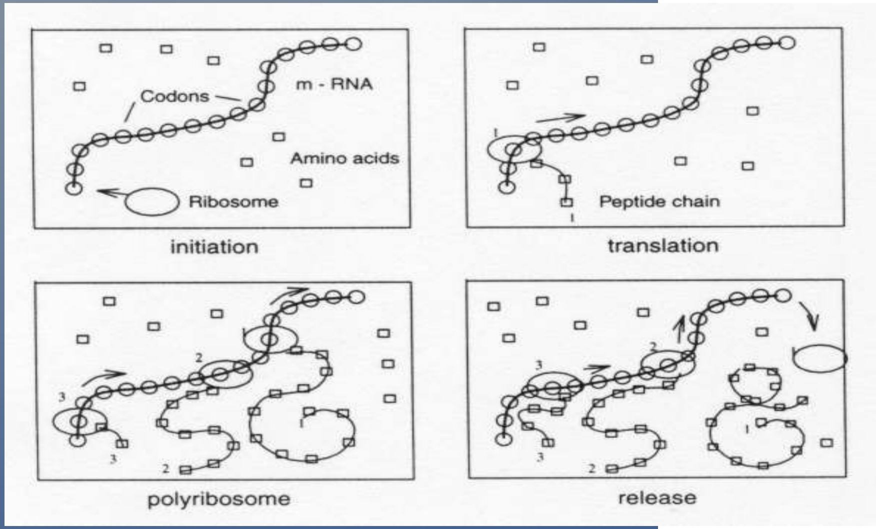

The simple ***ASEP*** (Ligget '95) is an exactly solved lattice gas

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

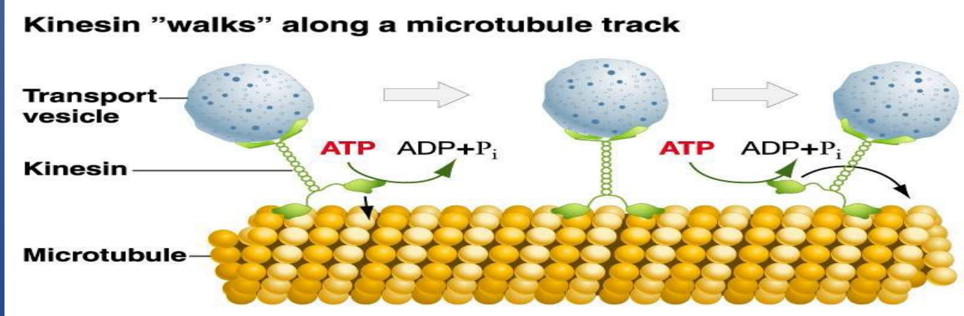
# Applications of ASEP

ASEP = "Ising" model of nonequilibrium physics

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

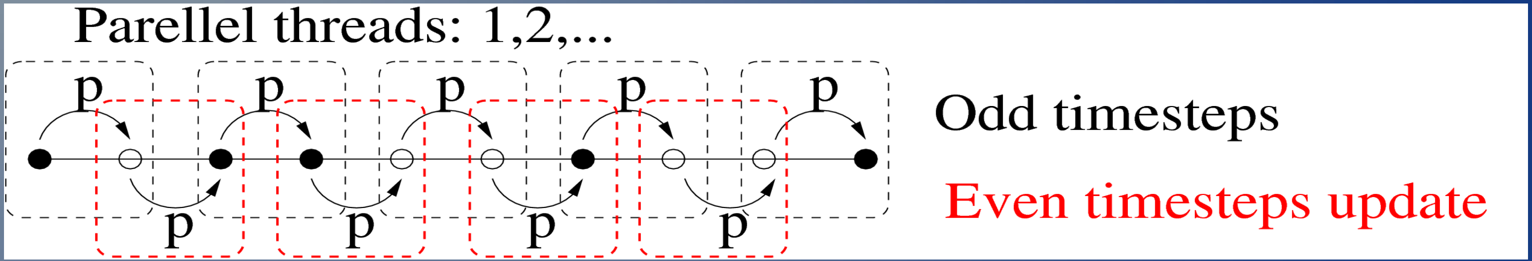



- Protein synthesis
- Surface growth
- Boundary induced phase transitions
- Real and/or Model Traffic
- Intracellular Transport
- Ant Trails



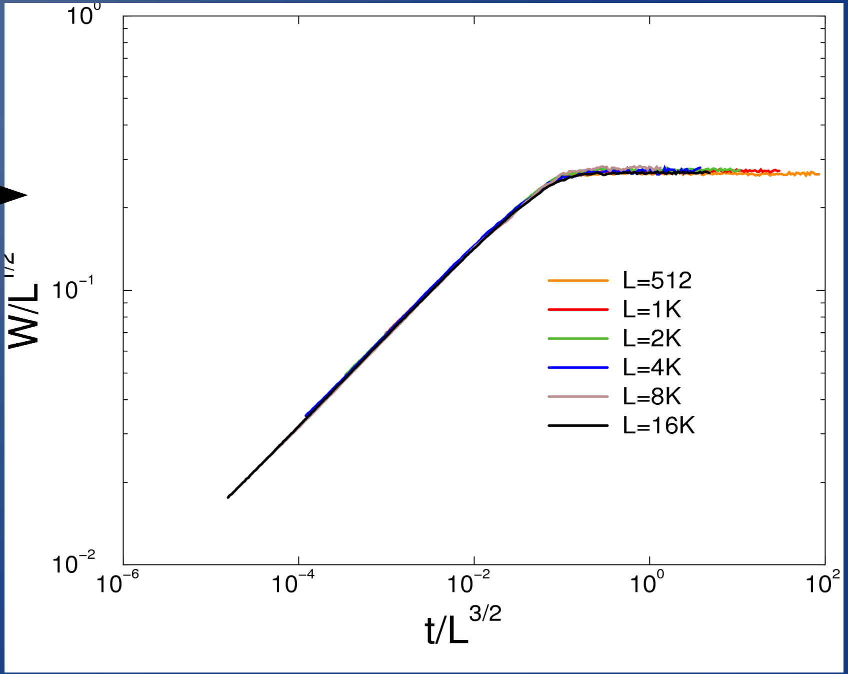
# Test of parallel update algorithms for 1d ASEP/KPZ

