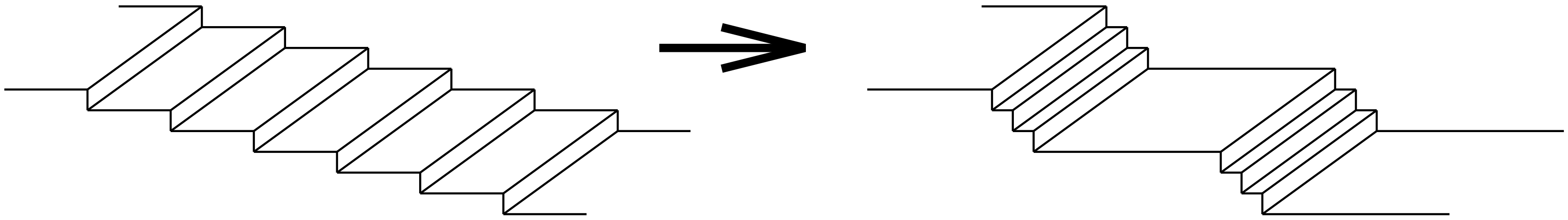
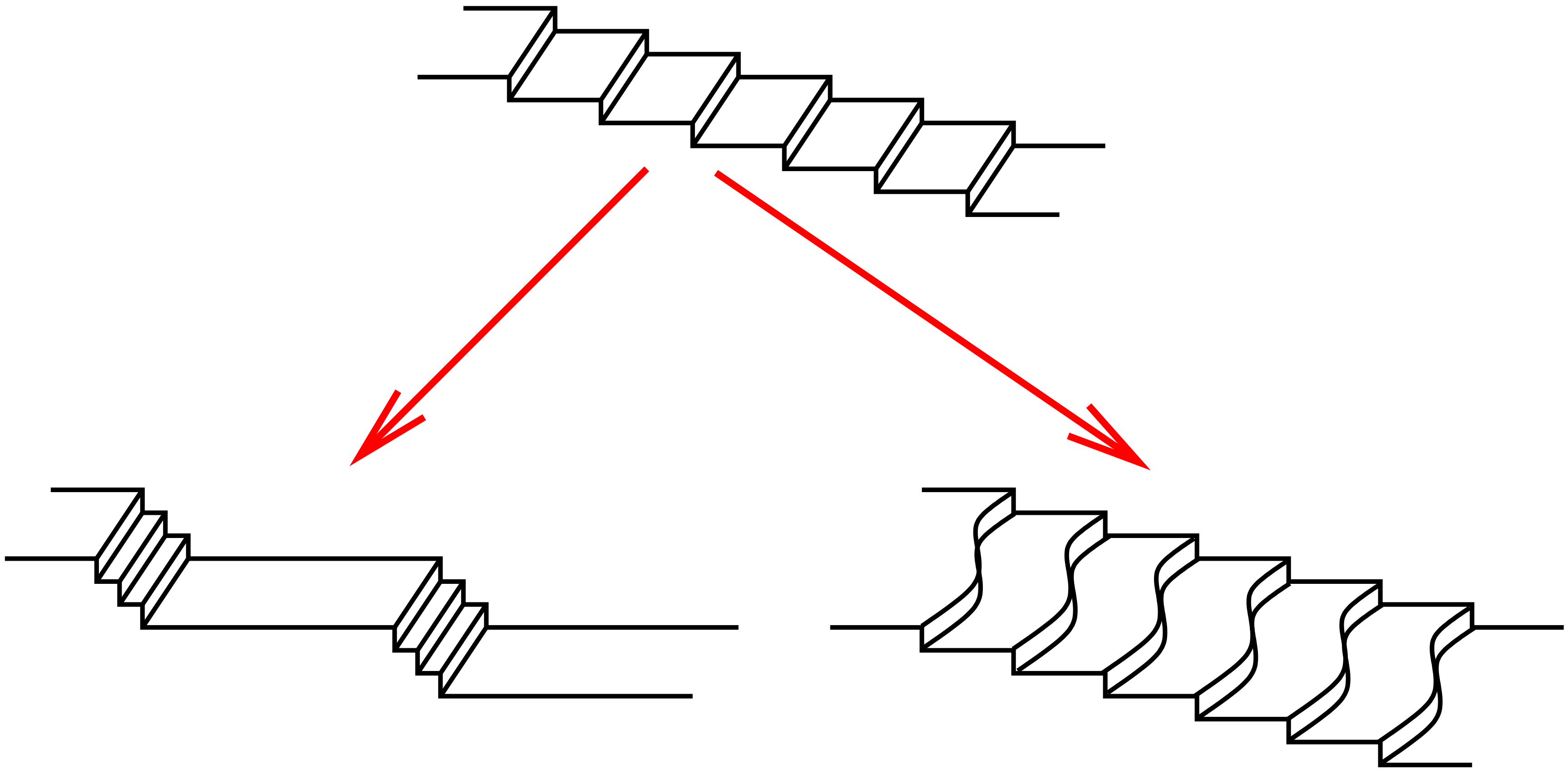
Condensation and coarsening of step bunches



- Step bunching instability of vicinal surfaces
- A minimal stochastic model (F. Slanina, M. Kotrla)
- Misanthropes, urns and worms (E.K.O. Hellén)
- Realistic step-step interactions (V. Popkov)

