Simulation of surface growth and lattices gases using GPUs

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Abstract

Restricted solid on solid surface growth models can be mapped onto binary lattice gases. We show that efficient simulation algorithms can be realized on GPUs either by CUDA or by OpenCL programming. We consider a deposition/evaporation model following Kardar–Parisi–Zhang growth in 1+1 dimensions related to the Asymmetric Simple Exclusion Process and show that for sizes, that fit into the shared memory of GPUs one can achieve the maximum parallelization speedup (~100 for a Quadro FX 5800 graphics card with respect to a single CPU of 2.67 GHz). This permits us to study the effect of quenched, columnar disorder, requiring extremely long simulation times. We compare the CUDA realization with an OpenCL implementation designed for processor clusters via MPI. A two-lane traffic model with randomized turning points is also realized and the dynamical behavior has been investigated. Doing extremely large scale (2^{17} x 2^{17}) simulations in 2+1 dimensions we uncover surface growth and aging behavior, proving the lack of fluctuation – dissipation relation.

The Kardar-Parisi-Zhang (KPZ) equation:

$$\partial_t h(\boldsymbol{x},t) = \nu + \sigma\nabla^2 h(\boldsymbol{x},t) + \lambda\big(\nabla h(\boldsymbol{x},t)\big)^2 + \eta(\boldsymbol{x},t)$$

- ν, λ the amplitudes of the mean and local growth velocity
- σ is a smoothing surface tension coefficient
- η roughens the surface by a zero-average Gaussian noise field

Surface width:

$$W(L,t) = \left[\frac{1}{L}\sum_{x=1}^{L} h_x^2(t) - \left(\frac{1}{L}\sum_{x=1}^{L} h_x(t)\right)^2\right]^{1/2}$$

Family-Vicsek scaling:

$$W(L,t) \propto t^{\beta}, \quad t_0 \ll t \ll t_s$$
$$\propto t^{\alpha}, \quad t \ll t_s$$

- α – roughness exponent
- β – surface growth exponent

Two-point functions

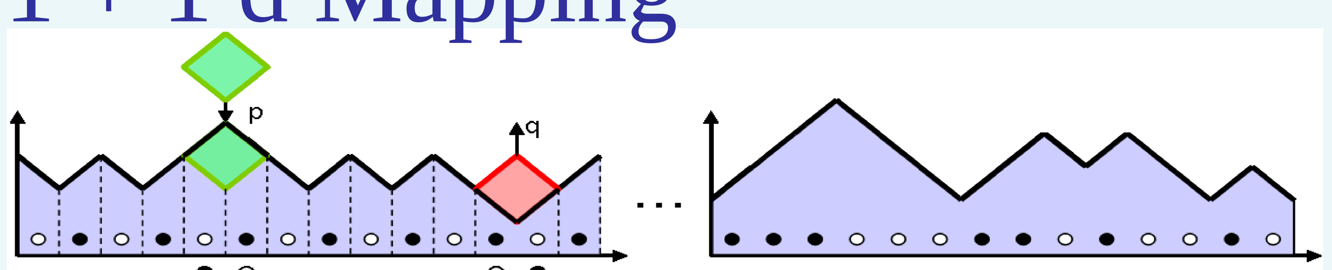
Auto-correlation

$$C(t,s) = \langle\phi(t)\phi(s)\rangle - \langle\phi(t)\rangle\langle\phi(s)\rangle = s^{-b} f_C\left(\frac{t}{s}\right) \quad \sim (t/s)^{-\lambda_C/z}$$

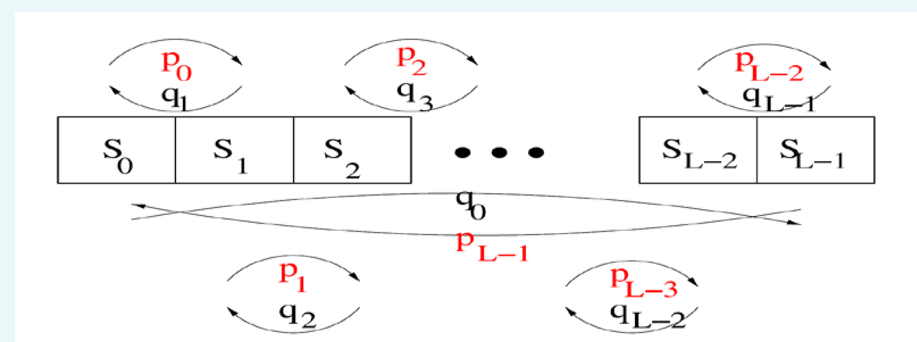
Auto-response

$$R(t,s) = \left.\frac{\delta\langle\phi(t)\rangle}{\delta j(s)}\right|_{j=0} = \left\langle\phi(t)\widetilde{\phi}(s)\right\rangle = s^{-1-\tilde{a}} f_R\left(\frac{t}{s}\right) \quad \sim (t/s)^{-\lambda_R/z}$$