- Parallel 2-sublattice 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< 64K programs fits into shared memory of multiprocessor blocks

→ **no communication losses,**

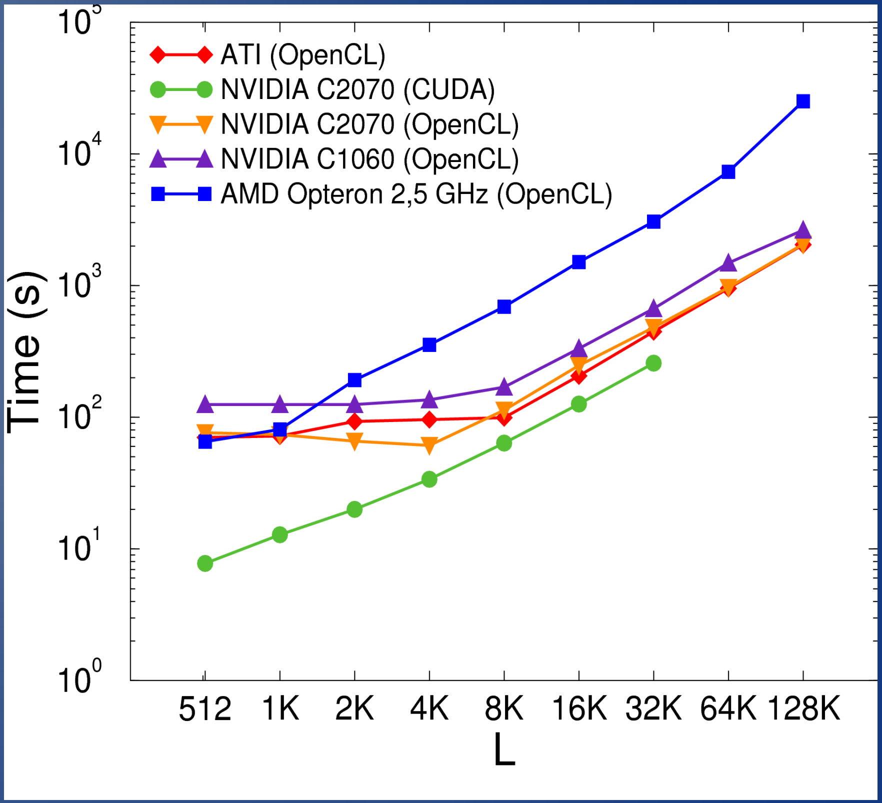
maximal speedup & scaling:

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

# General OpenCL code

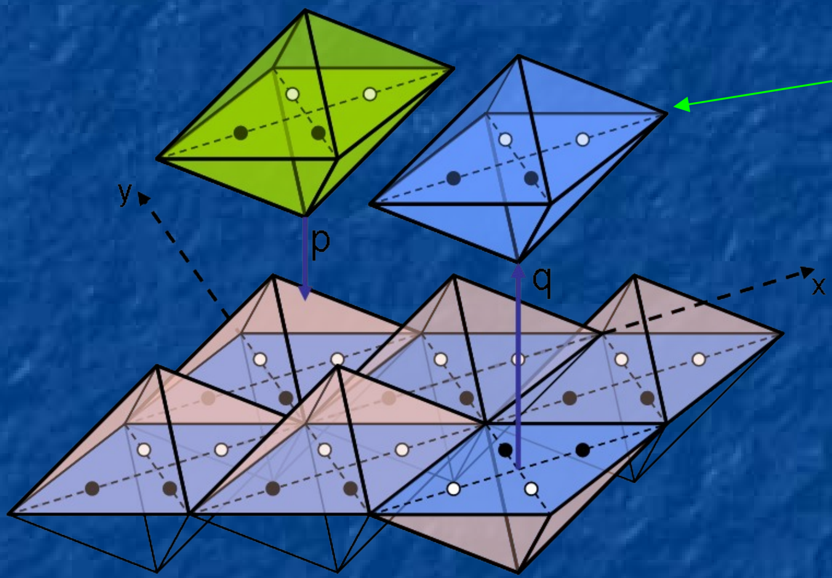
Tested for TASEP (KPZ) on ATI, NVIDIA, CPU clusters

- Portable for “any” parallel computers
- For larger system OCL speed is comparable with CUDA's
- Multi-GPU program with **M**essage **P**assing **I**nterface




Henrik Schulz, Géza Ódor, Gergely Ódor, Máté Ferenc Nagy, *Simulation of 1+1 dimensional surface growth and lattices gases using GPUs*, ***Comp. Phys. Comm. 182 (2011) 1467***

# Mapping of KPZ growth in *2+1* dimensions




- Generalized particle exchange:

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

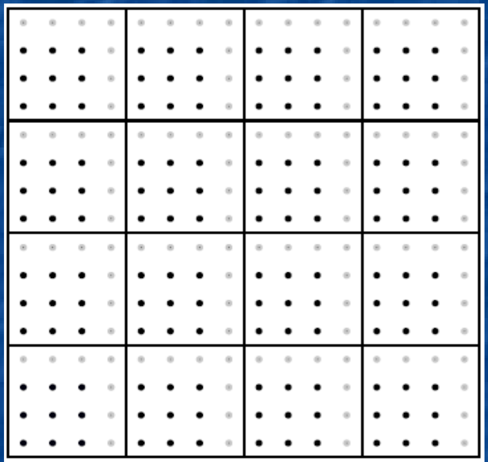
- **Octahedron model**

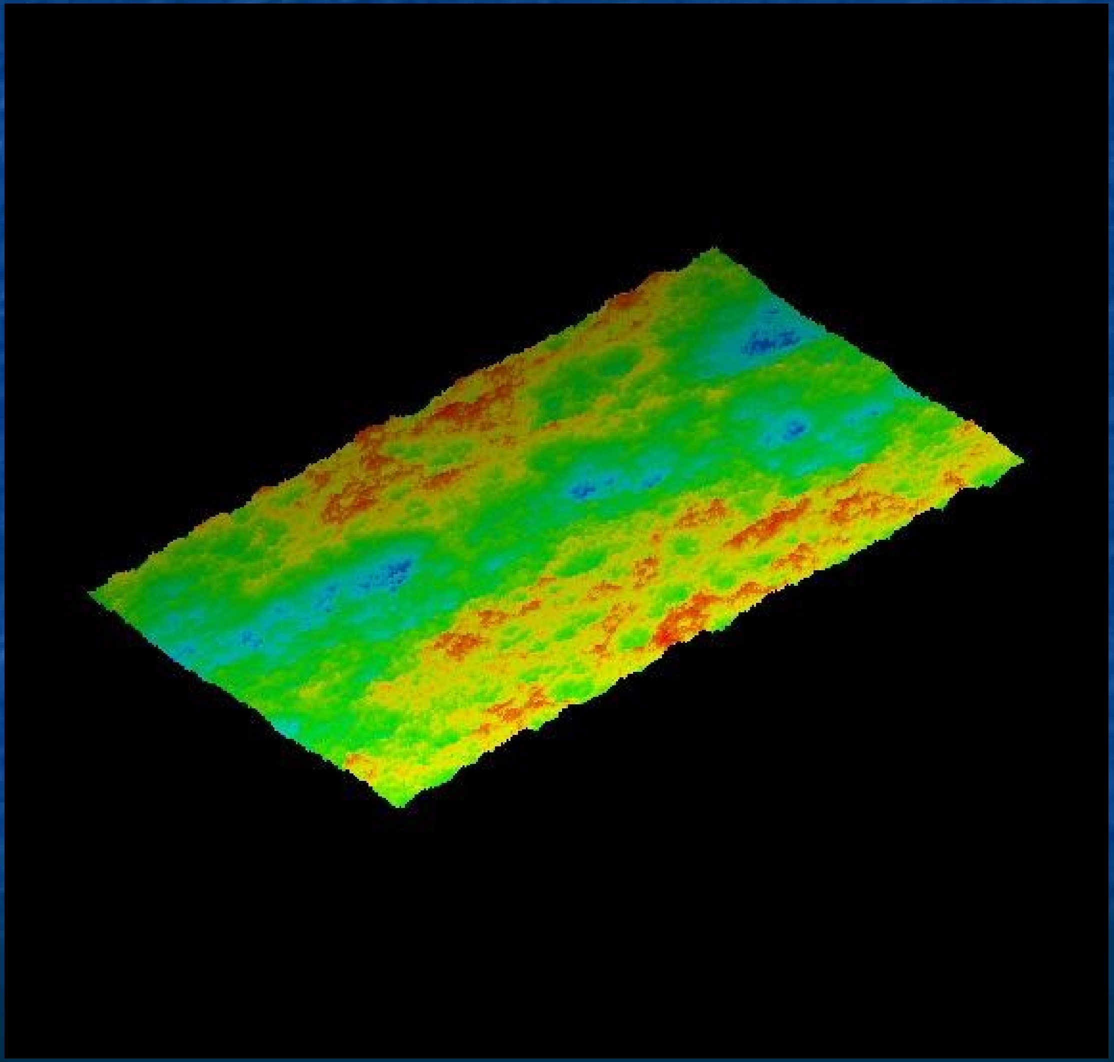
  **Driven diffusive gas of pairs (dimers)**

- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 031112 (2010)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 051114 (2010)*

# CUDA code for 2d KPZ

- Checkerboard decomposition
- Sub-systems are loaded in shared memory of GPUs updated with inactive boundaries:





- Each 32-bit word stores the slopes of 4x4 sites
- Origin of decomposition moves at every MCs
- **Speedup 430 x with respect a CPU of 2.8 GHz 131072 x 131972 size**

