Felületi mintázatképződés rácsgázok segítségével

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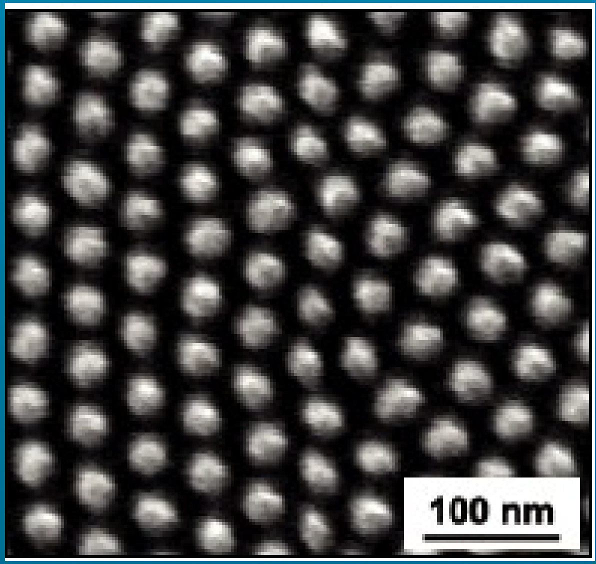
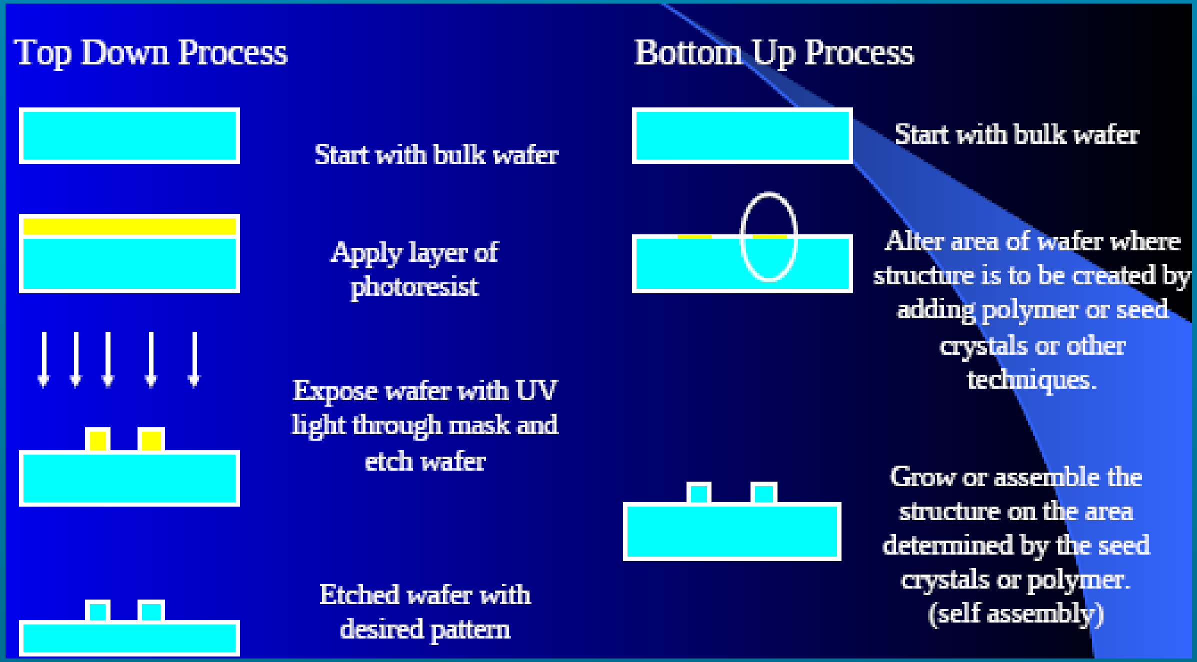
Motivation

In nanotechnologies large areas of **nanopatterns** 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 by STATPHYS

The Kardar-Parisi-Zhang (KPZ) equation/classes

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

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:

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

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

Characterization of surface growth:

