Felületnövekedési és rácsgáz modellek hatékony szimulációja GPU-val

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Kardar-Parisi-Zhang (KPZ) equation

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

σ : (smoothing) surface tension coefficient
λ : anisotropy, local growth velocity
η : roughens the surface by a zero-average Gaussian noise field:

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

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

Characterization of surface growth:

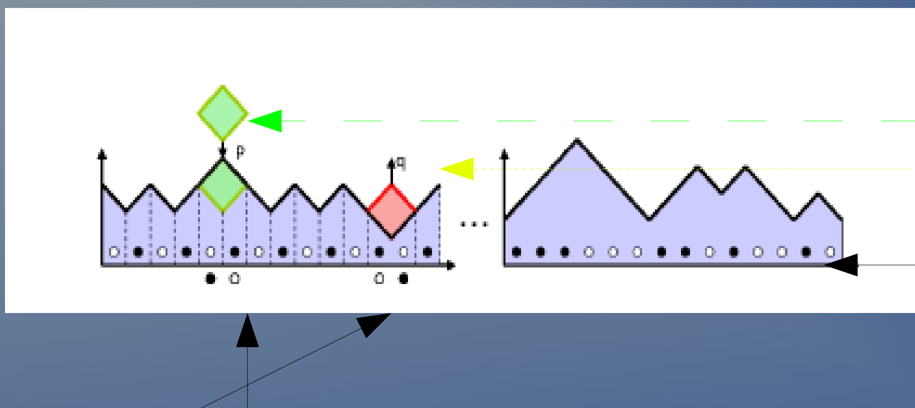
Width:

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

Family-Vicsek scaling:

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

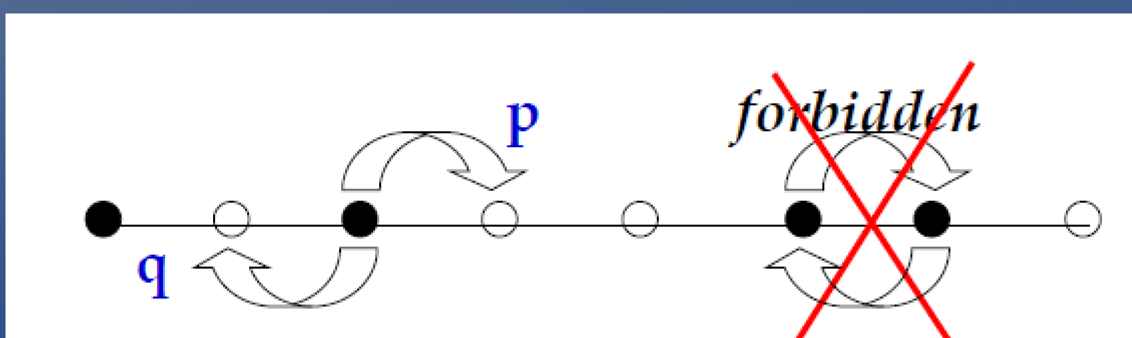
Mappings of KPZ onto lattice gas system in *1d*



'Kawasaki' exchange of particles

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

Attachment (with prob. ***p***) and Detachment (with prob. ***q***) -> Anisotropic diffusion of particles (**bullets**) along the *1d* base space (*M. Plischke, Rácz and Liu, PRB 35, 3485 (1987)*)

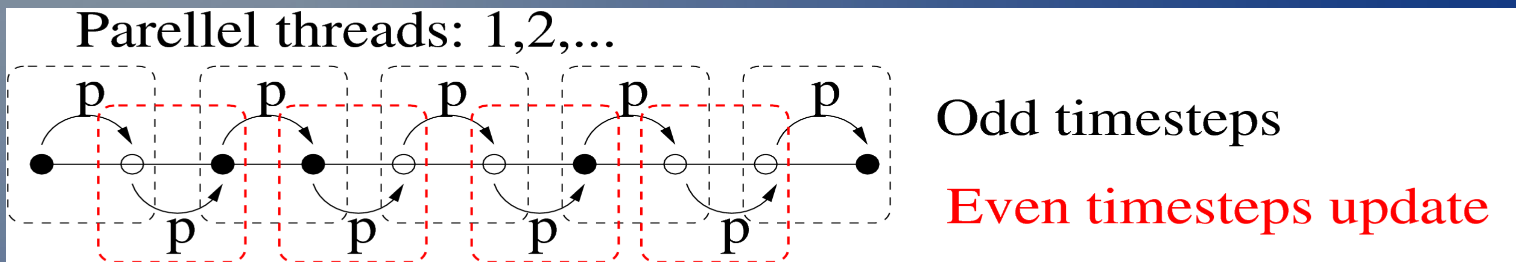


The simple ***ASEP*** (Ligget '95) is an exactly solved lattice gas

Many features (response to disorder, different boundary conditions ...) are known.