1 + 1 d Mapping

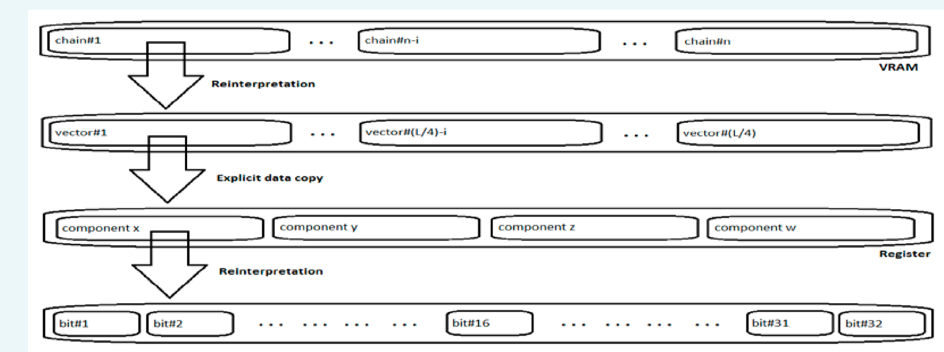


Mapping of the 1+1 dimensional surface growth onto the 1d **ASEP** model. Surface attachment (with probability ***p***) and detachment (with probability ***q***) corresponds to anisotropic diffusion of particles (bullets) along the 1d base space (M. Plischke, et. al, Phys. Rev. B 35, 3485 (1987))



The CUDA algorithm paralellizes the iterations by subdividing the lattice into groups of 2 sites. Odd and even steps use different groupings.

Furthermore, to allow lattices of nearly arbitrarily large sizes (compared to reasonable 1d sizes), and accelerating the algorithm, bit-level coding is used allowing for higher throughput of processing.



Although speed is lost regarding that bit masks or bit shifts are needed even to access data, higher cache hit ratio of reduced datasize results in overall speed-up.

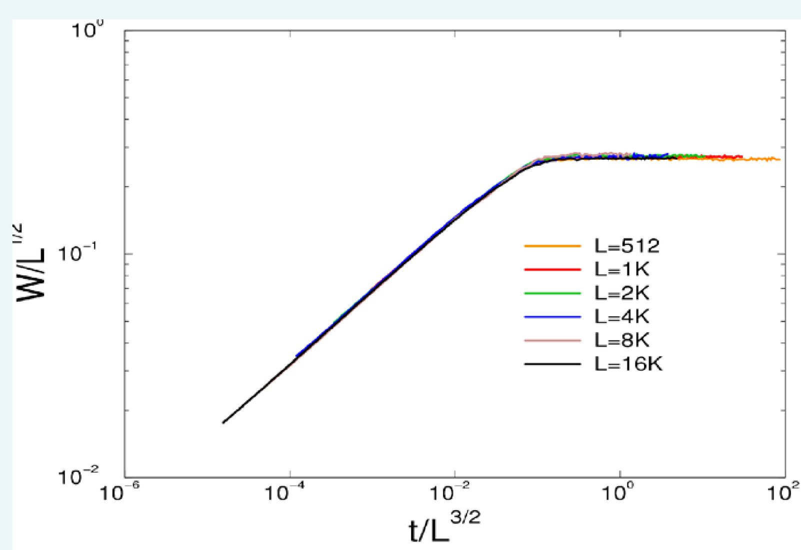
Pure, parallel update dynamics

- Up-down asymmetry

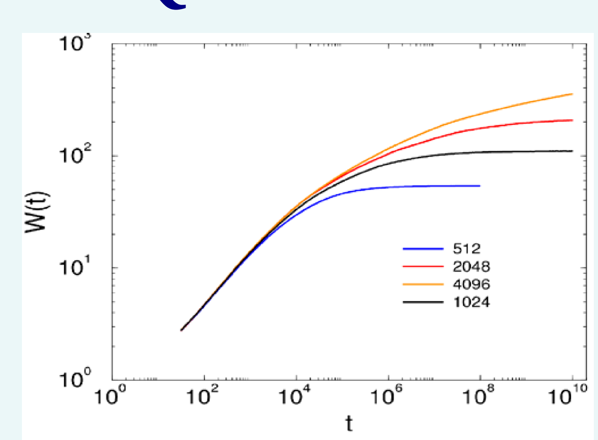
Kardar-Parisi-Zhang universality class scaling exponents:

α = ½, β = 1/3, z = α / β = 3/2

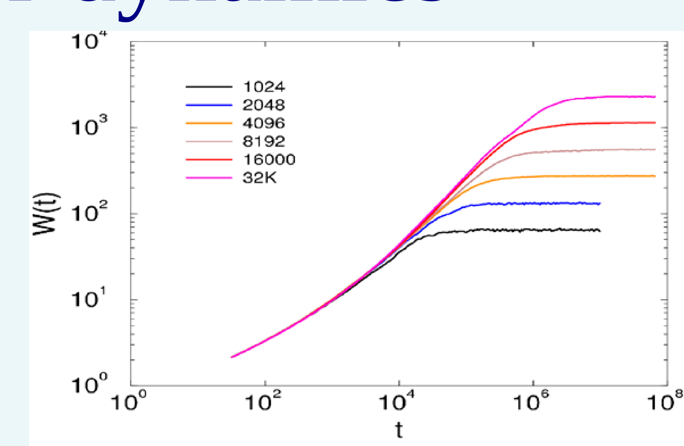
numerical agreement with the literature



Quenched disorder dynamics

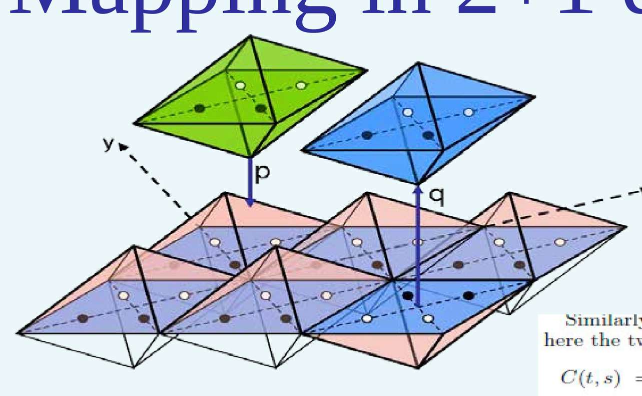


Left-right symmetric: PASEP



Left-right asymmetric: TASEP

Mapping in 2+1 dim.

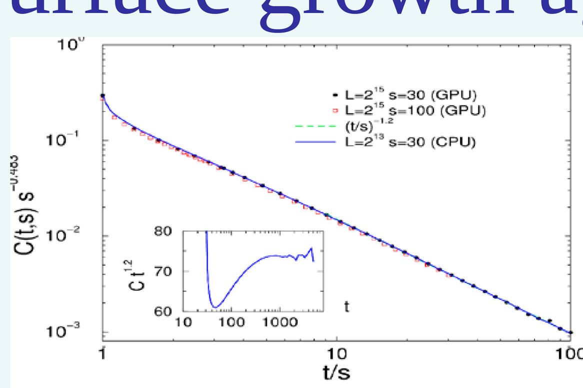


Similarly to the one-dimensional case we considered here the two-time temporal correlator

$$\begin{aligned} C(t,s) &= \langle (h(t;\vec{r}) - \langle\overline{h}(t;\vec{r})\rangle)\,(h(s;\vec{r}) - \langle\overline{h};\vec{r}(s)\rangle)\rangle \\ &= \langle h(t;\vec{r})h(s;\vec{r})\rangle - \langle\overline{h}(t;\vec{r})\rangle\langle\overline{h}(s;\vec{r})\rangle \\ &= s^{-b}F_C\left(\frac{t}{s}\right), \end{aligned} \tag{8}$$

were ⟨⟩ denotes averaging for sites and independent runs.

Surface growth aging



a	b	λ_R	λ_C	β	α
0.30(1)	−0.483(2)	2.03(1)	1.95(1)	0.2415(15)	0.393(4)

TABLE I: Scaling exponents of the $d = 2+1$ dimensional KPZ class.

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