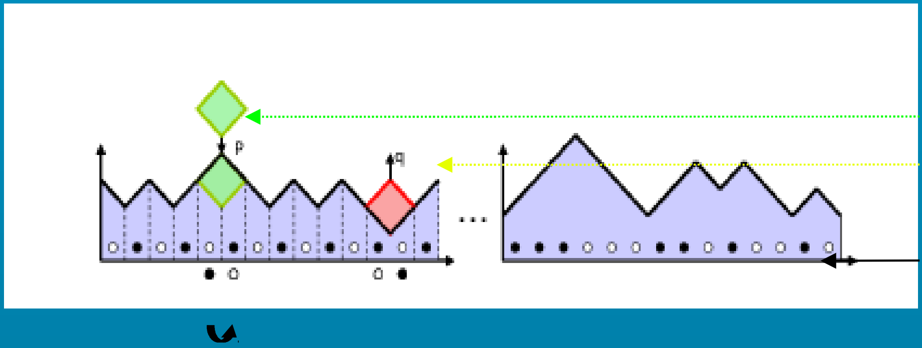
Interface Width:

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

Family-Vicsek scaling:

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

Mappings of KPZ onto lattice gas system in 1d

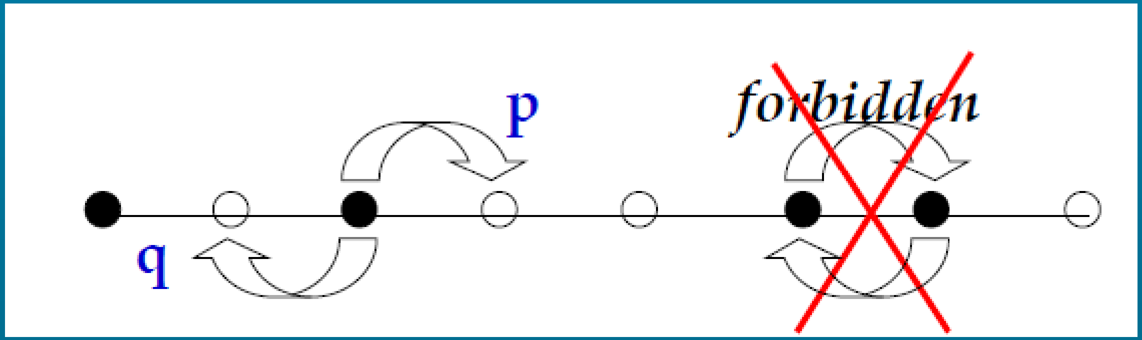


Kawasaki' exchange of particles

- 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)*)