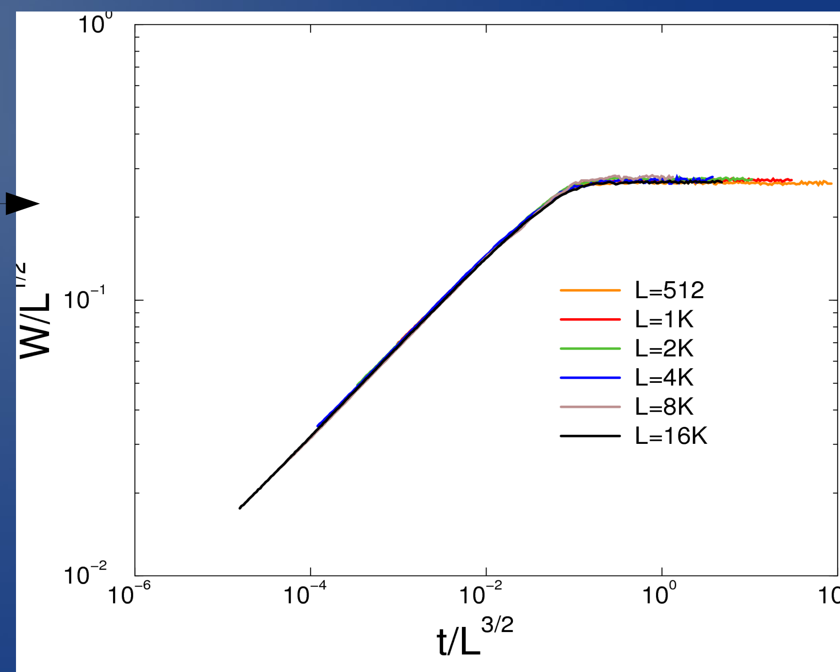
Test of parallel update algorithms for 1d ASEP/KPZ

Parallel updates on a ring of size *L*:



with probability *p* (reverse with *q*)

Scaling by the serial C and CUDA*:*
Agreement with 1d KPZ scaling



L< 64K programs fit into shared memory of multiprocessor blocks

→ **no communication losses,**

maximal speedup & scaling:

240 cores ~ **100 x** of a CPU (2.8 GHz)

The hardware

- Local supercomputer thanks to NVIDIA Professor Partnership:

  4 x Quadro FX 5800 GPUs
  960 cores, 16 GB dev. Mem.

  ~ 4 Teraflops theoretically

- For comparison the recently installed supercomputer in Győr ~ 3.3 Teraflops for 50 Million HUF !

Details of the CUDA code

- Independent random sequence by intelligent striding of *drand48()* LCRG by -> ***gpu-rng*** (GNU) cycle length > 2^{1024}