# 2d KPZ simulations

$$\beta_{\rm eff}(t) = \frac{\ln W(t, L\to\infty) - \ln W(t', L\to\infty)}{\ln(t) - \ln(t')}$$

$$\alpha_{\rm eff}(L) = \frac{\ln W(t\to\infty, L) - \ln W(t\to\infty, L/2)}{\ln(L) - \ln(L/2)}$$

$$\beta_{\rm eff}(t) = \beta + b_1\phi_1 t^{\phi_1}$$

$$\alpha_{\rm eff}(L) = \alpha + a_1\omega_1 L^{\omega_1}$$

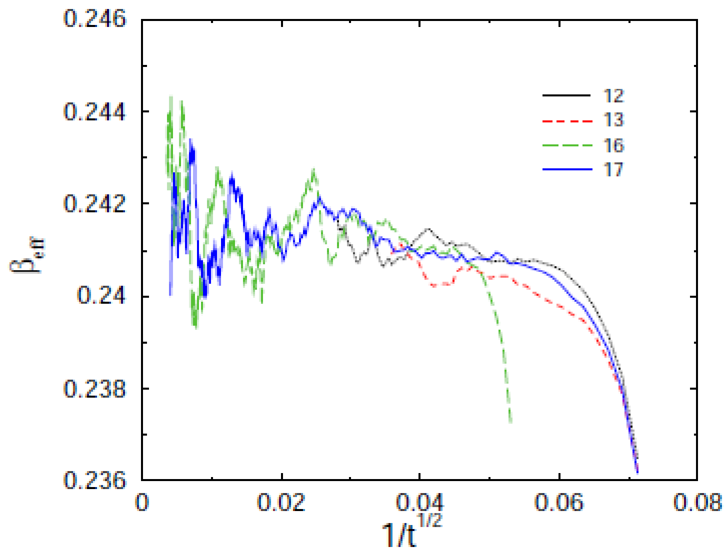



FIG. 3: (Color online) Local slopes of the surface growth for different sizes ($L = 2^{12}, 2^{13}, 2^{16}, 2^{17}$). Averaging was done over 20-100 independent runs.

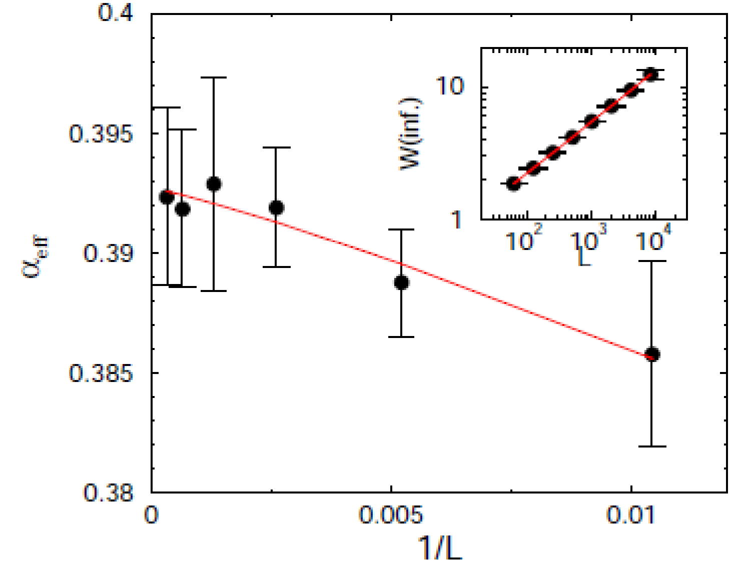



FIG. 4: (Color online) Local slopes of the roughness exponent for different sizes. The line shows a fit with the form (14). Inset: Surface width of the stationary state as the function of linear system size. The line corresponds to a fit with the form (10).

Jeffrey Kelling and Géza Ódor:
*Extremely large-scale simulation of a Kardar-Parisi-Zhang model using graphics cards,*
Phys. Rev. E 84 (2011) 061150

*α = 4/10, β =1/4*
ruled out

# 2d KPZ universal scaling function

$\Psi_L(x) = \langle W^2 \rangle P_L(W^2/\langle W^2 \rangle)$

$x^{-8}(10-x)\exp(-2/x^2)$

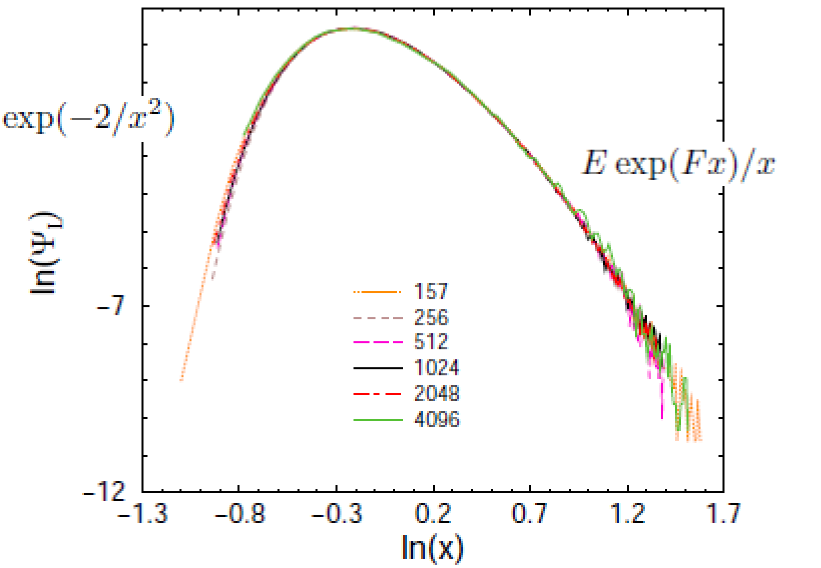



FIG. 6: (Color online) The universal scaling function $\Psi_L(x)$ in the steady state for $L = 2^8, 2^9, 2^{10}, 2^{11}, 2^{12}$. The dotted line shows the $L = 157$ results of [22].

