Ripples and dots generated by lattice gases

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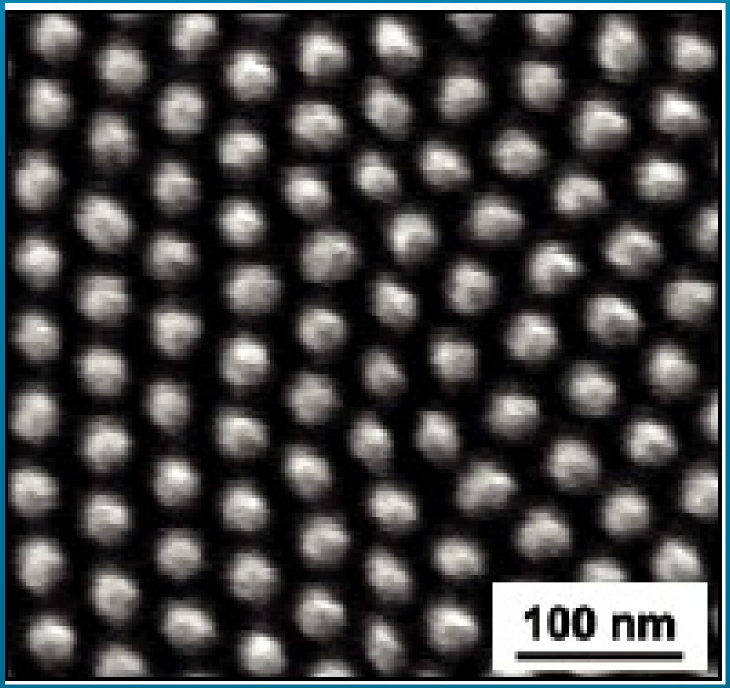
Motivation

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.



Better understanding of basic surface growth phenomena is needed !

See: Phys. Rev. E **79** 021125 (2009),
Phys. Rev. E **81** 031112 (2010),
Phys. Rev. E **81** 051114 (2010)

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:

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

$$z = \alpha/\beta$$

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

Exactly solvable in *1+1 d*, in higher dimension even the field theory failed being unable to access the strong coupling regime:

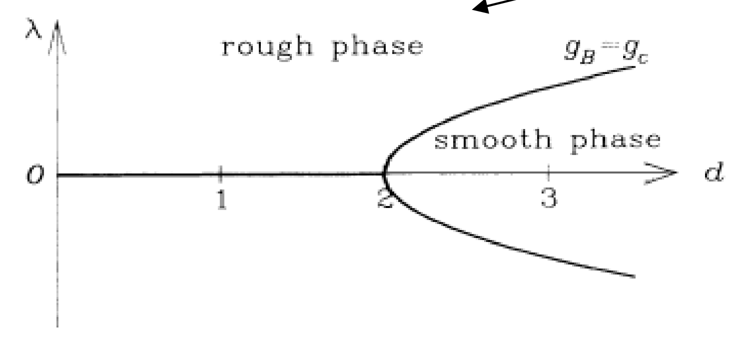


FIG. 1. Schematic phase diagram of the KPZ equation from the one-loop RG analysis. Transitions are marked by thick lines.

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

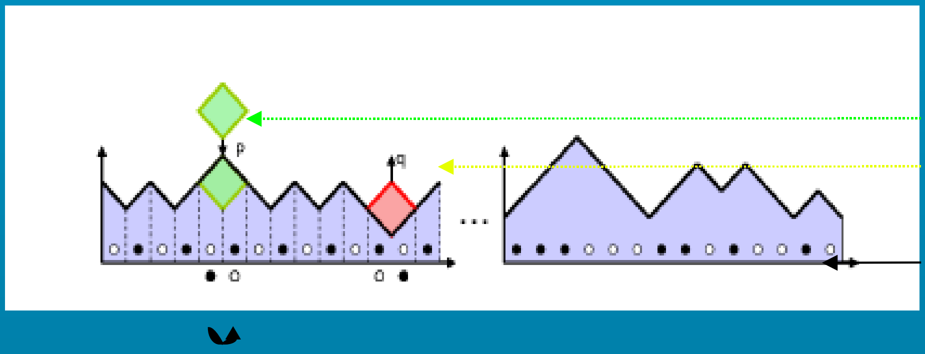
Open problems :

The upper critical dimension is still debated: $d_c = 2, 4, \ldots \infty$?