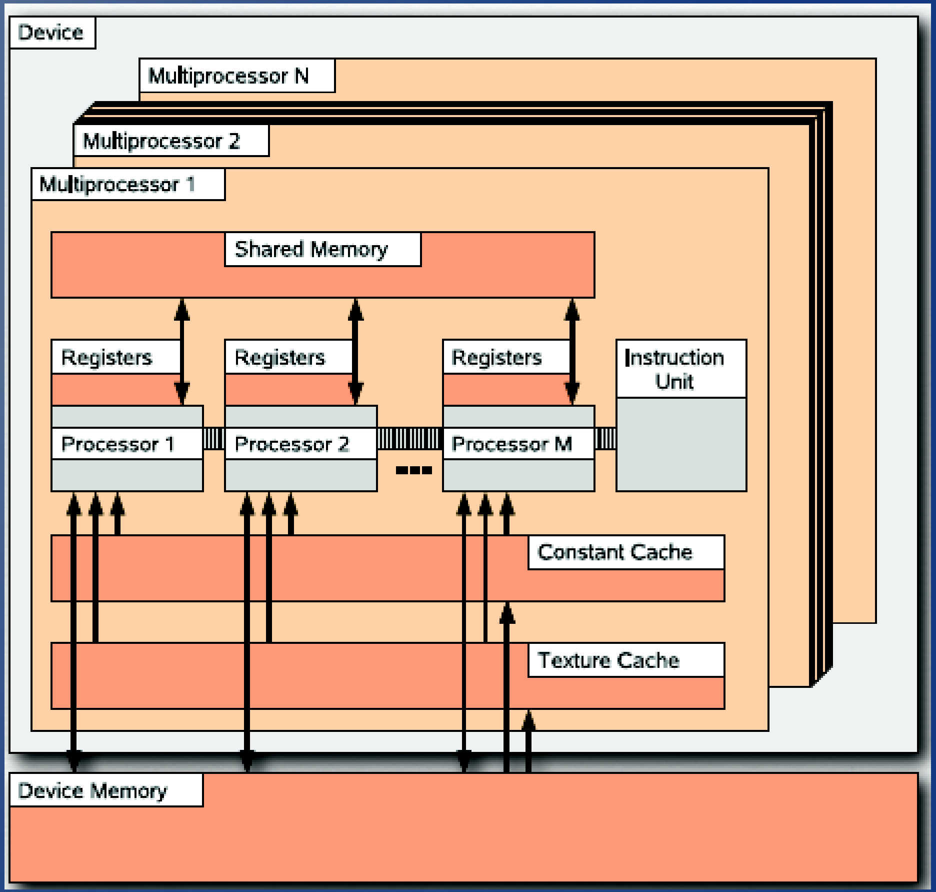
- Start from half filled initial state.

- Sampling of width:

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

by reconstructing heights from local derivatives (0/1) at times:

$$t_{i+1} = t_i * 1.05 \quad \text{if} \quad i \neq 0\,, \quad t_0 = 30$$



General OpenCL code

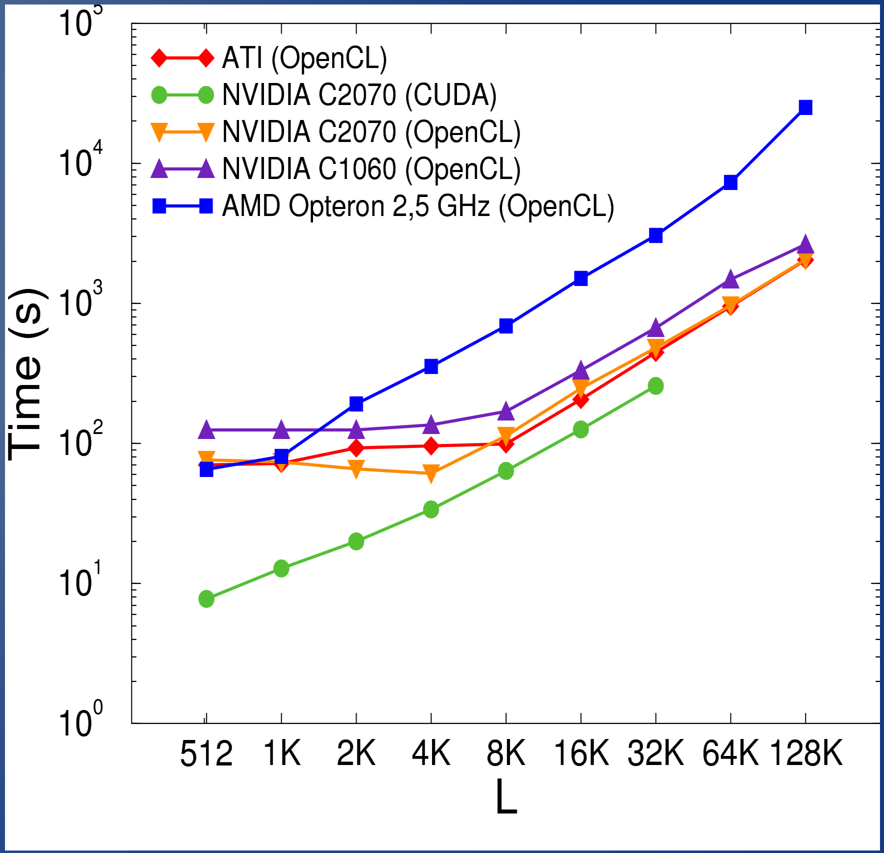
- Portable for “any” parallel computers

  Tested for TASEP (KPZ) on ATI, NVIDIA, CPU clusters

- Multi-GPU program using **M**essage **P**assing **I**nterface

- No size limitation by shared memory

- For larger system its speed is comparable to CUDA's



Disordered model (Q-TASEP)