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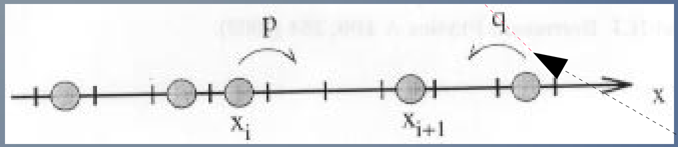
Phys. Rev. E 84 (2011) 061150

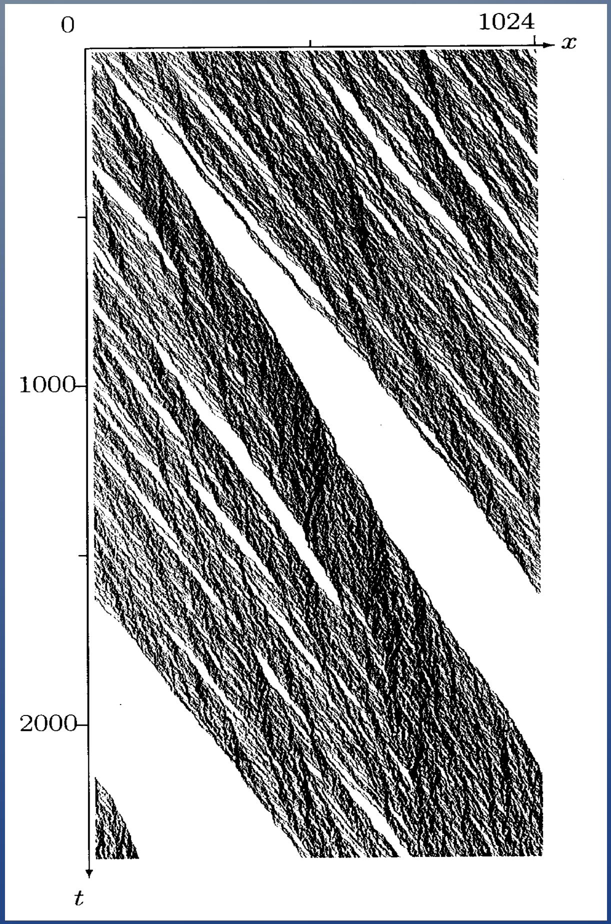
Corrections to scaling are negligible

# Disordered ASEP simulations

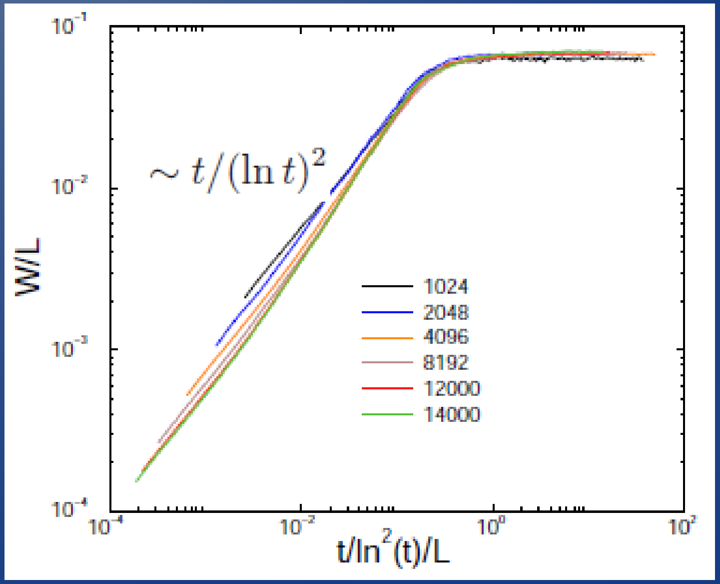



Bimodal, quenched, site-wise jump disorder distribution:

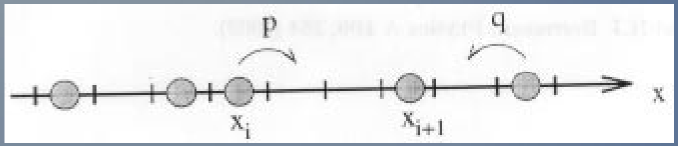
$$f(p_i) = (1-\phi)\delta(p_i - 1) + \phi\delta(p_i - r)$$




Totally asymmetric case:
only right jumps ($q_i$=0)