2-dim numerical estimates have a spread: $\alpha = 0.36 - 0.4$

Field theoretical conjecture by *Lässig :* $z = 4/10$, $\beta = 1/4$

Mappings of KPZ onto lattice gas system in 1d

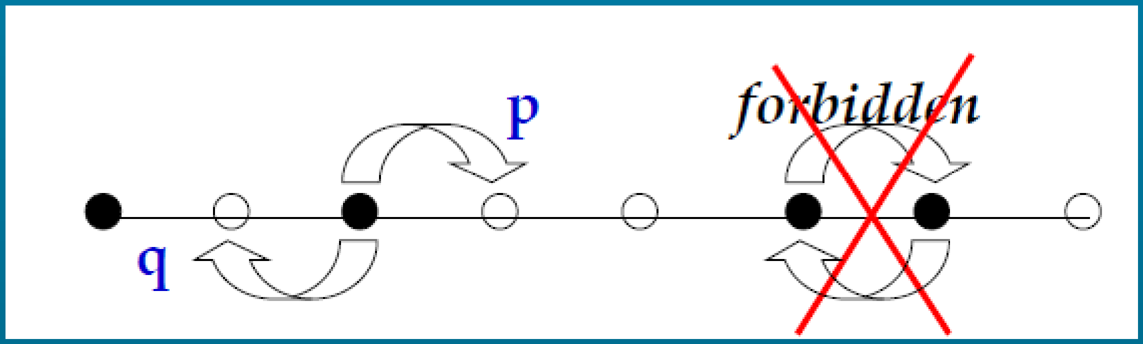


Kawasaki' exchange of particles

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

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

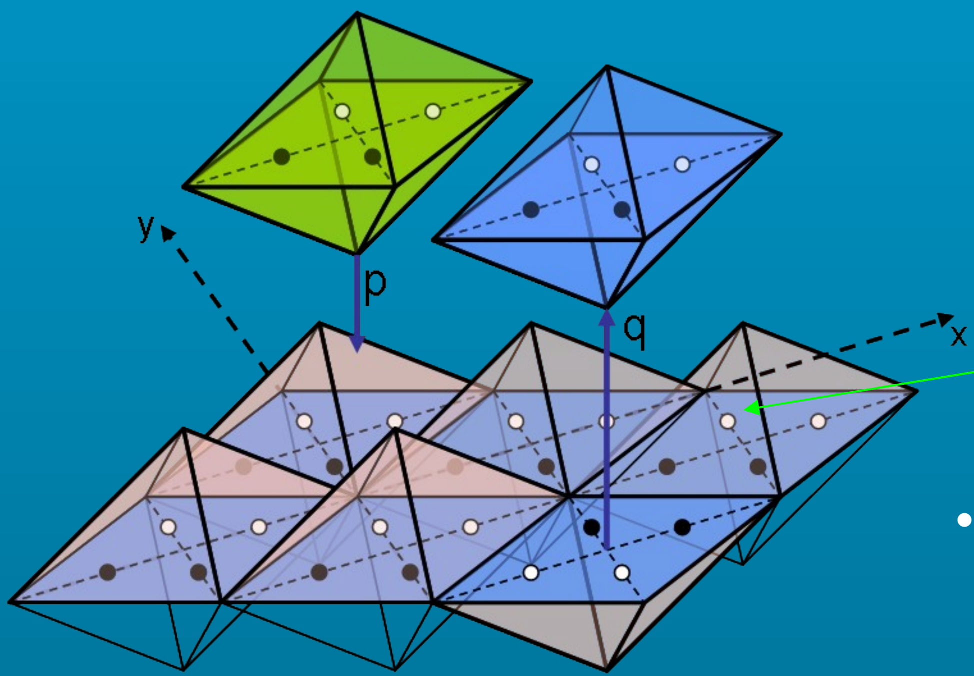
  to anisotropic diffusion of particles (bullets) along the *1d* base space (*M. Plischke, Rácz and Liu, PRB 35, 3485 (1987)*)



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)

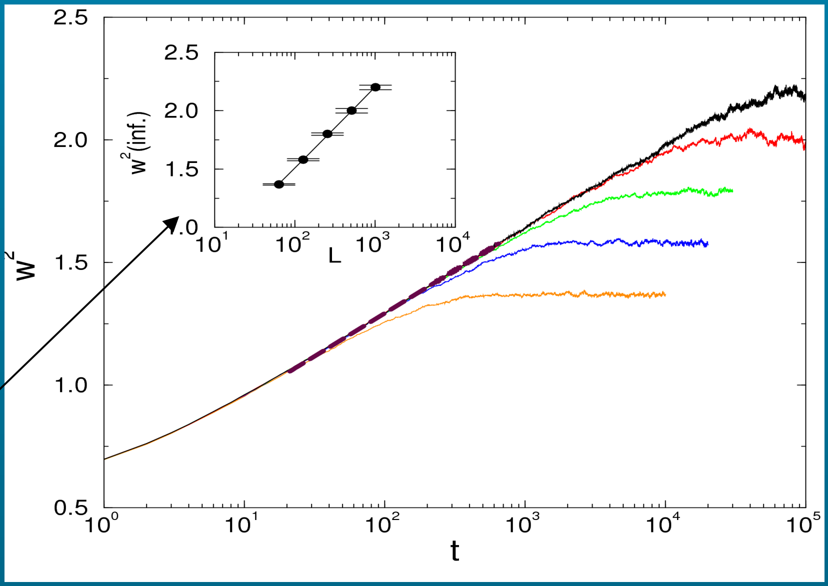
G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009)   derivation of mapping

Generalized Kawasaki update:

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

$$\lambda = 2\frac{p}{p+q} - 1$$

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



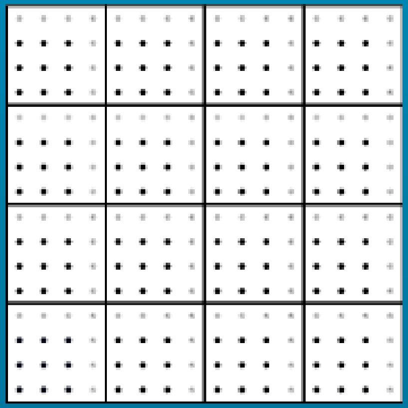
$W^2(t) = 0.152 \ln(t) + b$ for $t < t_{sat}$

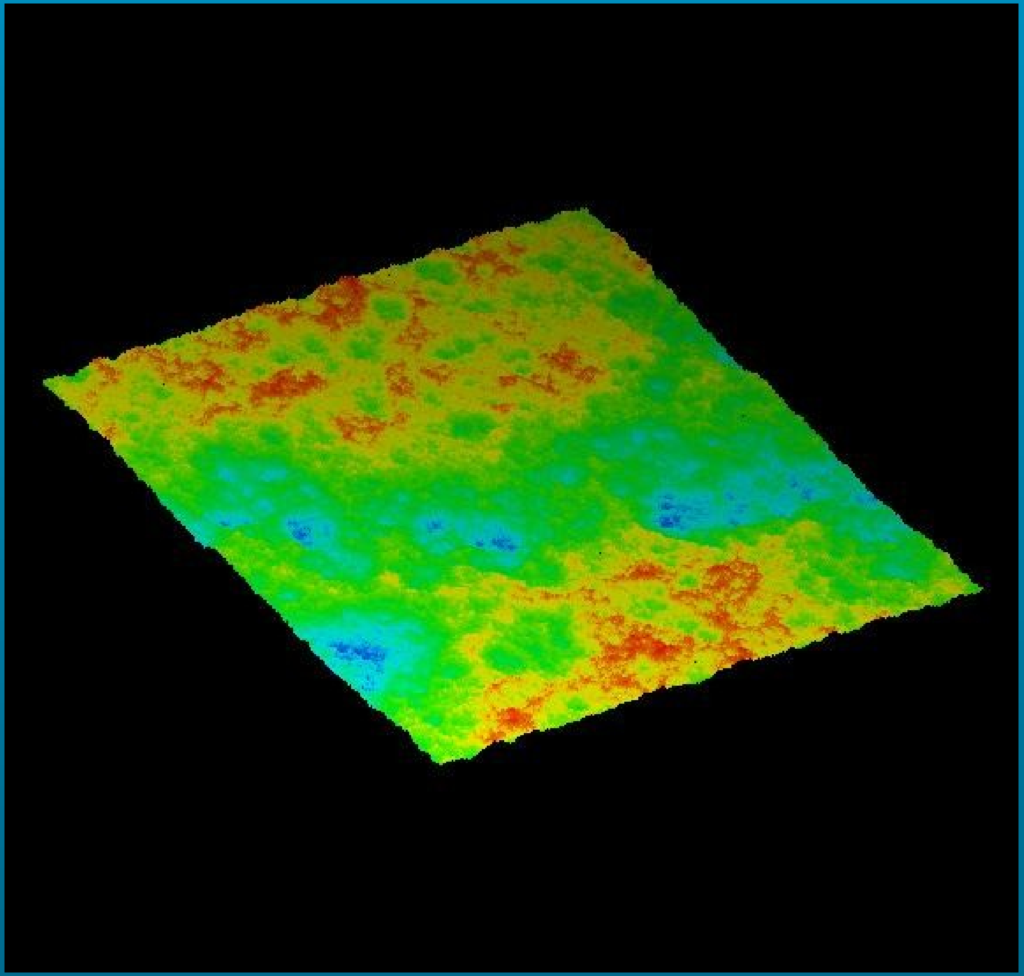
$W^2(L) = 0.304 \ln(L) + d$ for $t > t_{sat}$