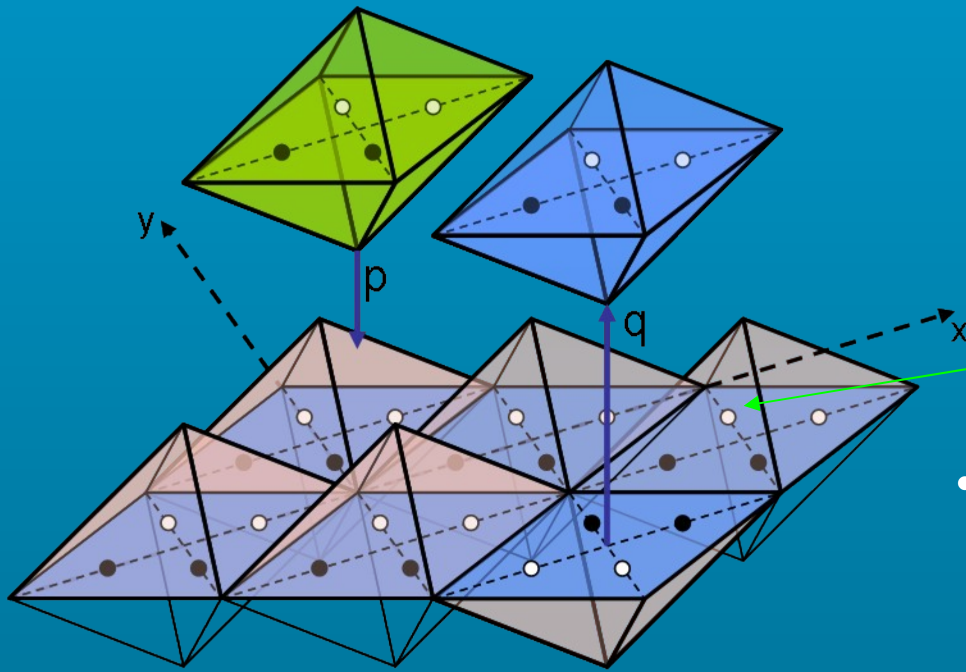


The simple ***ASEP*** (Ligget '95) is **exactly solved 1d lattice gas**

Many features (response to disorder, different boundary

conditions ...) are known.

Mappings of KPZ growth in *2+1* dimensions



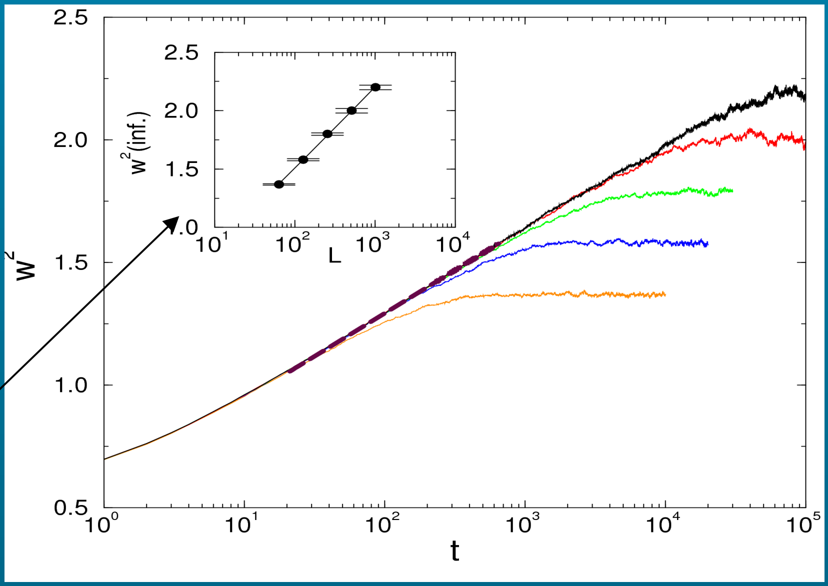
Octahedron model ~ Generalized ASEP:
Driven diffusive gas of pairs (dimers)

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

Generalized Kawasaki update:

$$\begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \underset{q}{\overset{p}{\rightleftharpoons}} \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}$$

- For ***p*** = ***q*** =***1*** Edwards-Wilkinson (EW) scaling:



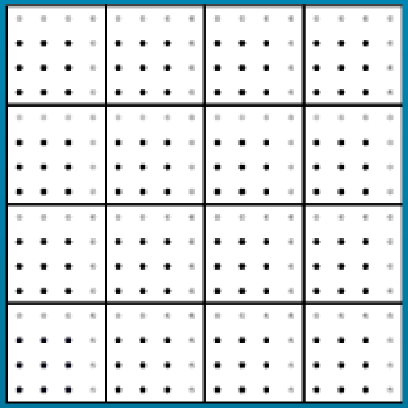
$W^2(t) = 0.152\ln(t) + b$ for $t < t_{sat}$