# Disordered ASEP simulations

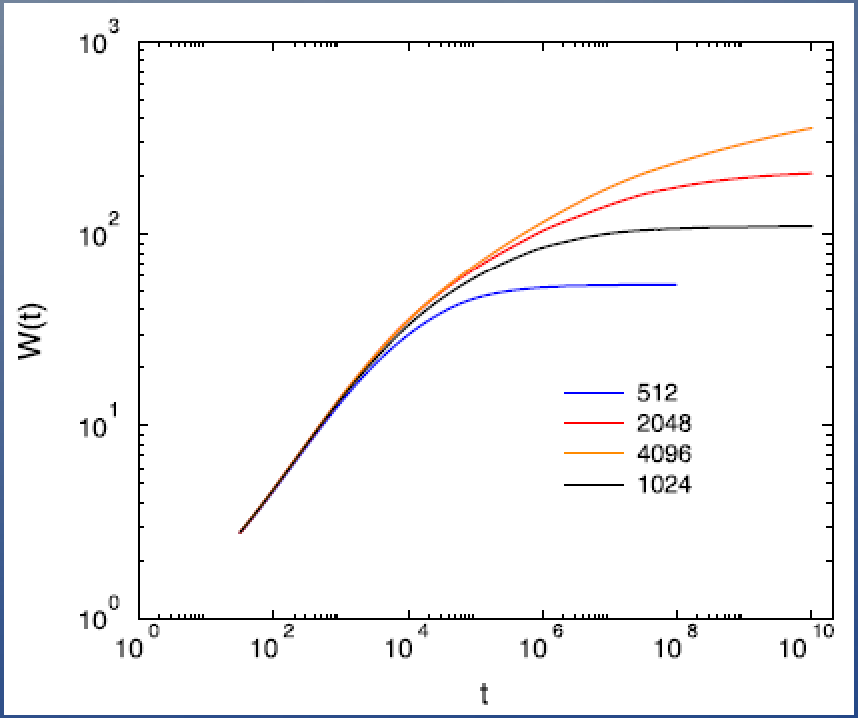


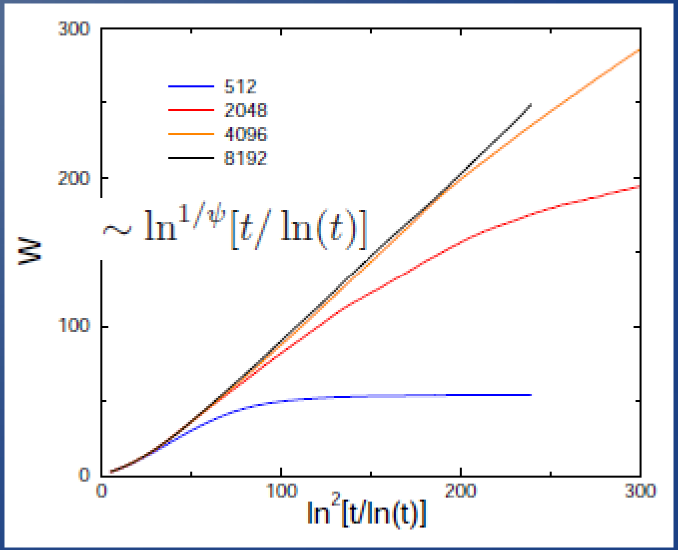

Bimodal, quenched, site-wise jump disorder

Partially asymmetric case:

Left/right jumps ($p_i$, $q_i$ >0)

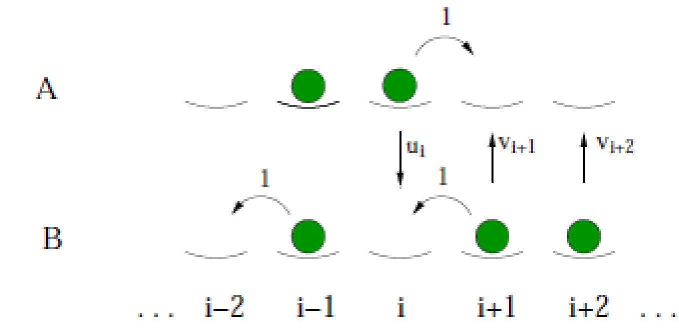
Ultra-slow, logarithmic dynamics:




R. Juhász, G. Ódor
Anomalous coarsening in disordered exclusion processes,
arXiv:1206.1248

# Dynamics of a bidirectional, two-lane exclusion process with random lane change rates

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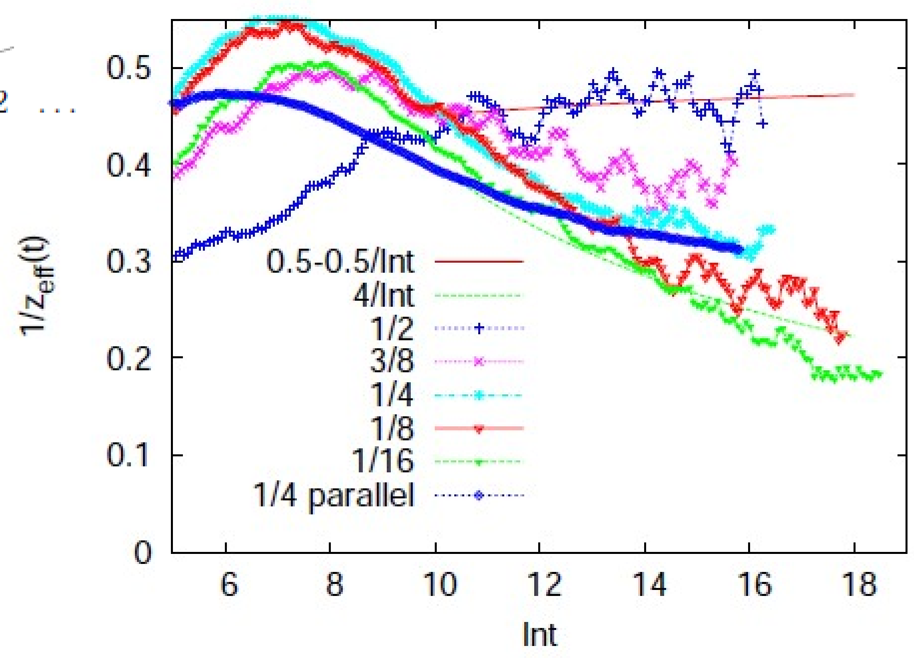



**Figure 8.** Effective dynamical exponents of coarsening in the bidirectional two-lane model measured in Monte Carlo simulations performed at different global densities $N/2L = 1/2, 3/8, 1/4, 1/8, 1/16$ with the random sequential update, except one of them which was obtained by parallel update for $L = 48000$ and $10^2$ samples.