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:



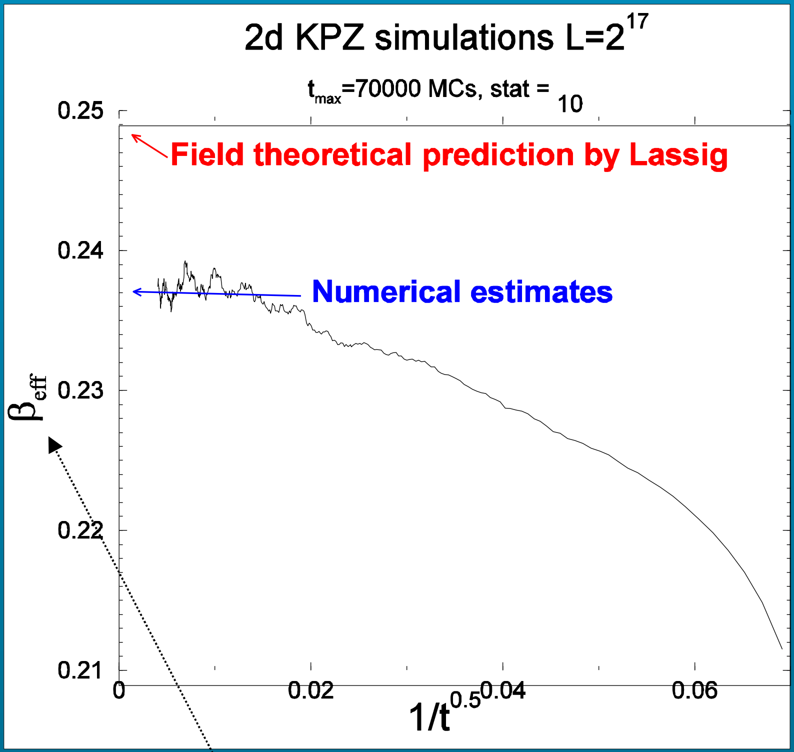


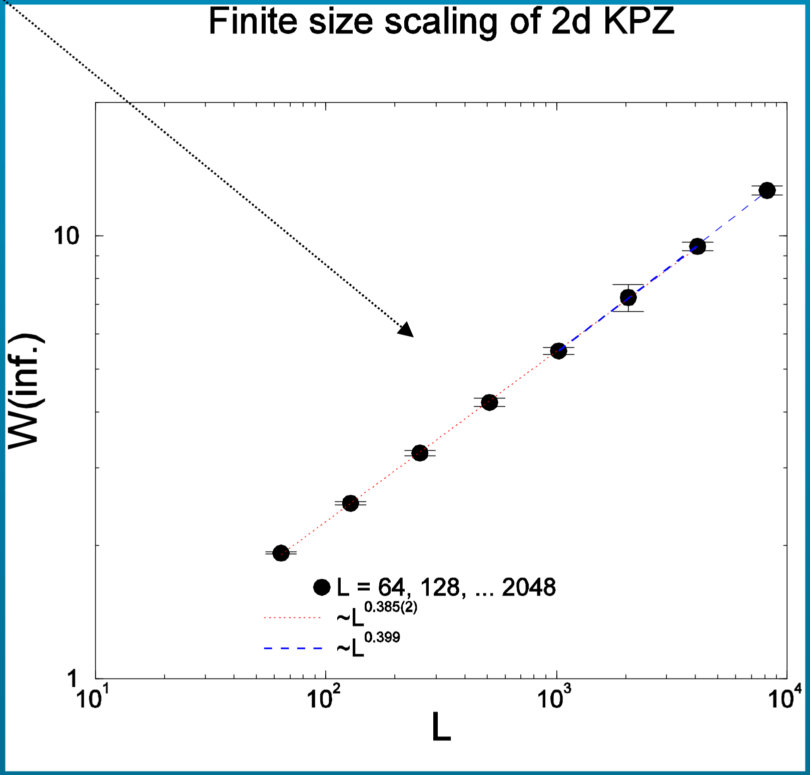
- Each 32-bit word stores the slopes of 4 x 4 sites
- Origin of decomposition moves at every MCs
- **Speedup 240 x with respect a 2.8 GHz CPU**