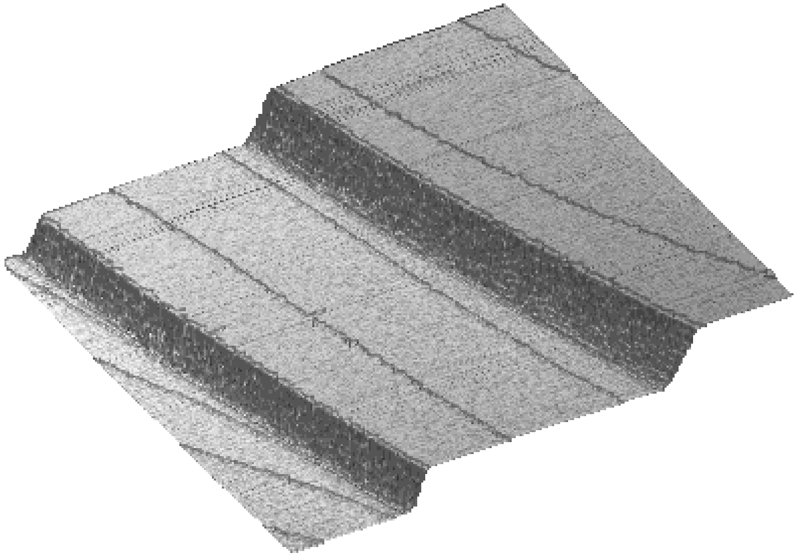
Nonequilibrium instabilities of vicinal surfaces

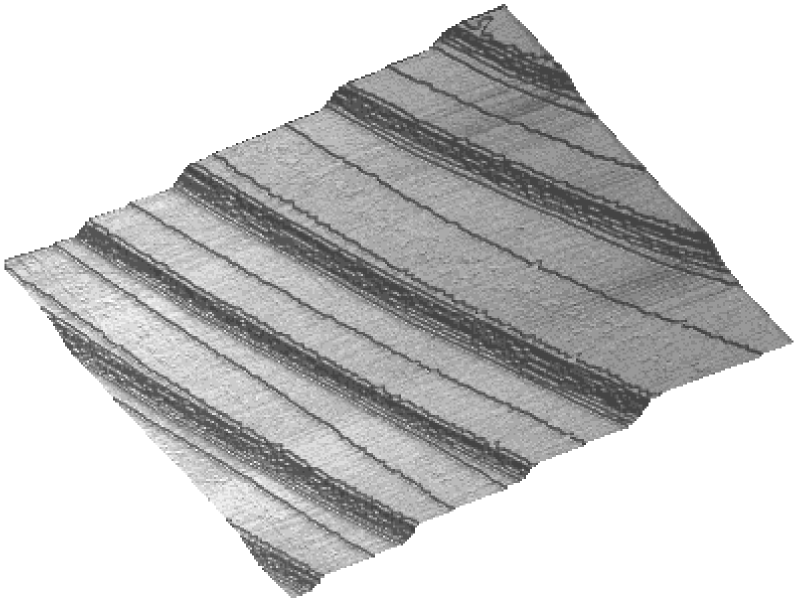


step bunching

step meandering

Electromigration-induced step bunches on Si(111)



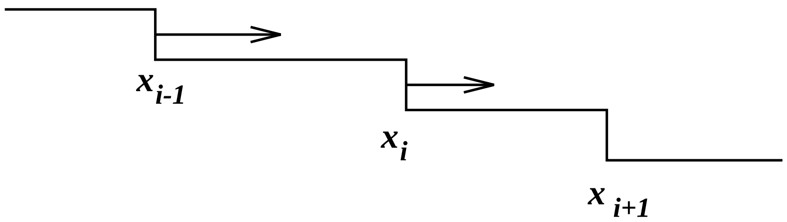


Courtesy of E.D. Williams, University of Maryland

Stability of step trains during growth

- evolution of straight steps:

$$\frac{dx_j}{dt} = f_+(x_{j+1} - x_j) + f_-(x_j - x_{j-1})$$



$f_\pm(x)$: flux from lower/upper terrace

- homogeneous step train: $x_j^{(0)} = [f_+(l) + f_-(l)]t + jl$ l: mean step spacing

  linear stability analysis: $x_j(t) = x_j^{(0)} + \varepsilon_j(t) \quad \Rightarrow \quad \varepsilon_j(t) \sim e^{i\phi j + \omega t}$ with

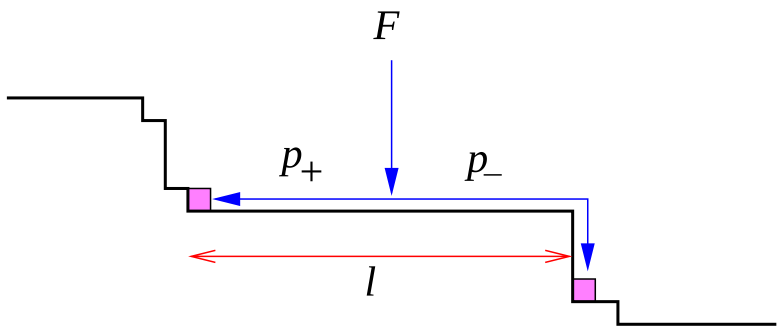
$$\mathscr{R}(\omega(\phi)) = -(1 - \cos\phi)[f'_+(l) - f'_-(l)]$$

  $\Rightarrow$ step train is stable iff $f'_+(l) - f'_-(l) > 0$

- step bunching during growth requires preferential attachment from the **upper** terrace