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

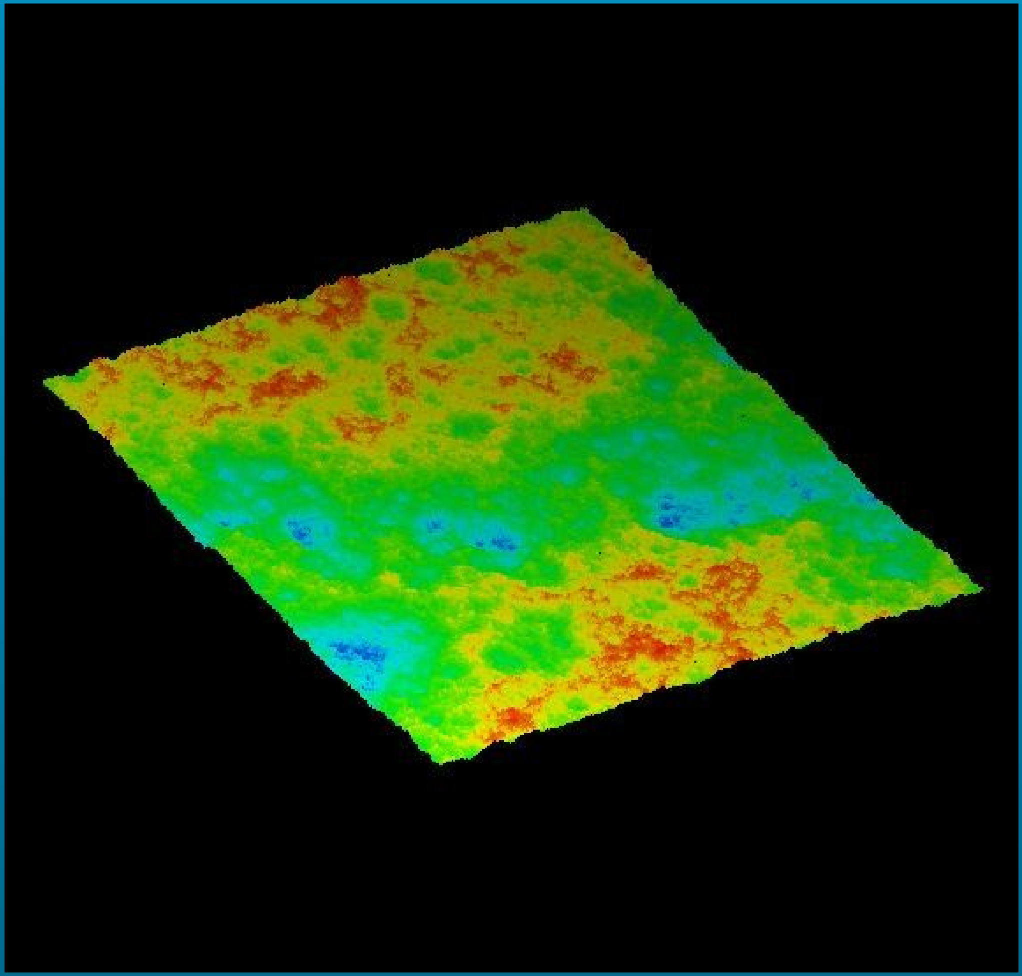
2d problem is reduced to quasi 1d dynamics of reconstructing dimers

Simulation on graphics card (GPU)