First KPZ scaling results with GPU

p = 1, q = 0

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

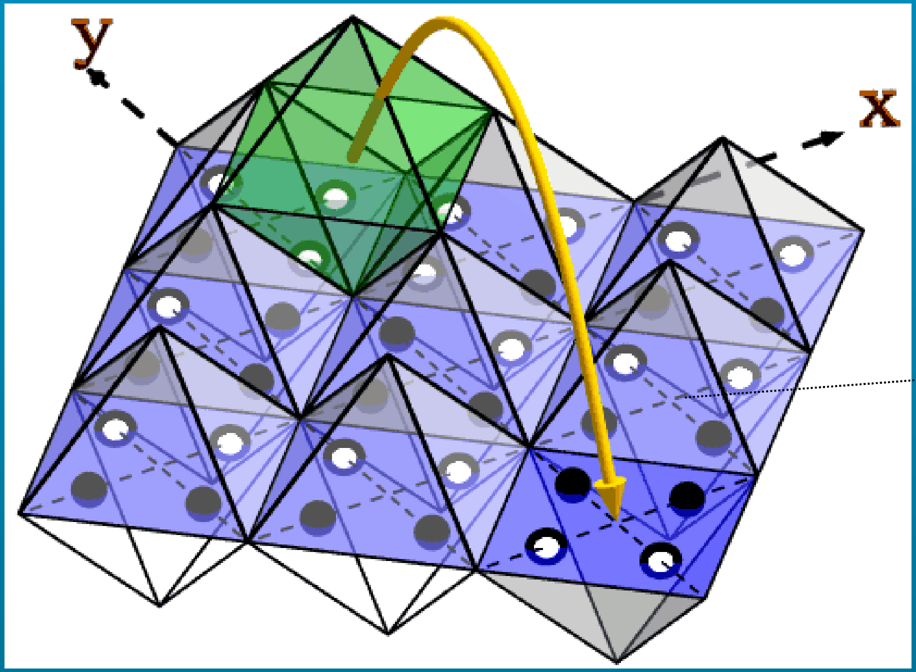


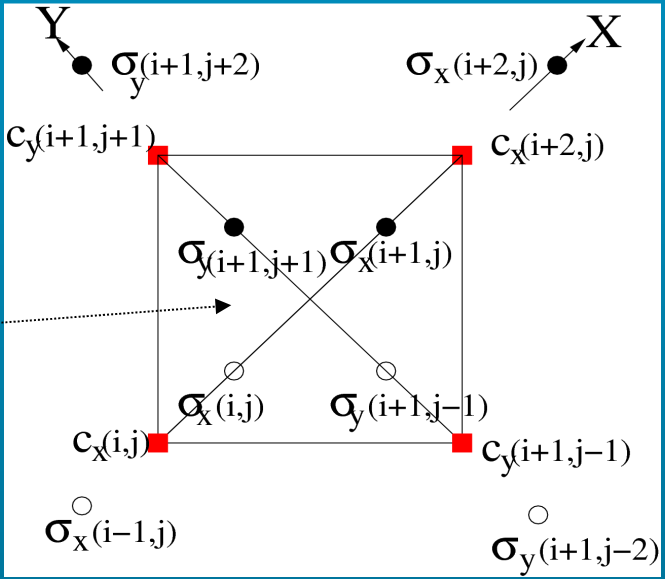


Effecitve β exponent: $\partial\, ln(W) \,/\, \partial\, ln(t)$

Surface diffusion (Molecular Beam Epitaxy classes)

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





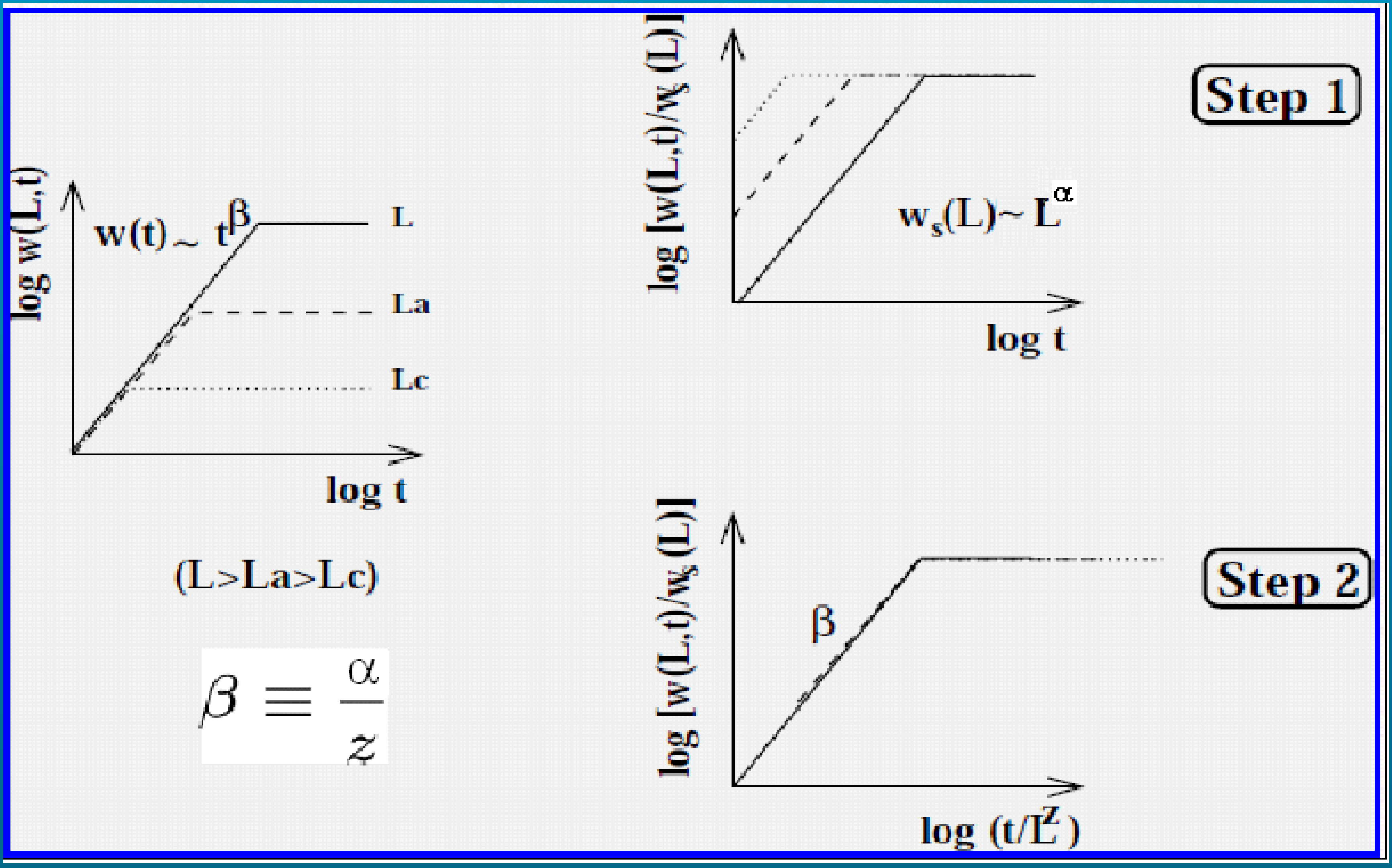
- Two versions based on local configurations
- a) Larger height octahedron model LHOD
- b) Larger curvature octahedron model LCOD: /\
  \/\/ → \/ \/

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

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

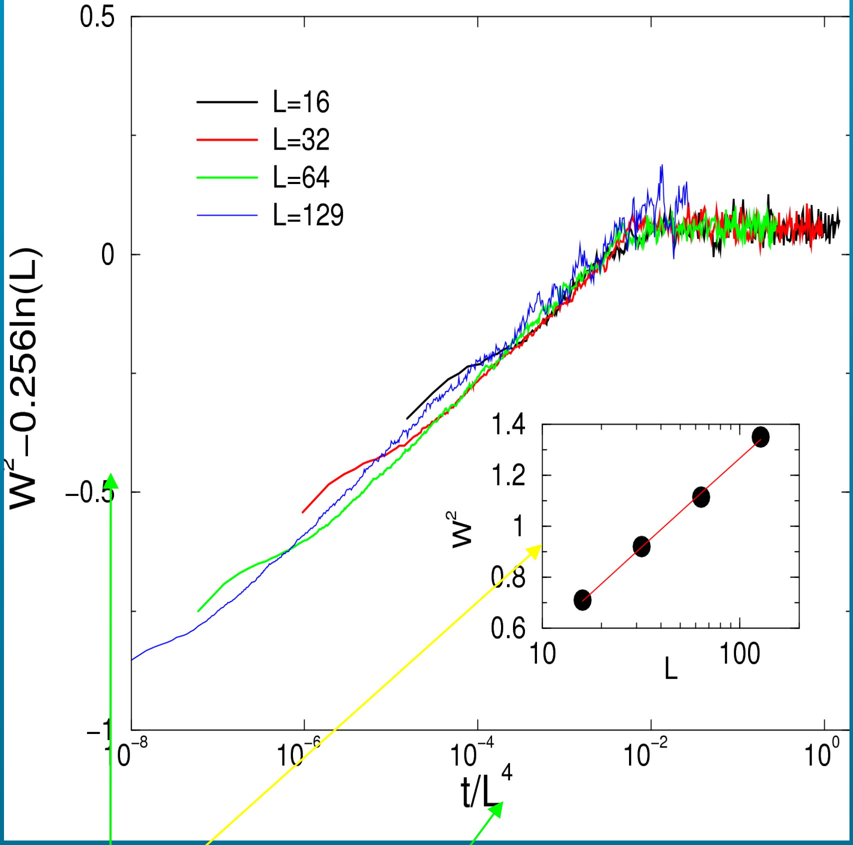
$$w_{i\to i'} = 1/2[1 - a \tanh(-\Delta H^2)]$$