A minimal stochastic model with hard core step repulsion

F. Slanina, JK, M. Kotrla, PRE **71**, 041605 (2005)



$$p_{\pm}(l) = \frac{1}{2}\frac{(1 \pm b + dl)}{(1+dl)}$$

b: attachment asymmetry

d: inverse kinetic length

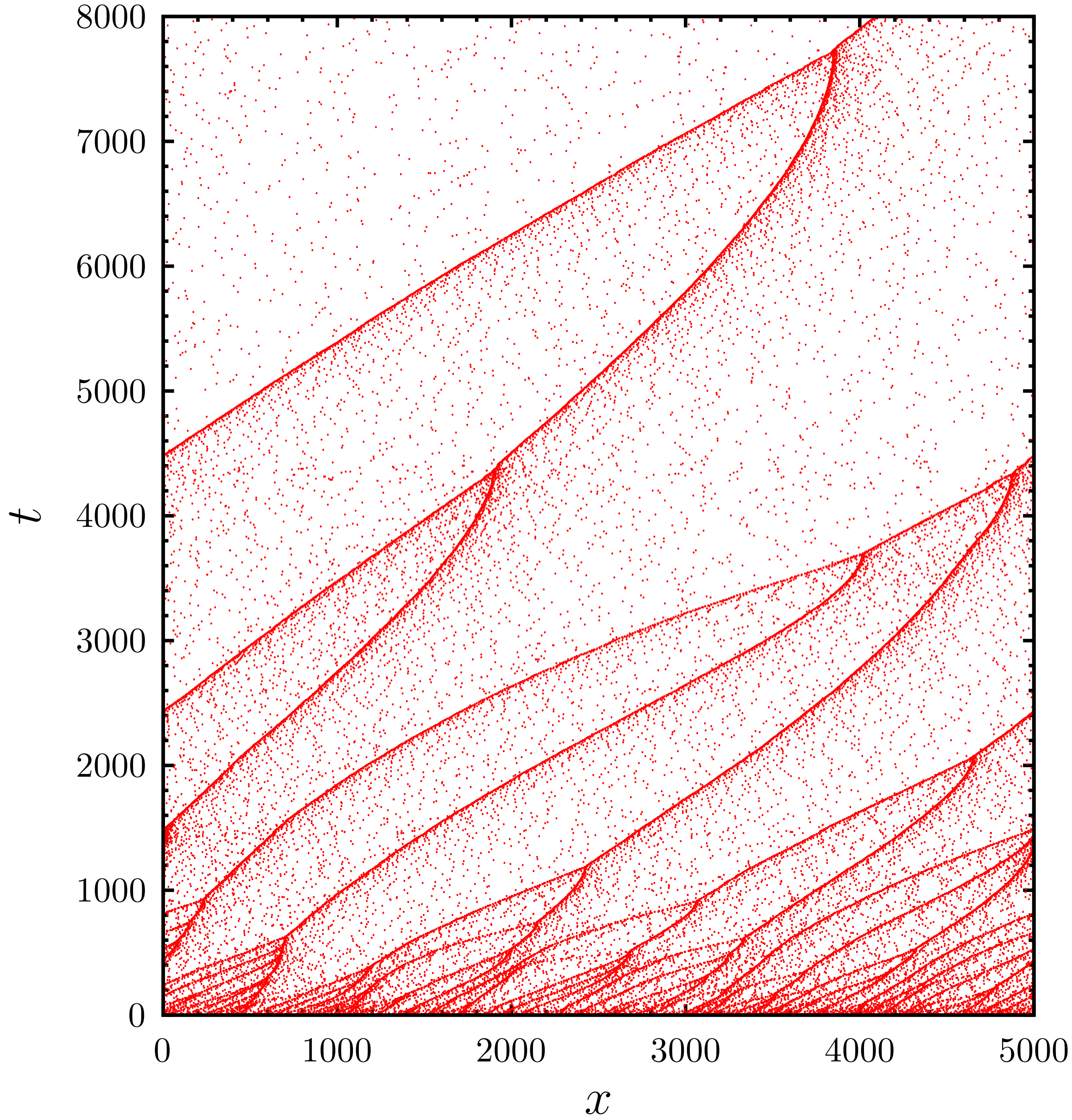
- Microscopic picture: Deposited atoms with concentration $n(x)$ diffuse along the terrace and attach to the ascending (descending) step at rate k_+ (k_-):

$$D\frac{d^2n}{dx^2} + F = 0, \quad D\frac{dn}{dx}|_{x=0,l} = \pm k_{\pm} n|_{x=0,l}$$