- Site-wise binary quenched disorder

$$P(p_i) = (1-D)\delta(p_i - p) + D\delta(p_i - rp)$$

- Corresponds to KPZ + columnar disorder:

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

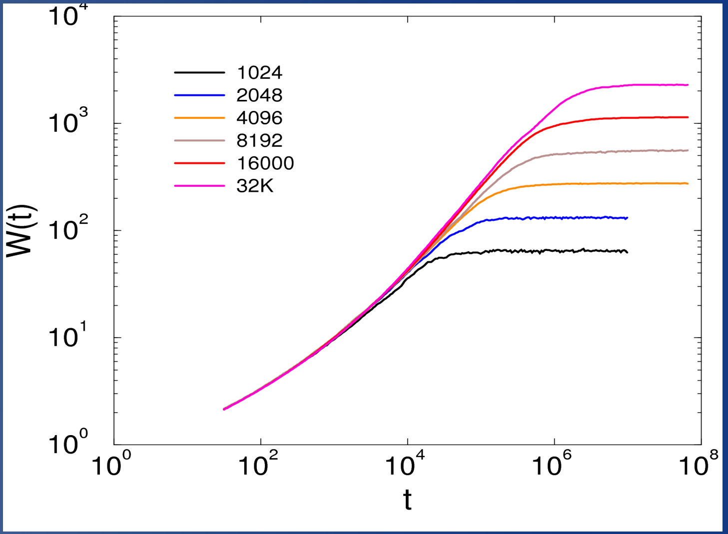
- Q-TASEP: p_i=0.8 or 0.2, q_i=0

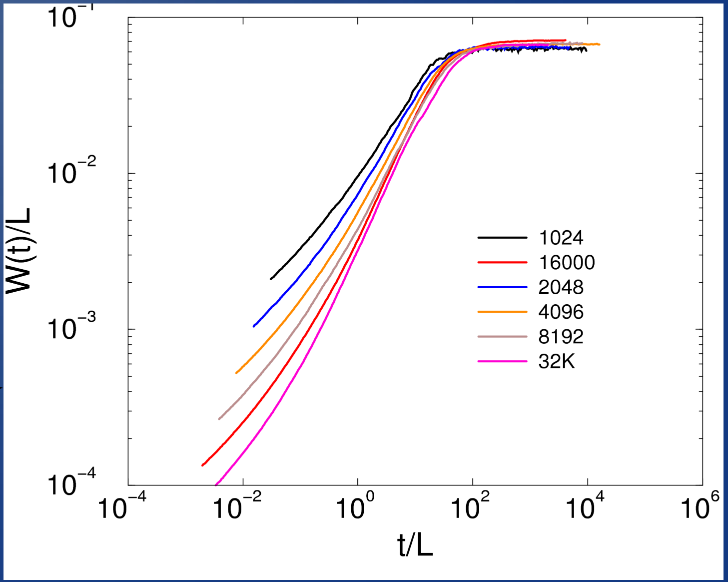
  L=1024, 2048,....14000

  t_{max} *= 10⁸ MCs*

- *Studied by Krug et al. 1999, Stinchcombe et al. 2008*
- *Data collapse with* $\beta = \alpha$ *= z = 1 faster than KPZ !*
- *Logarithmic corrections :*