Schematics of finite size data collapse via dynamic scaling

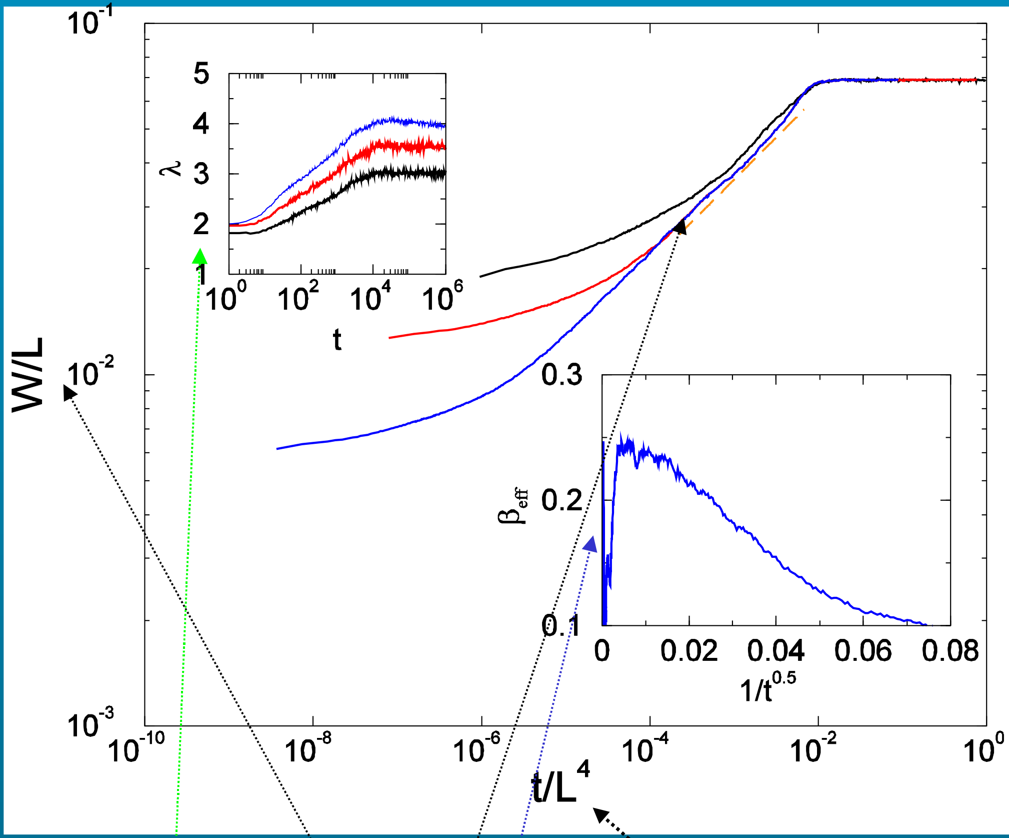


Scaling behavior of LCOD
Test of MH diffusion

For *p=q=0*



p=q=0.05



MH with conserved (diffusive) noise

$\alpha = \beta = 0$, $z=4$

W^2 grows logarithmically

MH with non-conserved noise

$\alpha = 1$, $\beta = 1/4$, $z = 4$

λ grows logarithmically

Pattern formation by the octahedron model

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

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

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

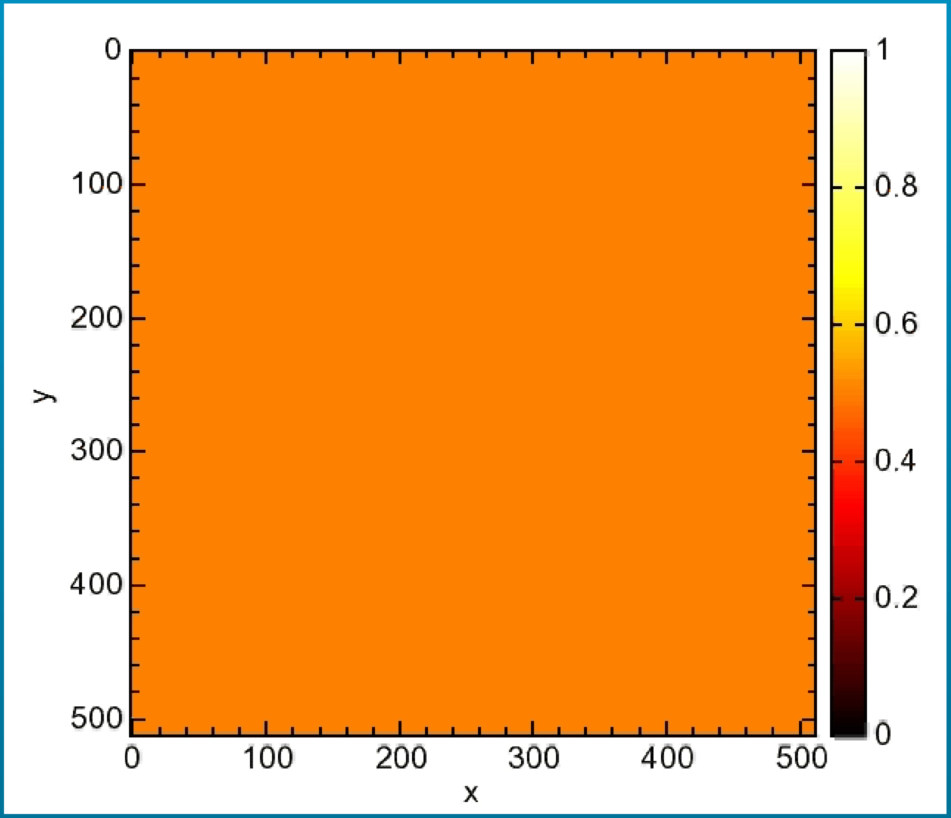
To generate **patterns inverse** (uphill) diffusion is needed !
in fact inverse KS is studied here: signs of couplings are reversed