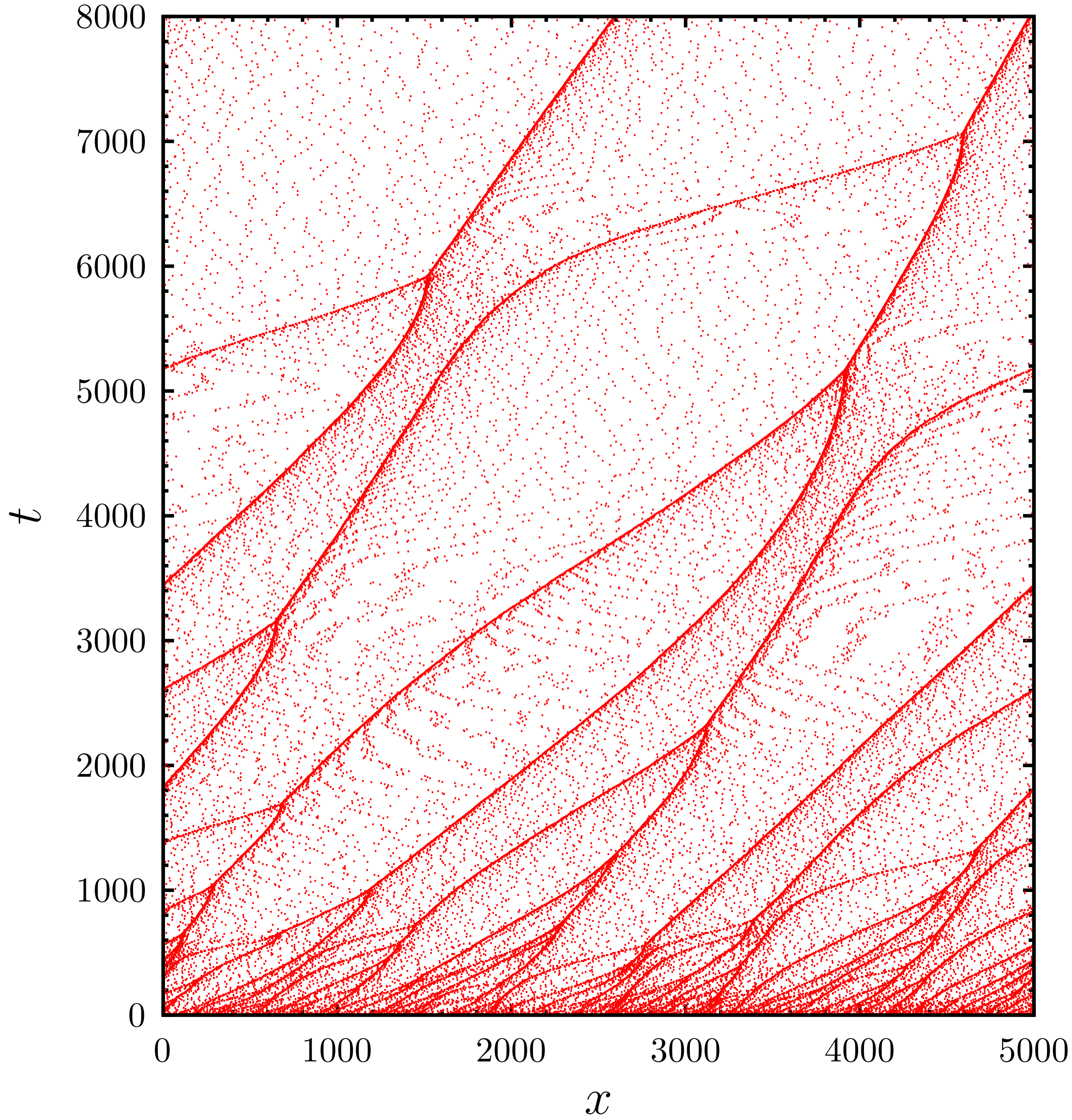
$$\Rightarrow \quad b = \frac{k_+ - k_-}{k_+ + k_-}, \quad d = \frac{1}{D/k_+ + D/k_-}$$

- Step bunching occurs for $b < 0$

Coarsening for $d = 0$



Coarsening for $d > 0$



Coarsening laws

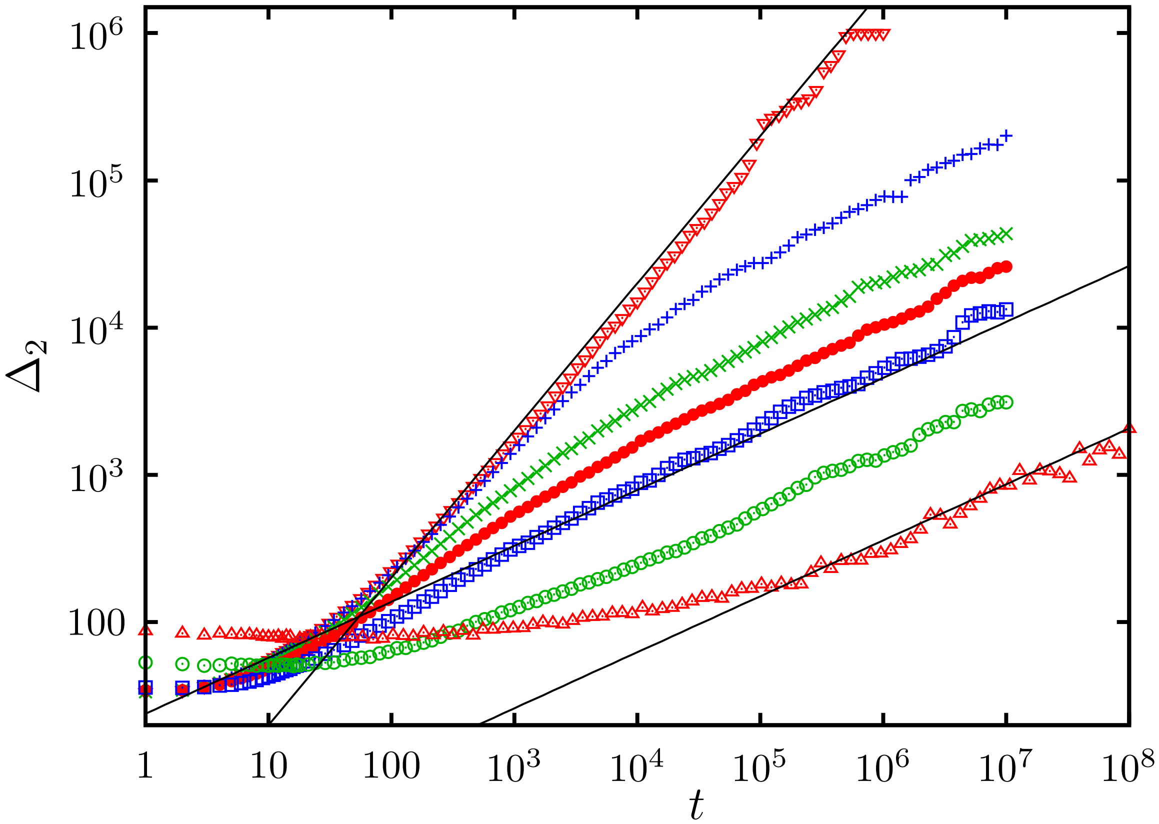
- coarsening measure: $\Delta_2 = L^{-1}\sum_i (X_i - X_{i-1})^2$ L: system length
  X_i: positions of bunches containing at least 2 steps