$$\xi(t) \propto \frac{t/t_0}{\ln(t/t_0)}$$

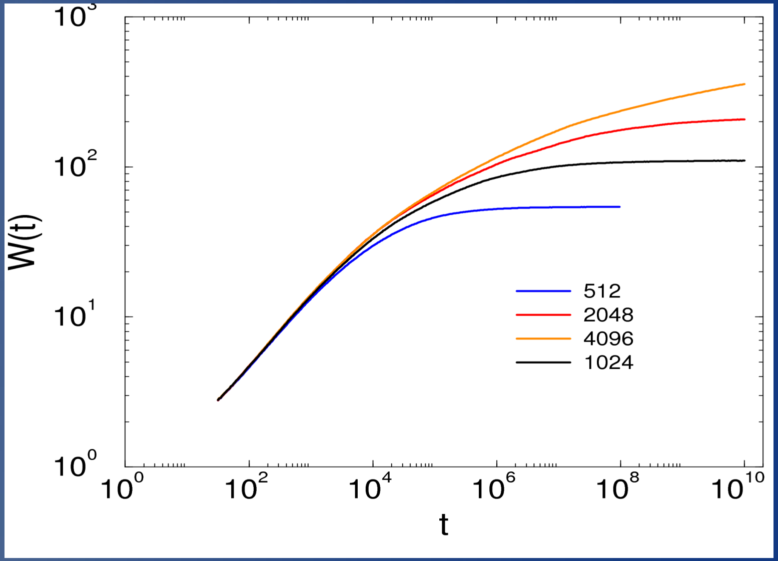




Disordered model (Q-SSEP)

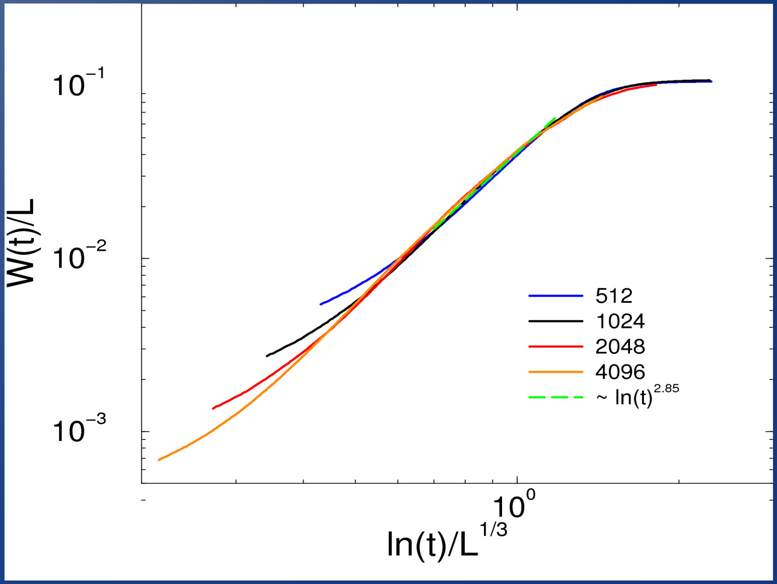
- Quenched disorder, left-right symmetry: p_i, q_i = *0.8 or 0.2*
- *Ultra-slow (log.) time dependences*

$$W(t,L) \propto \ln(t)^{\bar{\beta}}$$

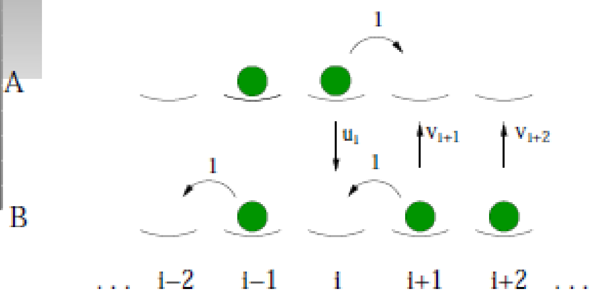


- Studied by *R. Juhász et al.* analytically (RG)
- Agreement, but due to wide distributions the typical values scale (ψ = *1/3*) differently than mean values (ψ = *½*)

$$\ln(\tau) \propto \xi^{\psi}$$



Bidirectional two-lane model



- single particle, homogeneous system: active diffusion (Klumpp & Lipowsky 2005)
- single particle in random environment
- many-particle system is qualitatively different from the disordered PASEP