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

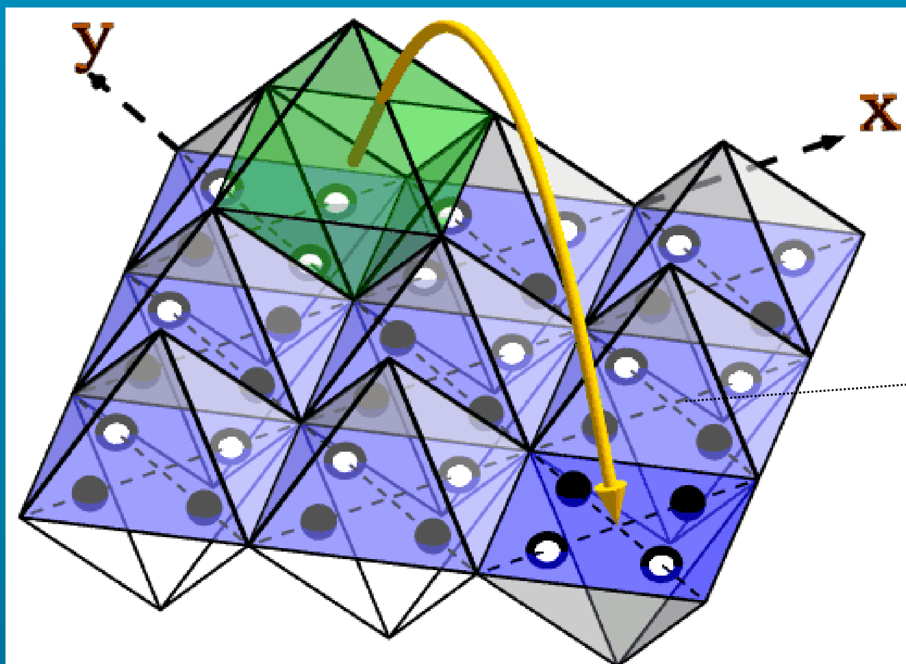


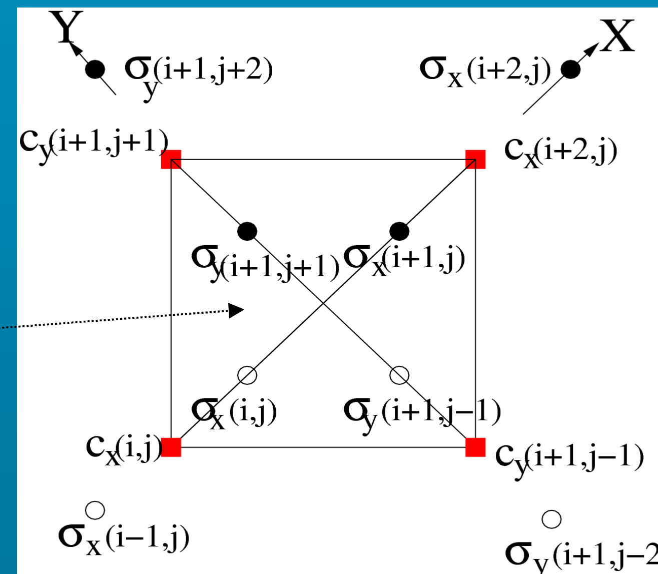
- Each 32-bit word stores the slopes of 4 x 4 sites
- Origin of decomposition moves at every MCs
- **Speedup 240 x to 2.8GHz CPU on 128.000 x 128.000 lattices**



Surface diffusion (Molecular Beam Epitaxy classes)

- Simultaneous octahedron deposition/removal: Attracting (smoothening diffusion) or repelling (roughening diff.) dimers





- Two versions based on local configurations
- a) Larger height octahedron model LHOD
- b) Larger curvature octahedron model LCOD:

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

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

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

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

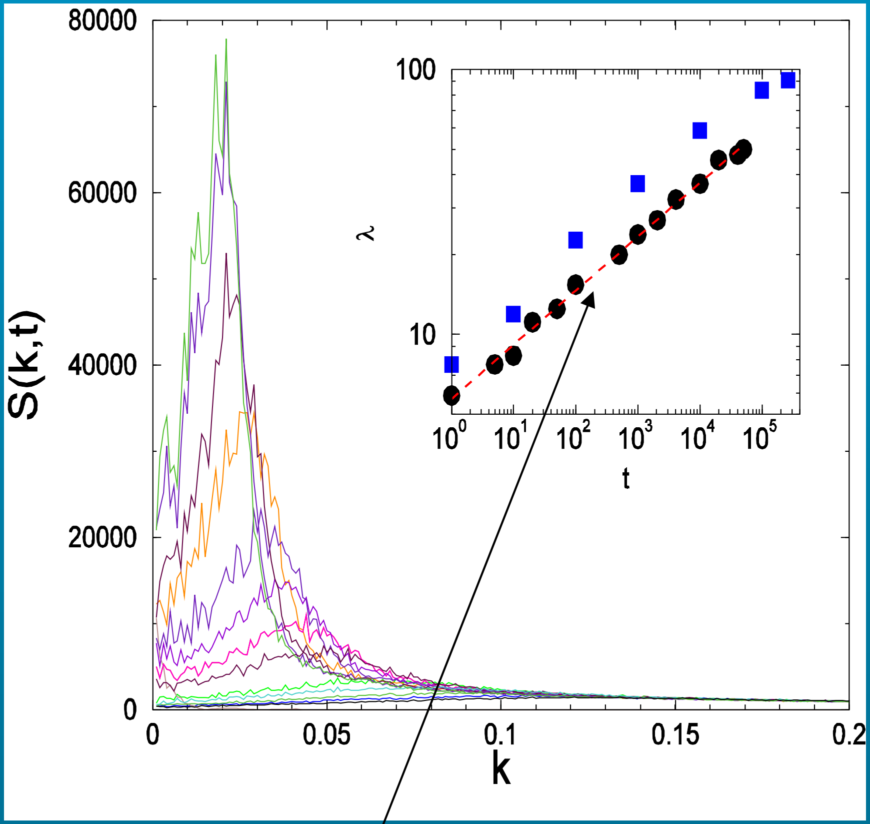
Alternating application of deposition/removal (probabilities.: p, q)
and surface diffusion (probabilities: D_x, D_y)