- attachment-limited:
  $(d = 0)$

  $\Delta_2 \sim t$

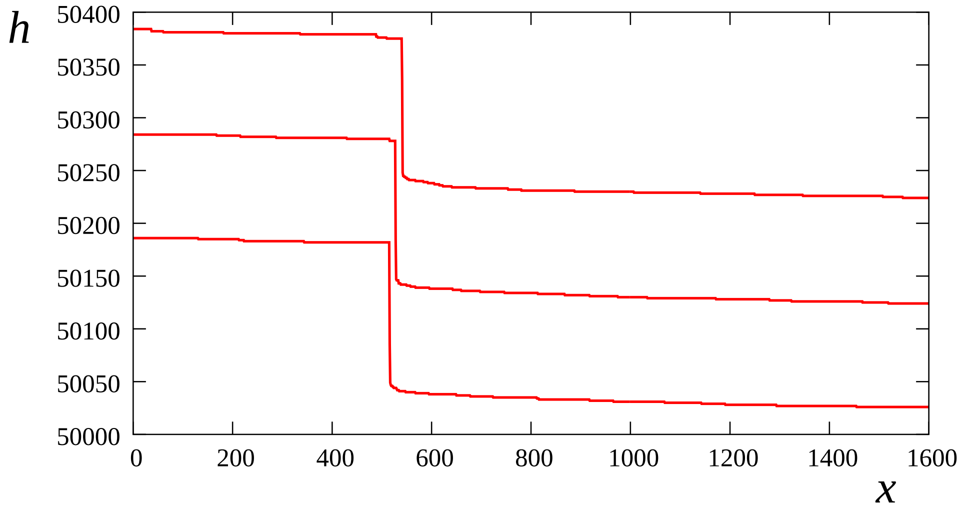
- diffusion-limited:
  $(d > 0)$

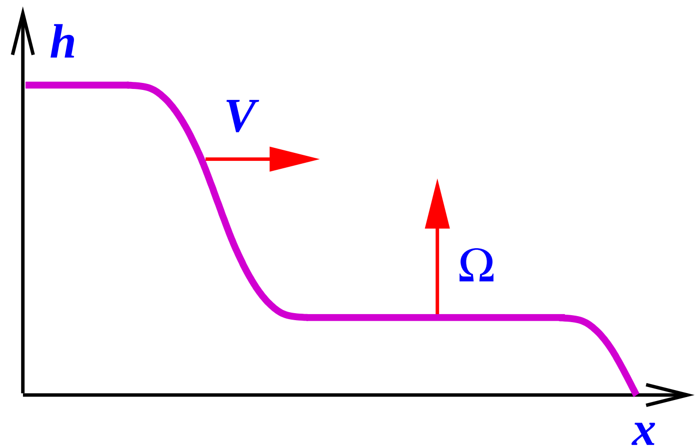
  $\Delta_2 \sim t^{0.38}$



$b = -0.9,\ d = 0, 10^{-4}, 10^{-3}, 3\times 10^{-3}, 0.01, 0.1, 1$

Stationary bunches for $d = 0$





$b = -0.1, d = 0$

- Stationary traveling bunch: $h(x,t) = f(x - Vt) + \Omega t$ with $\Omega + m_0 V = F$

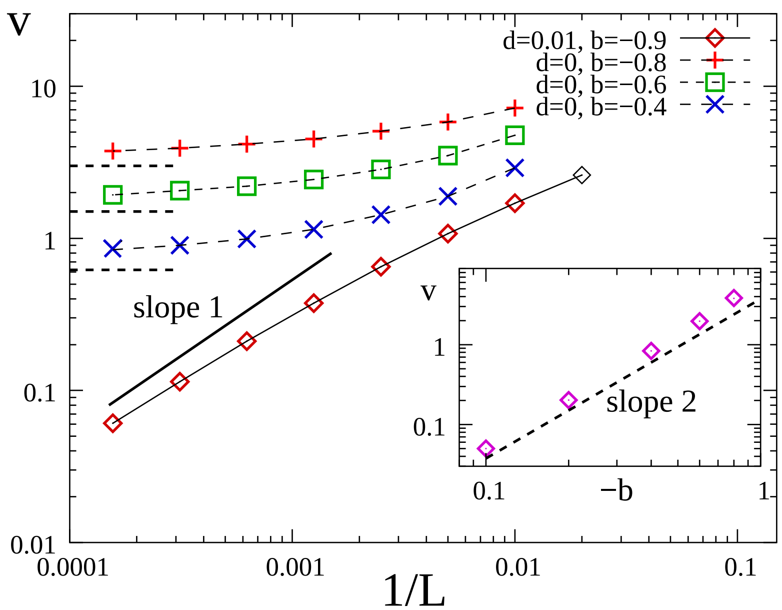
- Dynamics of mean terrace lengths:

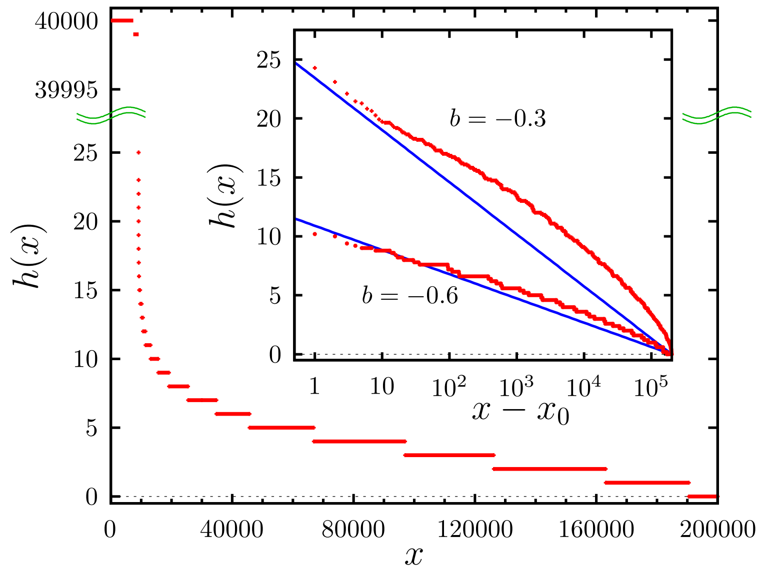
$$\frac{d\langle l_i \rangle}{dt} = \frac{1}{2}(1+b)\langle l_{i+1} \rangle - \frac{1}{2}(1-b)\langle l_{i-1} \rangle - b\langle l_i \rangle$$

- Ansatz: $\langle l_i \rangle = e^{Q(i+\Omega t)}$ $\Rightarrow$ $\Omega Q = \sinh(Q) + |b|[1 - \cosh(Q)]$

- Dynamics selects **minimal** value of Ω $\Rightarrow$ **maximal** value of V

- Strong finite size effects in V due to fluctuation effects?





- Stationary height profile: $h(x_0)-h(x)=Q^{-1}\ln(x-x_0)$ x_0: bunch position

- Lateral bunch speed **vanishes** asymptotically when $d>0$

Bunch speed and bunch coarsening

A.A. Chernov, Sov. Phys. Usp. **4**, 116 (1961)

- Power law relation between lateral bunch speed V and bunch spacing L:

$$V \sim L^{-\nu}$$

- Typical time between coalesence events: $t^* \sim L/V \sim L^{1+\nu}$

$$\Rightarrow \quad L \sim t^{\beta} \quad \text{with} \quad \beta = \frac{1}{1+\nu}$$

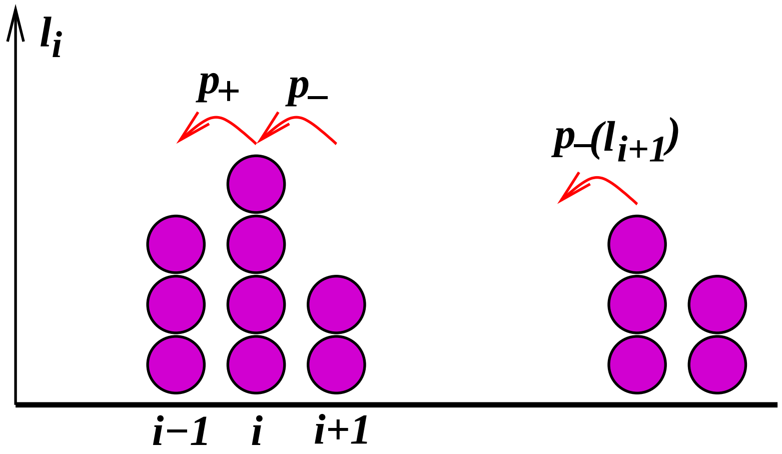
- $d = 0 \quad \Rightarrow \nu = 0, \quad \beta = 1$

- $d > 0 \quad \Rightarrow \beta \approx 0.38, \quad \nu \approx 1.6$ **????**

- In the presence of realistic step-step interactions generically $\nu = 1$ and $\beta = 1/2$

V. Popkov, J.K., Europhys. Lett. **72**, 1025 (2005)

Terrace dynamics as a particle system



- $b = 1, p_- = 0$: ZRP with rate $p_+(l) = l \Rightarrow$ stationary Poisson distribution

  J.K., M. Schimschak, J. Phys. I **5**, 1065 (1995)