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



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

The wavelength λ defined as the longest uniform interval in LG grows

logarithmicallz λ scaling

LHOD model scaling

Inverse MH + KPZ case

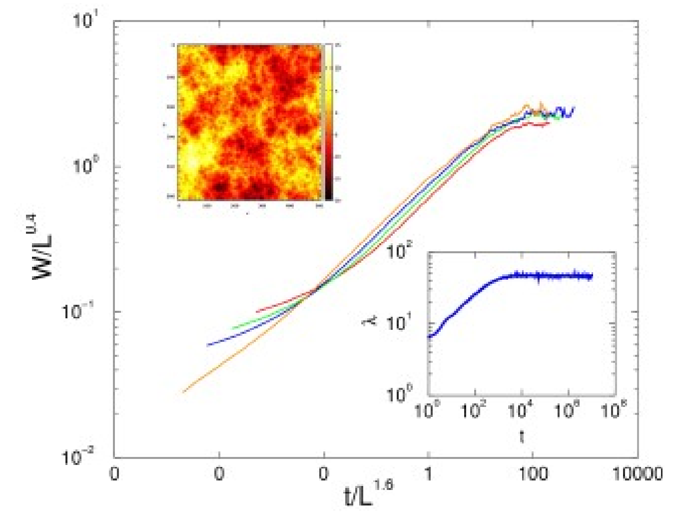


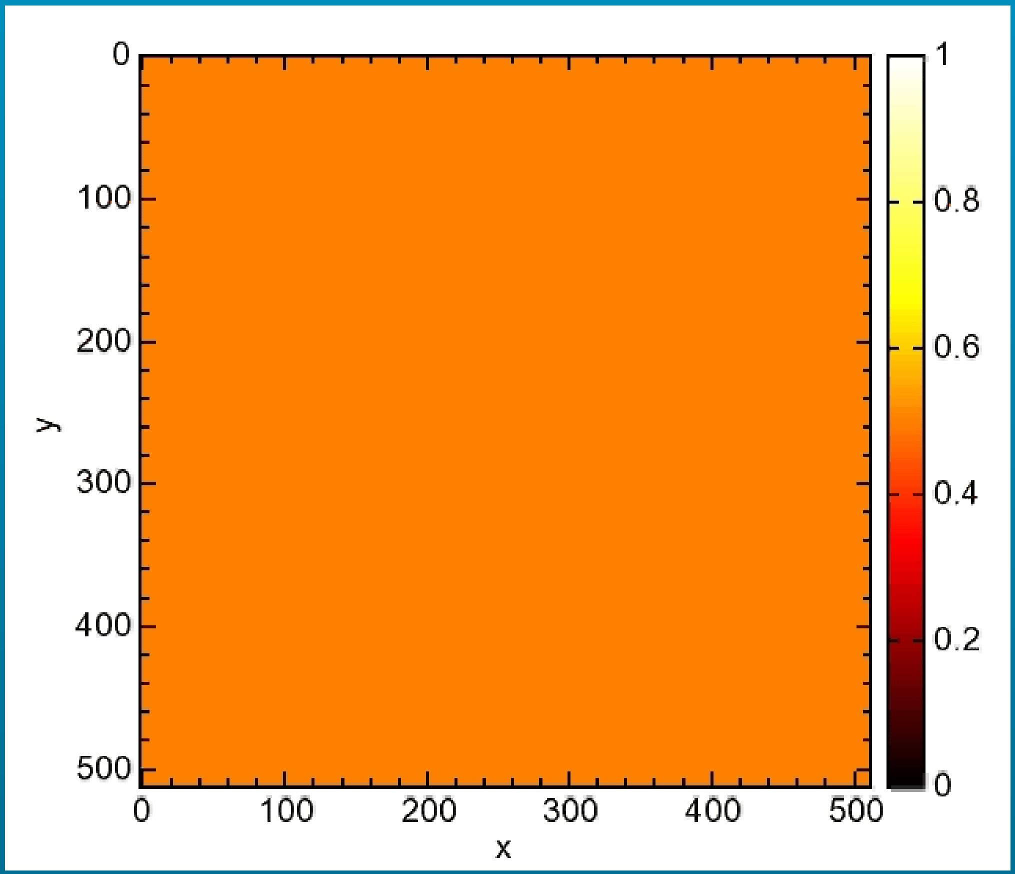
FIG. 11: (Color online) Data collapse of the $L = 128, ...1024$ LHOD model ($p_{\pm x} = p_{\pm y} = 1$) with a competing deposition ($p = 1$) process. One can see very a slow crossover towards KPZ scaling. The right insert shows the growth of λ for $L = 512$. The left insert is a snapshot of the steady state, corresponding to the smeared KPZ height distribution.

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

iKS ~ KPZ in 2d

Anisotropic surface diffusion:

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



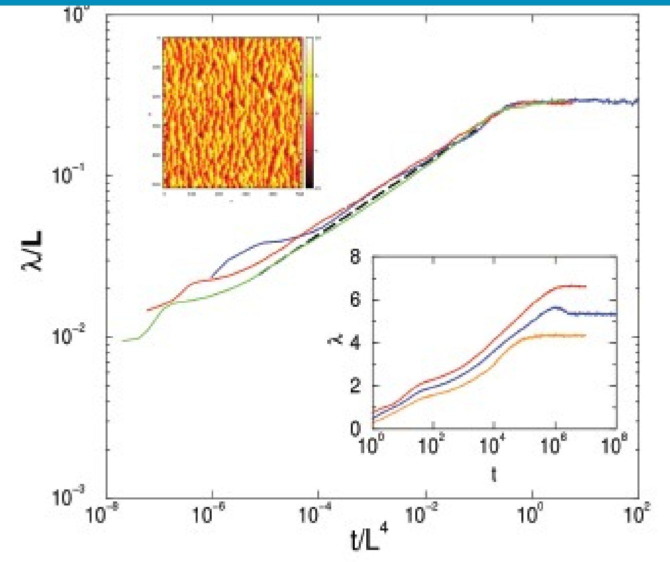


FIG. 8: (Color online) The wavelength growth in the LHOD model for anisotropic diffusion with steady DC current $p_y = 1$, $p = q = 0.005$ for sizes $L = 32, 64, 128$ (top to bottom at the beginning). Dashed line: power-law fit with the exponent $\beta = 0.24(1)$. The left insert shows the corresponding pattern. The right insert corresponds the isotropic diffusion case $p_{\pm x} = p_{\pm y} = 1$, where $\lambda(t)$ grows logarithmically.