Scaling behavior of 2d **Kuramoto-Sivashinsky ~ KPZ** ???
Field Theoretical hypothesis 1995 (*Cuerno et al.)*

Isotropic surface diffusion

Dimer lattice gas simulation

Power Spectrum Density



$D_x = D_y = 1$, $p = q = 0.005$

The wavelength λ calculated from the PSD:

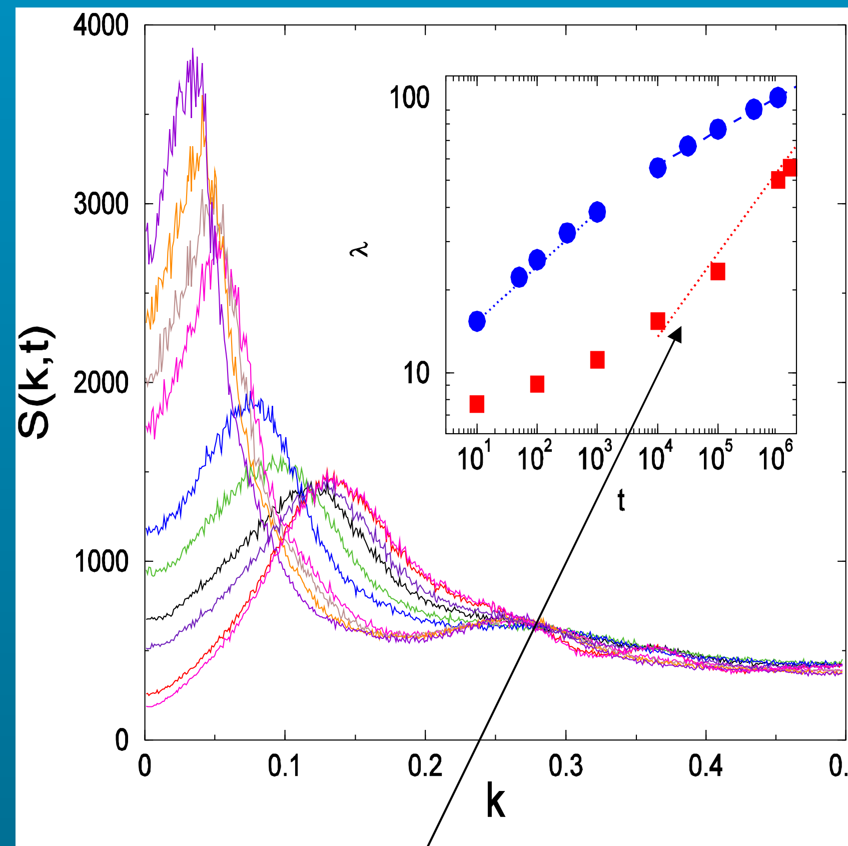
$\lambda \propto t^{0.2}$

Both for the LHOD, LCOD cases

Anisotropic surface diffusion:

$\kappa_x \partial_x^4 h(x,t) + \kappa_y \partial_y^4 h(x,t)$

Power Specrtum Density



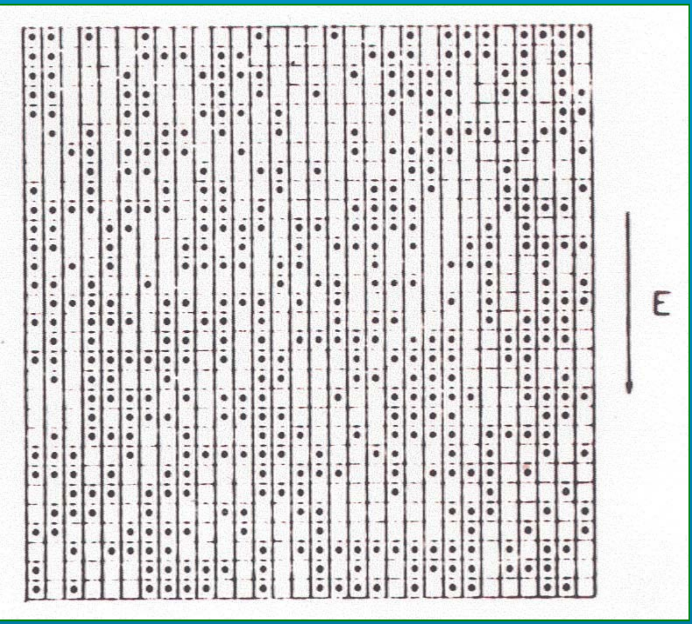
$D_x = 0, D_y = 1,$ $p = q = 0.005$

The wavelength in LHOD model

λ grows $\propto t^{0.35}$ **In agreement with the two-field model** (Cuerno et al)

In LCOD: $\lambda \propto t^{0.2}$

Mapping between Ising Lattice Gas
and surface growth



Disordered dimer LG state

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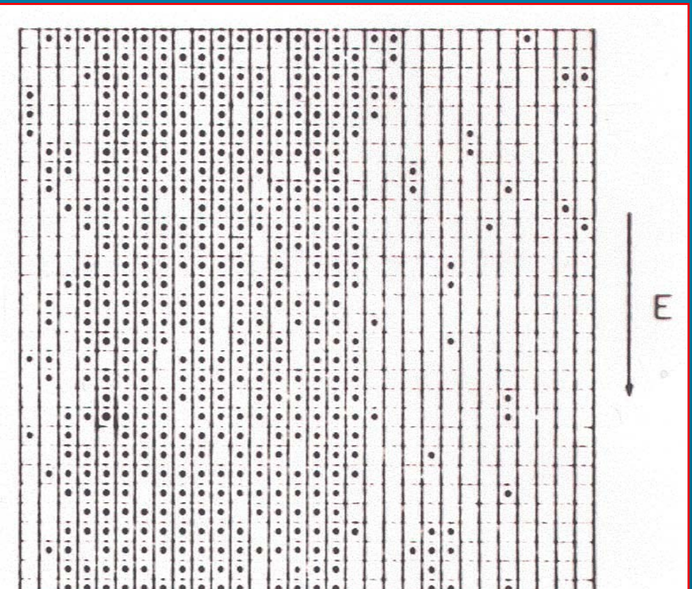
„Smooth”, structureless surface



Phase separeted state of LG

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Surface Patterns

Exploiting analogies with LG

Handy tool to study surfaces, Langevin eqs.

Summary

- KPZ, LHOD, LCOD models created exhibiting MBE, MH scaling in 2d
- Precise numerical results for EW, KPZ, KS scaling exponents, functions
- Understanding of surface growth phenomena via driven lattice gases
- Efficient method to explore scaling and pattern formation $\rightarrow$ GPUs
- For pattern formation : competing reactions : ***KPZ + MBE***
- Wavelength growth scaling via **PSD** analysis
- **UNIVERSALITY DUE TO: $\xi \rightarrow \infty$, CURRENTS, NONEQUILIBRIUM**
- See: **Phys. Rev. E 79** 021125 (2009), **81** 031112 (2010), **81** 051114 (2010) arXiv:1109.2717 (Applied Surface Science in press)
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