- In general, rate depends on departure site **and target site**

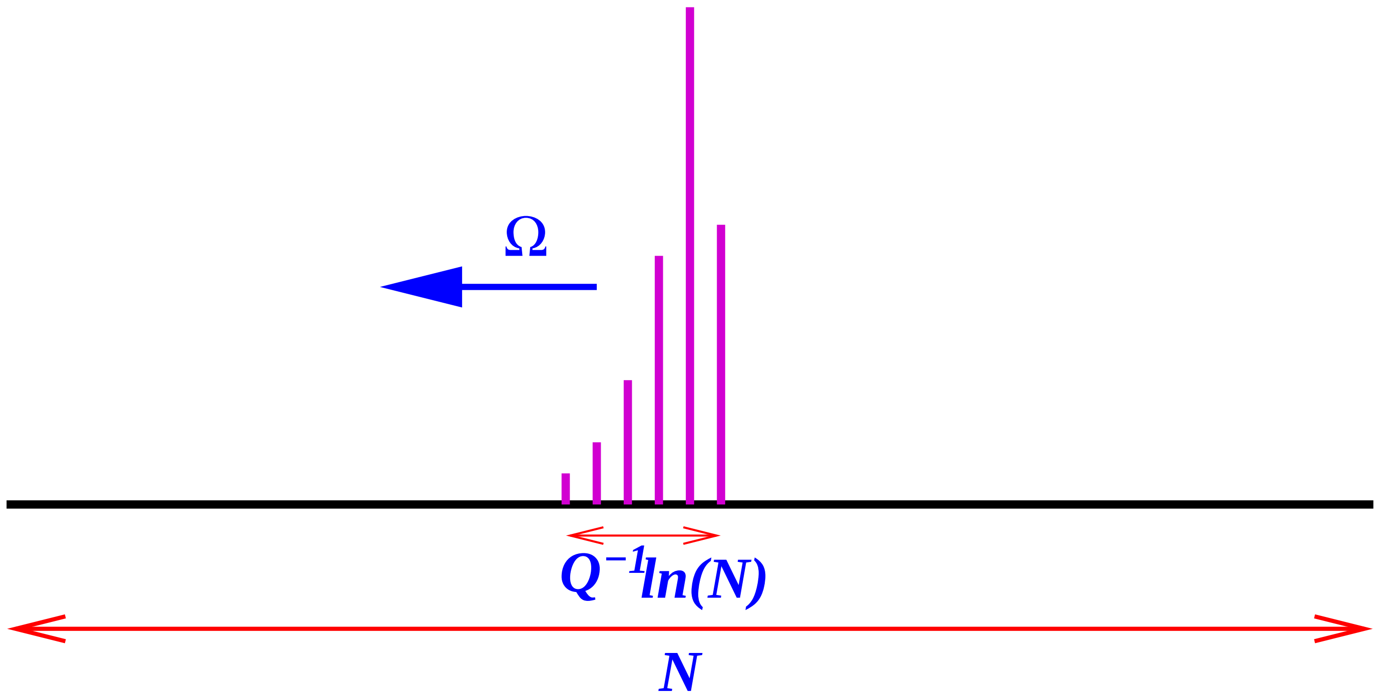
  $\Rightarrow$ misanthrope-like process

- In the presence of empty sites dynamics becomes **nonlocal**

- Edwards-Wilkinson universality class for any $b > 0$

- Conserved KPZ-behavior for $b = 0$

The step bunch as a condensate



- Velocity selection analogous to "pulled fronts"?

  W. van Saarloos, Phys. Rep. **386**, 29 (2003)

- Is the nonlocal interaction between the front and back end of the bunch important?

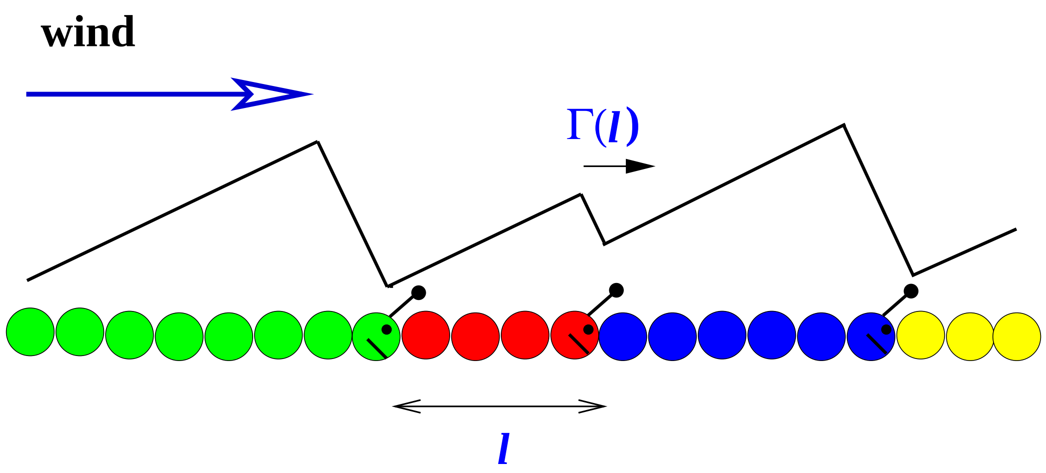
Mass transfer models for sand ripples

E.K.O. Hellén, J.K., Phys. Rev. E **66**, 011304 (2002)

- Misanthrope process with rate $\Gamma(l_i)$ depending only on mass l_i at target site: Site i **robs** mass from its neighbor(s)