Exploration of extremely slow (scaling) behavior: **Fits GPUs**

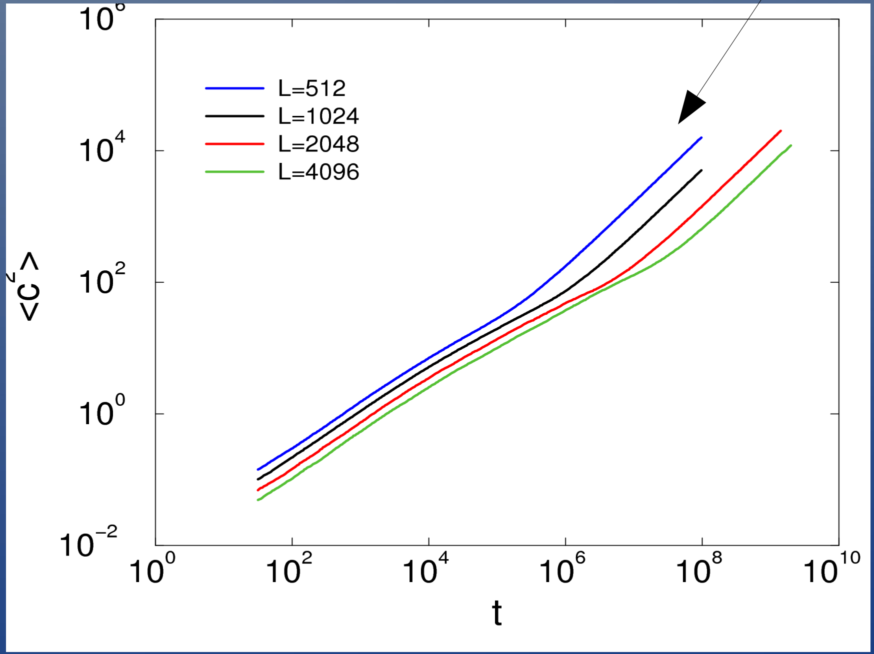
Two-lane PASEP

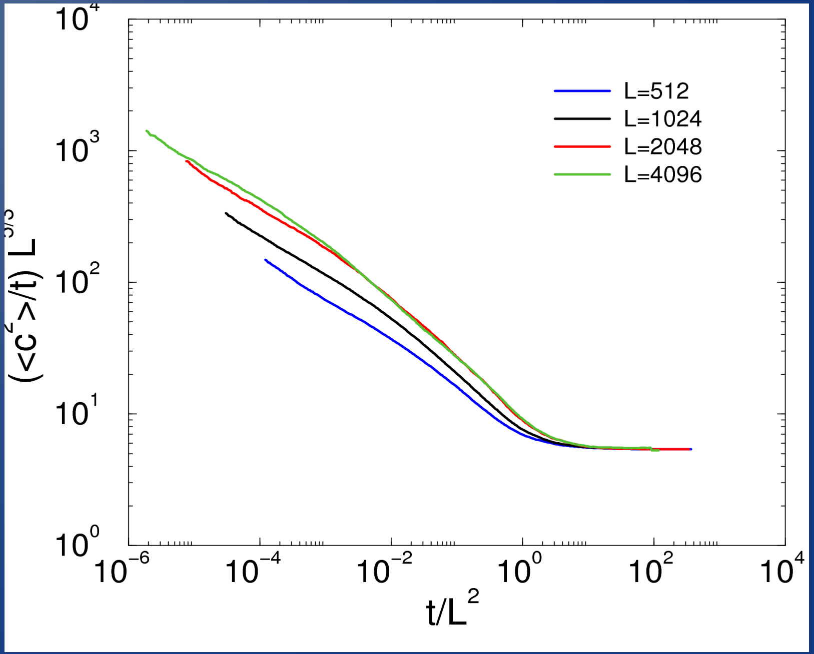
- Parallel SCA version of the original model checked by Robert: C code
- GPU version developed by Gergely and Géza for CUDA

1. Even-sub-lattice updates, with probabilities $p = 0.8$,
2. $A \to B$ lane-changes, with probabilities u_i,
3. Odd-sub-lattice updates, with probabilities $p = 0.8$,
4. Closing boundaries, with probabilities $p = 0.8$,
5. $B \to A$ lane-changes, with probabilities v_i.

- The total current (every exchange) is followed. $c = (J/L)^2$

In the steady state it's **fluctuation** becomes linear -> FSS, ***z=2 ?***





Mappings of KPZ growth in *2+1* dimensions

Generalized Kawasaki update:

$$\begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \rightleftharpoons \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}$$