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

The wavelength λ grows
power-law manner
in case of **DC current**

Scaling behavior: inverse-MH & KPZ

Anisotropic diffusion case *$D_x = 0$, $D_y = 1$*

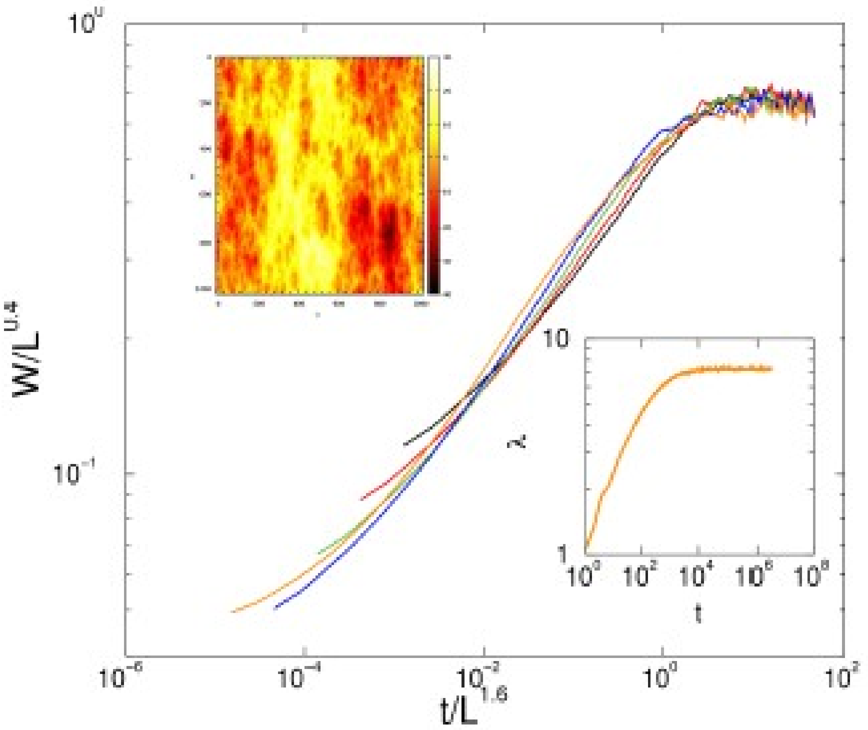


FIG. 9: (Color online) Data collapse for deposition ($p = 1$, $q = 0$) and anisotropic, inverse diffusion $p_{\pm x} = 1$ in the LHOD model with KPZ class exponents for $L = 64, 128, 256, 512, 1024$ (top to bottom curves at the right side). Right insert: $\lambda(r)$ for $L = 1024$, left insert the blurred ripple structure.

- If the deposition is strong: ***p = 1***

  A-iKS ~ A-KPZ ~ KPZ

KPZ + normal Mullins: no patterns, but crossover to mean-field

- For **strong** diffusions:
  Smooth surface:
  Logarithmic growth, but **not EW** coefficients *(a=0.4 ↔ 0.151)*
- Wavelength :

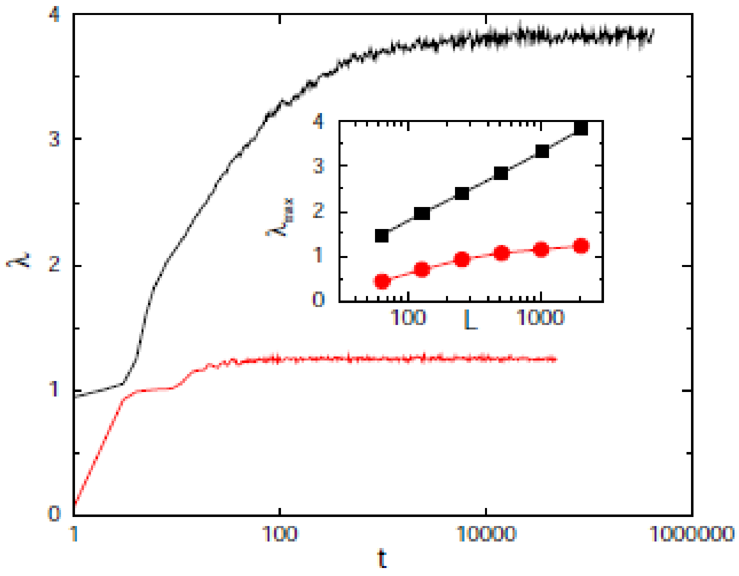


FIG. 14: (Color online) The wavelength saturates quickly for KPZ + weak LHOD (higher curve) and KPZ + strong LHOD (lower curve) diffusion ($L = 2048$). The insert shows λ_{max} versus L.

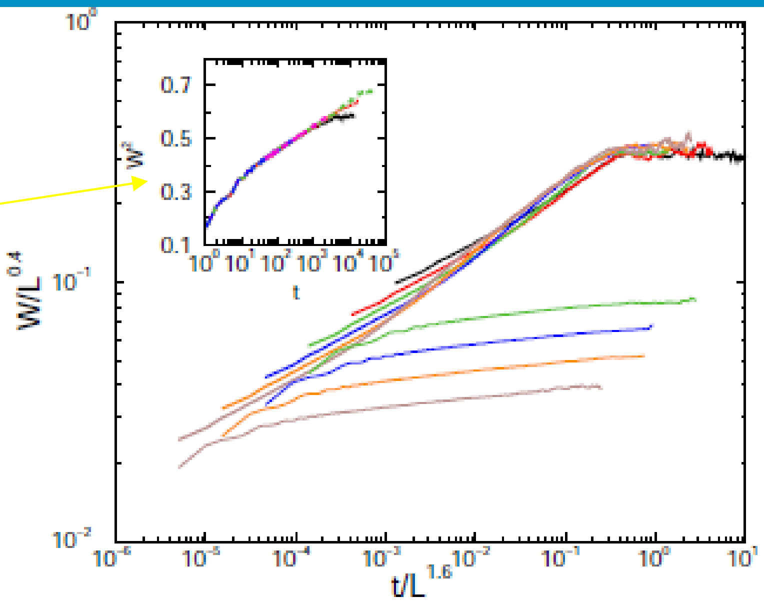


FIG. 13: (Color online) Data collapse of KPZ deposition ($p = 1$) and weak, isotropic normal LHOD (higher curves) for $L = 64, 128, ...2048$ (top to bottom). In case of strong diffusion (lower curves) the KPZ scaling disappears and as the insert shows logarithmic growth can be observed.