- $\Gamma(l) = 1/l$: Worm model

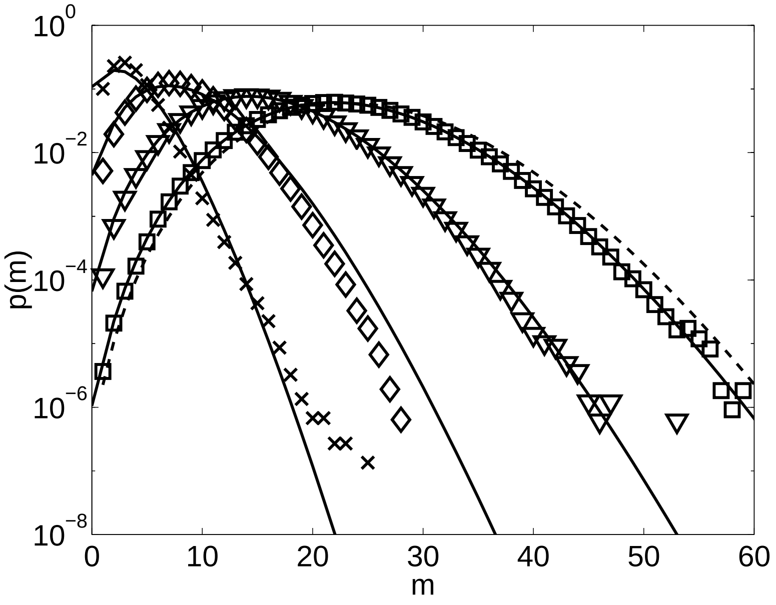
B.T. Werner, D.T. Gillespie, PRL **71**, 3230 (1993)



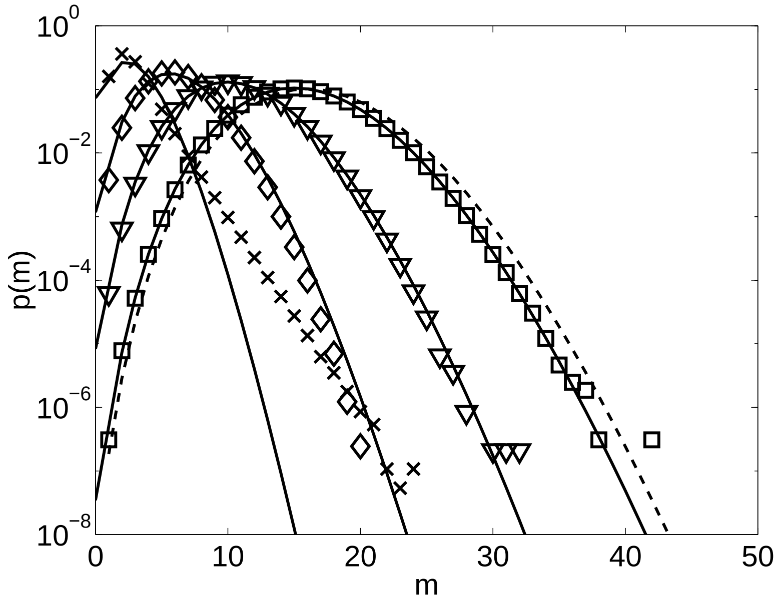
- Empty sites are eliminated $\Rightarrow$ merging of ripples

- Logarithmic coarsening for $\Gamma(l) \sim l^{\gamma}$, $\gamma < 0$

- Power-law coarsening $\sim t^{1/(1-\gamma)}$ for $0 < \gamma < 1$ and $\sim t^{1/2}$ for $\gamma = 0$
- Exponential coarsening for $\Gamma(l) \sim l$
- Approximate product measure is established when merging events are rare $(\gamma < 0)$



$\gamma = -0.5$



$\gamma = -1$

Realistic step-step interactions

- Real steps repel each other via long-ranged entropic and elastic interactions

- Minimal description of the dynamics of straight steps:

$$\frac{dx_i}{dt} = \frac{1+b}{2}(x_{i+1} - x_i) + \frac{1-b}{2}(x_i - x_{i-1}) + U(2f_i - f_{i-1} - f_{i+1})$$

$$f_i = (x_i - x_{i-1})^{-3} - (x_{i+1} - x_i)^{-3}$$

- Interplay between destabilizing fluxes and stabilizing interactions leads to rich scaling behavior of bunches
  J.K., V. Tonchev, S. Stoyanov, A. Pimpinelli, Phys. Rev. B **71**, 045412 (2005)

- Hydrodynamic description works well for $0 > b > -1$
  V. Popkov, J.K., Europhys. Lett. **72**, 1025 (2005)

- Dynamic phase transition at $b = -1$ V. Popkov, J. K., cond-mat/0602216

Conclusions

- Vicinal surfaces provide a conceptually simple yet rich & experimentally accessible arena for nonequilibrium dynamics $\Rightarrow$ **“Experimental statistical mechanics”** (Ellen D. Williams)

- Step bunching as a condensation-like phenomenon with possibly nontrivial coarsening exponents

- Mechanism of bunch velocity selection may be related to front propagation into unstable states

- New examples of misanthrope-like processes with additional features (nonlocality or extinction of sites)

A vicinal poem

Lord Yarborough’s Defence

The land
in question,
by the slow, gradual
and imperceptible projection,
alluvion, subsidence, and accretion
of ooze, soil, sand, and other matter, being
slowly, gradually, and by imperceptible increase,
in a long time cast up, deposited, and settled by and from
the flux and reflux of the tide and water of the sea in upon and against
the outside and extremity of the demesne lands of the manor, hath been formed,
and hath been settled grown and accrued upon against and unto the said demesne land.

Lavinia Greenlaw