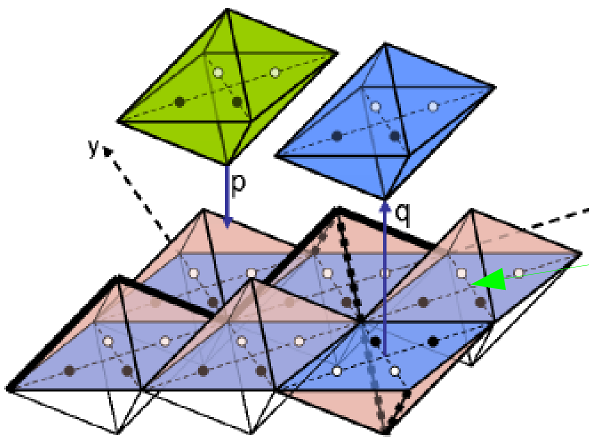


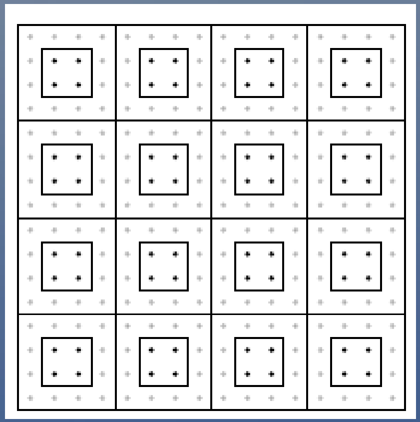
FIG. 2: (Color online) Mapping of the $2+1$ dimensional surface growth onto the $2d$ particle model (bullets). Surface attachment (with probability p) and detachment (with probability q) corresponds to Kawasaki exchanges of particles, or to anisotropic diffusion of dimers in the bisectrix direction of the x and y axes. The crossing points of dashed lines show the base sub-lattice to be updated. Thick solid/dashed lines on the surface show the x/y cross-sections, corresponding to the $1d$ model (Fig. 1.)

- **Octahedron model**
  Driven diffusive gas of pairs (dimers)

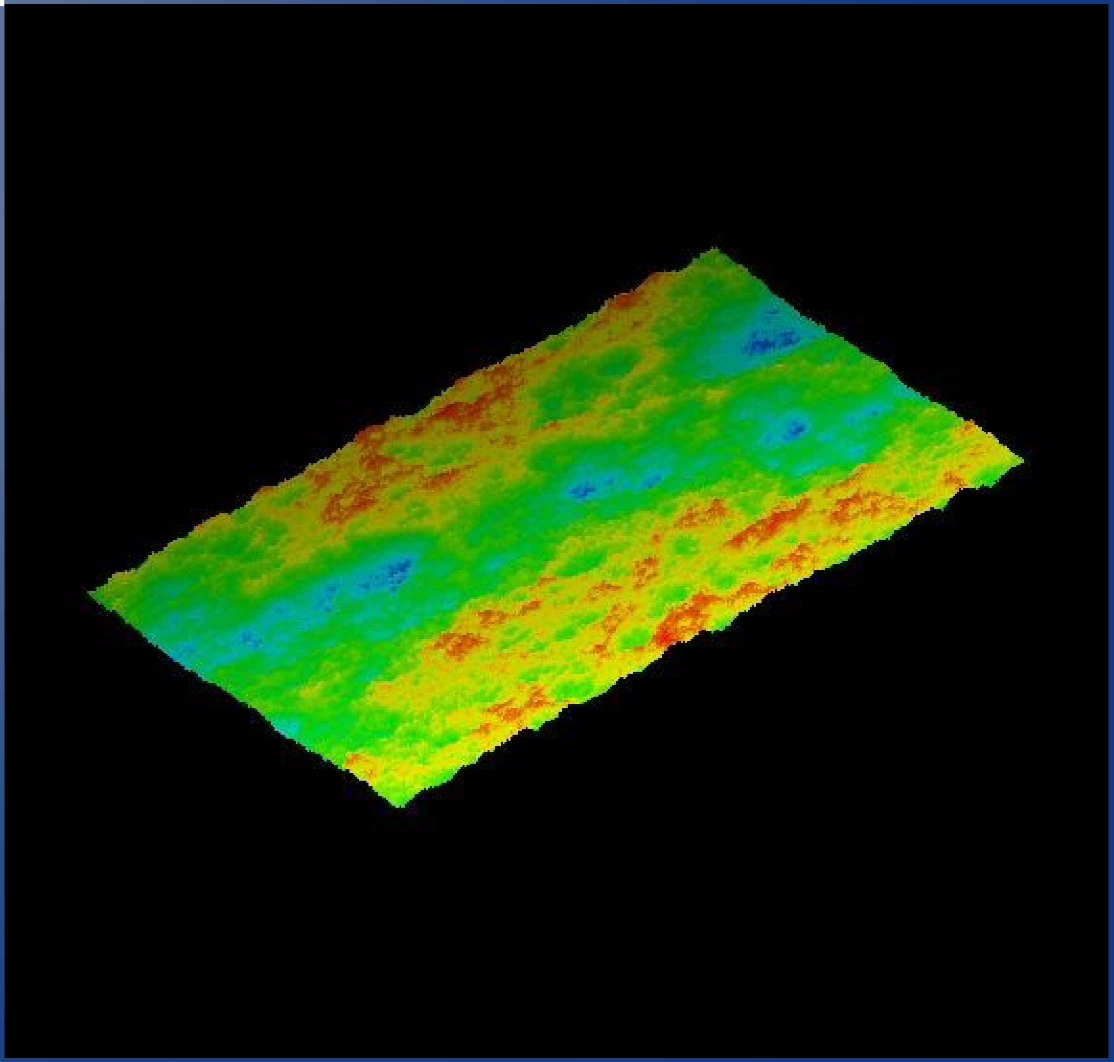
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 031112 (2010)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 051114 (2010)*

