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:

\[ \langle \eta(x,t) \eta(x',t') \rangle = 2D \delta^d (x-x')(t-t') \]

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

Characterization of surface growth:

**Interface Width:**

\[ W(L,t) = \left[ \frac{1}{L^2} \sum_{i,j} h^2_{i,j}(t) - \left( \frac{1}{L} \sum_{i,j} h_{i,j}(t) \right)^2 \right]^{1/2} \]

\[ W(L,t) \propto t^\beta, \text{ for } t_0 \ll t \ll t_s \]

\[ \propto L^\alpha, \text{ for } t \gg t_s \]

\[ z = \frac{\alpha}{\beta} \]
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:

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

- 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))

Kawasaki' exchange of particles

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:
\[
\begin{pmatrix}
-1 & 1 \\
-1 & 1
\end{pmatrix}
\begin{pmatrix}
p \\
q
\end{pmatrix}
\rightarrow
\begin{pmatrix}
1 & -1 \\
1 & -1
\end{pmatrix}
\]
\[\lambda = 2 \frac{p}{p+q} - 1\]

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

\[W^2(t) = 0.152 \ln(t) + b \quad \text{for} \quad t < t_{sat}\]
\[W^2(L) = 0.304 \ln(L) + d \quad \text{for} \quad t > t_{sat}\]

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:
  
  
  ![Checkerboard decomposition diagram]

- 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

\[ p = 1, \ q = 0 \]

\[ W(L,t) \propto t^\beta, \text{ for } t_0 \ll t \ll t_s \]
\[ \propto L^\alpha, \text{ for } t \gg t_s. \]

Effective \( \beta \) 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: \[ \vee \lightning \rightarrow \vee \vee \]

\[ c_x(i, j) = \sigma_x(i, j) \sigma_x(i + 1, j) \]

\[ \Delta H = \Delta \sum_{x=x,y} \sum_{(i,j)} c_x(i, j) + \Delta \sum_{x=x,y} \sum_{(i',j')} c_x(i', j') \]

\[ w_{i \rightarrow i'} = 1/2[1 - a \tanh(-\Delta H^2)] \]
Schematics of finite size data collapse via dynamic scaling

\[
\begin{align*}
\log w(L, t) \sim t^\beta & \quad \text{(Step 1)} \\
\log \left[ w(L, t)/w_s(L) \right] & \sim \log t \\
\beta & \equiv \frac{\alpha}{\nu} \\
\log \left[ \frac{w(L, t)}{w(L_c)} \right] & \sim \log \left( \frac{t}{L_c^\beta} \right) 
\end{align*}
\]
Scaling behavior of LCOD
Test of MH diffusion

For \( p=q=0 \)

MH with conserved (diffusive) noise

\[ \alpha = \beta = 0, \; z=4 \]

\( W^2 \) grows logarithmically

For \( p=q=0.05 \)

MH with non-conserved noise

\[ \alpha = 1, \; \beta = 1/4, \; z = 4 \]

\( \lambda \) 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 \(\sim\) KPZ ???

Field Theoretical hypothesis 1995 (Cuerno et al.)
Isotropic surface diffusion

Dimer lattice gas simulation

LHOD model scaling

Inverse MH + KPZ case

\[ D_x = D_y = 1, \quad p=q=0.005 \]

The wavelength \( \lambda \) defined as the longest uniform interval in LG grows logarithmically \( \lambda \) scaling

\[ D_x = D_y = 1, \quad p=1, \quad q=0 \]

iKS \( \sim \) KPZ in 2d

FIG. 11: (Color online) Data collapse of the \( L = 128, \ldots, 1024 \) 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 \( \lambda \) for \( L = 512 \). The left insert is a snapshot of the steady state, corresponding to the smeared KPZ height distribution.
Anisotropic surface diffusion:

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

Lattice gas simulation

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

The wavelength $\lambda$ grows power-law manner in case of DC current.
Scaling behavior: inverse-MH & KPZ

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

If the deposition is strong: $p = 1$

$A-iKS \sim A-KPZ \sim KPZ$
KPZ + normal Mullins: no patterns, but crossover to mean-field

- For **strong** diffusions:
  - Smooth surface:
  - Logarithmic growth, but **not** EW coefficients \((a=0.4 \leftrightarrow 0.15)\)
- Wavelength:

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

**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 \(\lambda_{\text{max}}\) versus \(L\).
Probability distributions

KPZ in different dimensions

Agreement with former KPZ class distribution results

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).
Mapping between Ising Lattice Gas and surface growth

Disordered dimer LG state

\[ \uparrow \]

„Smooth”, structureless surface

Phase separated state of LG

\[ \uparrow \]

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
inv-anis. Diffusion
strong-depo weak-depo
KPZ
MBE(MH)

Dots
inv-Diffusion
strong-depo weak-depo
KPZ
MBE(MH)

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

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