Probability distributions

KPZ in different dimensions

KPZ + surface diffusion

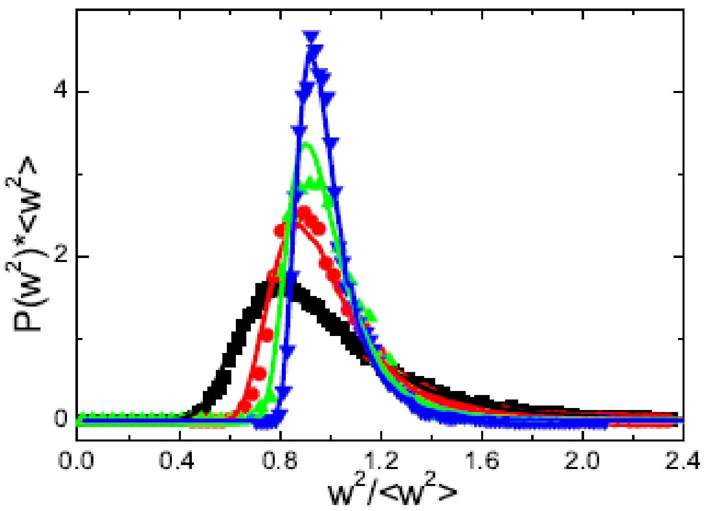


FIG. 15: (Color online) Comparison of the $P(W^2)$ of the higher dimensional octahedron model results (symbols) with those of [60] (lines) in $d = 2, 3, 4, 5$ spatial dimensions (bottom to top).

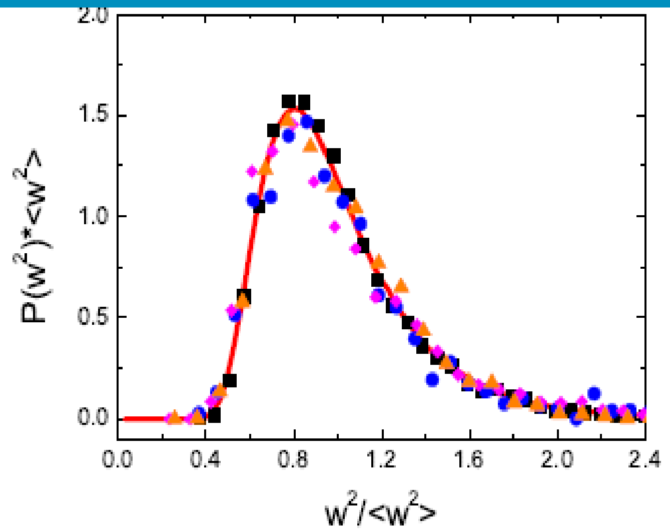
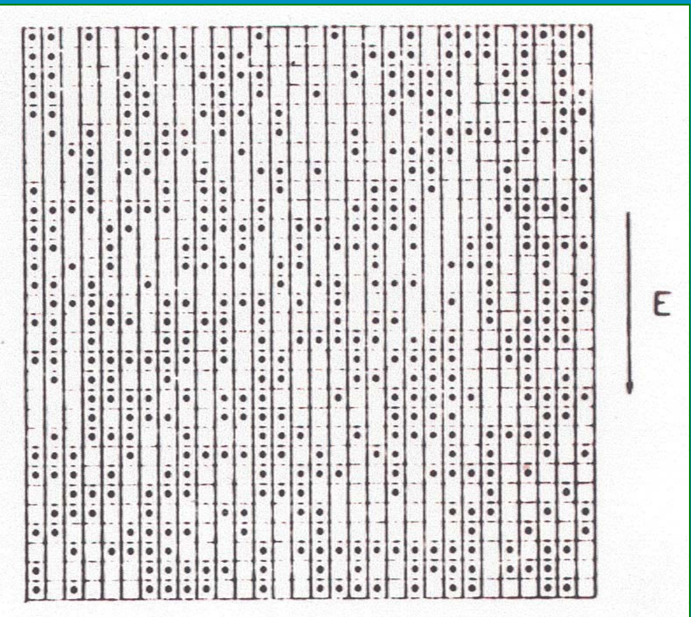


FIG. 16: (Color online) Comparison of $P(W^2)$ of the KPZ+LHOD (black boxes); KPZ+inverse LHOD (blue dots); KPZ+inverse, anisotropic LHOD (pink rhombuses); KPZ+inverse LCOD (orange triangles) with that of the KPZ from ref.[60] (solid line).

Agreement with former KPZ class distribution results

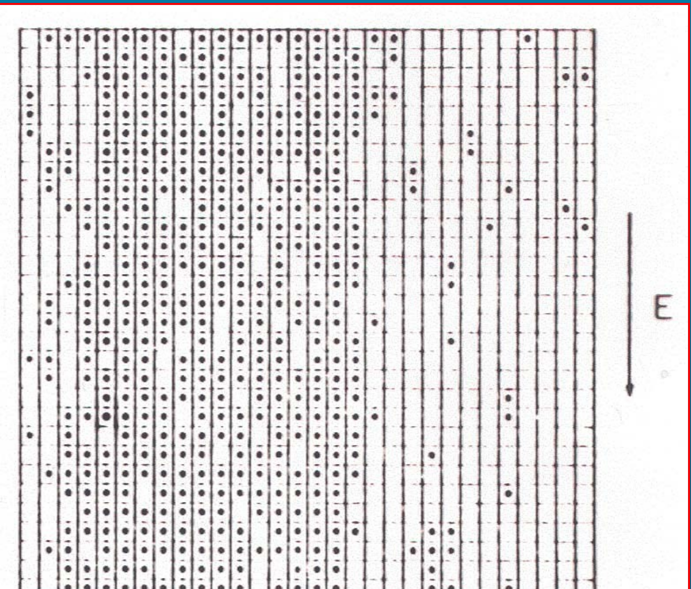
Mapping between Ising Lattice Gas
and surface growth



Disordered dimer LG state

↕

„Smooth”, structureless surface



Phase separeted state of LG

↕

Surface Patterns

Exploiting analogies with LG

Handy tool to study surfaces, Langevin eqs.

Summary

- KPZ, LHOD, LCOD models exhibiting MBE, MH scaling in 2d
- Precise numerical results for EW, KPZ, KS scaling exponents, distributions
- Understanding of surface growth phenomena via driven lattice gases
- Efficient method to explore scaling and pattern formation -> GPUs
- For pattern formation competing reactions (KPZ & inverse MBE) needed
- For strong (power-law), coarsening: DC current needed (otherwise log.)
- Numerical evidence for: iKS ~ KPZ scaling

Surface Diffusion + KPZ growth (deposition)

Ripples Dots

inv-anis. Diffusion		inv-Diffusion		normal-Diffusion	
strong-depo	weak-depo	strong-depo	weak-depo	strong-D	weak-D
KPZ	*MBE(MH)*	*KPZ*	*MBE(MH)*	*KPZ-MF*	*KPZ*

- See: Phys. Rev. E **79** 021125 (2009), **81** 031112 (2010), **81** 051114 (2010)
- Support from grants : DAAD/MÖB, OTKA (T77629), NVIDIA, DFG-FG845