CUDA code for 2d KPZ

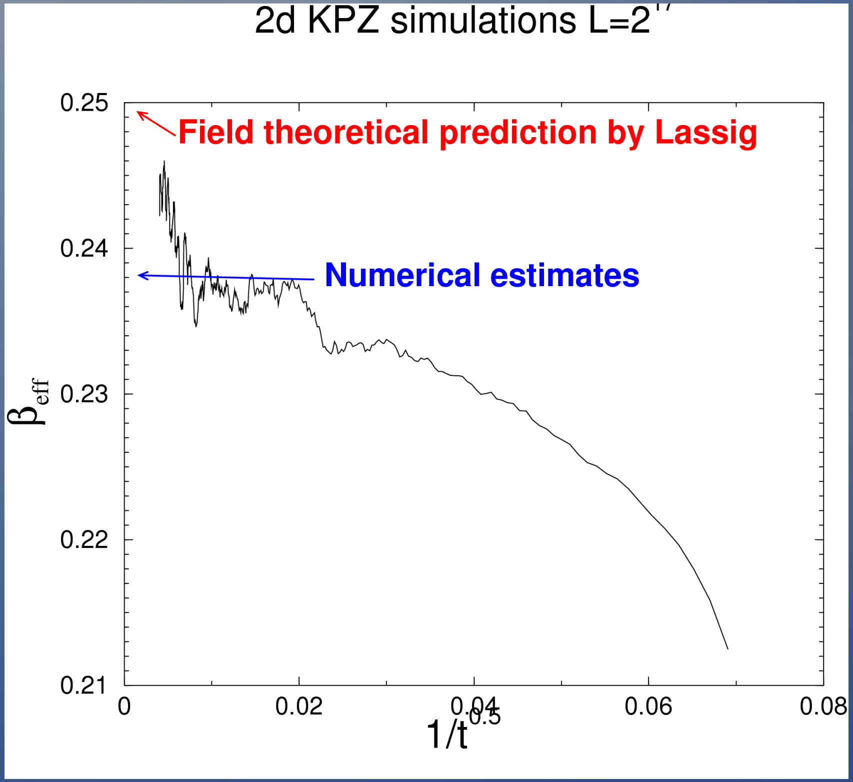
- Checkerboard decomposition
- Sub-systems are loaded in shared memory of GPUs updated with inactive boundaries:



- Each 32-bit word stores the slopes of 4x4 sites
- Origin of decomposition moves at every MCs
- **Speedup 240 x with respect the CPU**



Conclusions



- Preliminary results with the 2d KPZ CUDA simulations
- H. Schulz, G. Ódor, J. Kelling, K.-H. Heinig, B. Liedke, N. Schmeisser, *Computing the KPZ Equation Using GPU Acceleration*, 3rd International Workshop Innovation in Information Technologies - Theory and Practice, Dresden (2010).
- Henrik Schulz, Géza Ódor, Gergely Ódor, Máté Ferenc Nagy, *Simulation of 1+1 dimensional surface growth and lattices gases using GPUs, arXiv:1012.0385*
- Further studies in 2d : disorder, surface diffusion, scaling and pattern formation...