# Conclusions

- Efficient GPU simulations in 1 and 2 dim. for ASEP type of models
- CUDA and OpenCL realizations are compared
- Due to mapping surface growth dynamics has be studied
- Effect of disorder has been investigated
- Pattern formation could be the next step
- Acknowledgements: OTKA, NVIDIA, FP7, DAAD/MÖB
- Publications :

Henrik Schulz, Géza Ódor, Gergely Ódor, Máté Ferenc Nagy: *Simulation of 1+1 dimensional surface growth and lattices gases using GPUs,* Comp. Phys. Comm. 182 (2011) 1467

Jeffrey Kelling and Géza Ódor: *Extremely large-scale simulation of a Kardar-Parisi-Zhang model using graphics cards,* Phys. Rev. E 84 (2011) 061150

J. Kelling, G. Ódor, M. F. Nagy, H. Schulz, K.-H. Heinig: *Comparison of Different Parallel Implementaions of the 2+1-Dimensional KPZ Model and the 3 Dimensional KMC Model,* arXiv:1204.5072, to appear in EPJST

R. Juhász, G. Ódor, *Anomalous coarsening in disordered exclusion processes*, arXiv:1206.1248, submited to JSTAT

# Pattern formation by the octahedron model

Competing KPZ and surface diffusion (following Bradley-Harper theory):

Noisy **Kuramoto-Sivashinsky (KS)** 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 added !

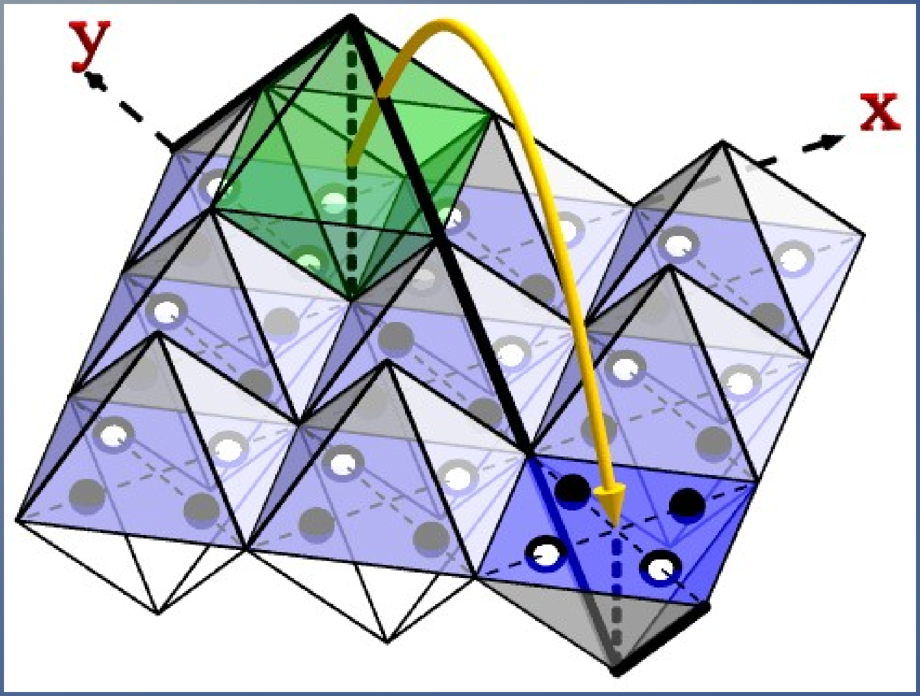
Inverse KS is studied here, signs of couplings are flipped

Alternating application of deposition/removal (probabilities.: $p$, $q$) and surface diffusion (probabilities: $D_x$, $D_y$)

Scaling behavior of 2d **Kuramoto-Sivashinsky ~ KPZ** ???

Field Theoretical hypothesis 1995 (*Cuerno et al.)*

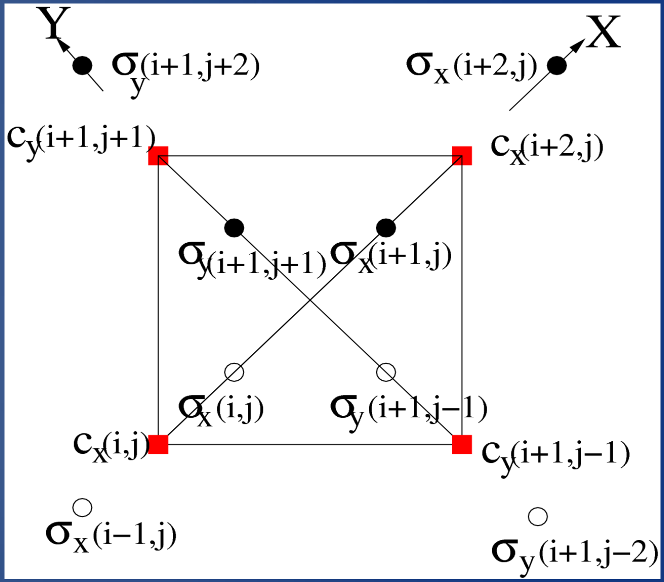
# Surface diffusion (Molecular Beam Epitaxy classes)




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**

/\
\/\/\/ → \/ \/

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

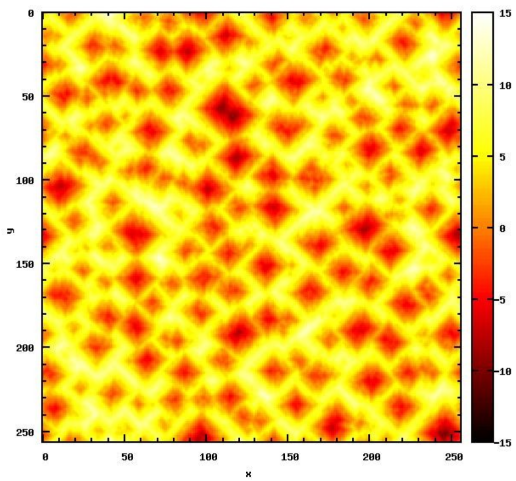
**Arrhenious type update probability** →

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

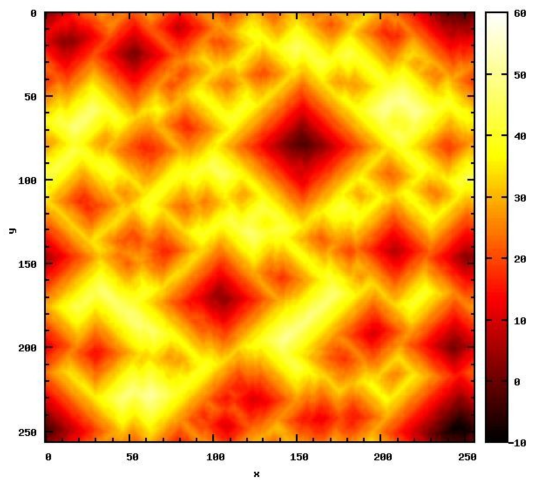
# Patterns generated

## Isotropic surface diffusion

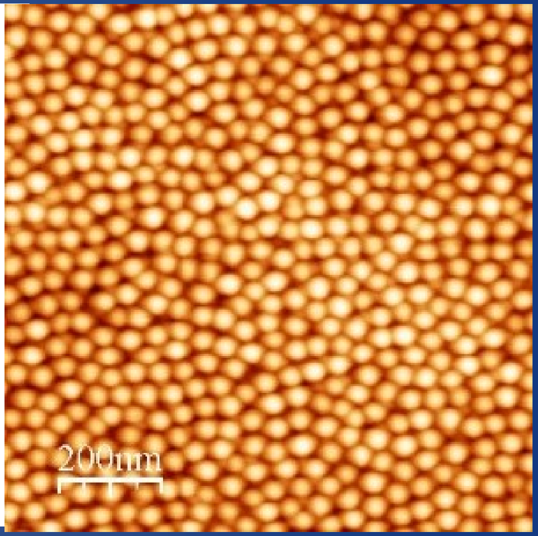
1KMCS




10KMCS




Experiment



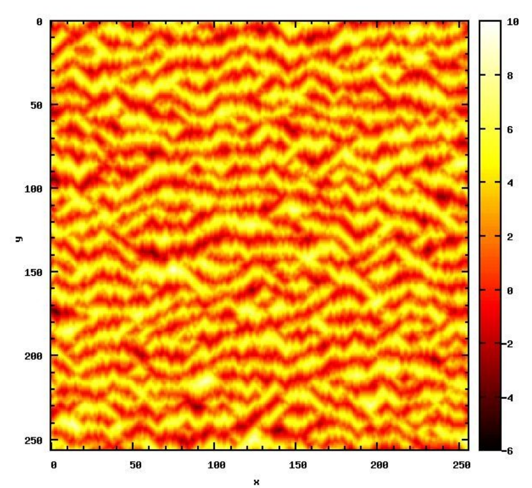

GaSb surface after normal 500 eV Ar+ sputtering. The periodicity and the height of the dots are both 30 nm.

## Coarsening dots

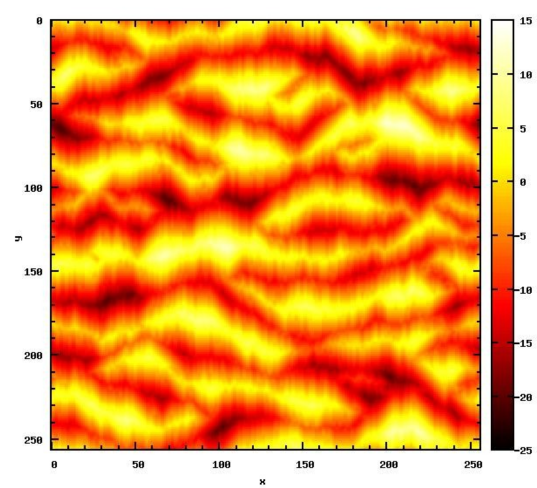
# Surface hight patterns generated by the dimers

## Anisotropic surface diffusion

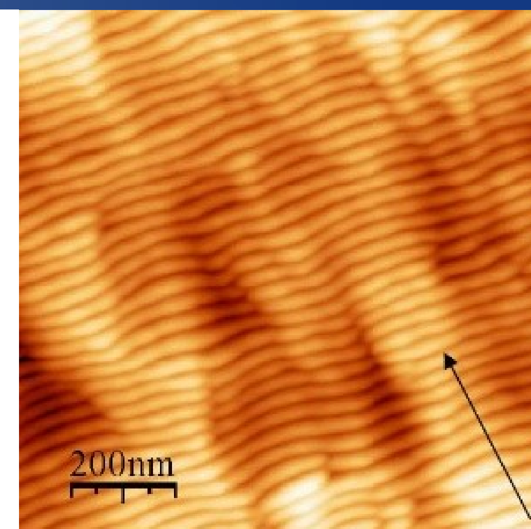
10KMCS




30KMCS




Experiment




Géza Ódor, Bartosz Liedke, Karl-Heinz Heinig and Jeffrey Kelling:
Ripples and dots generated by lattice gases
Applied Surface Science 258 (2012) 4186

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

Geza Odor