Rácsgáz és felületnövekedési modellek GPUs szimulációja

Géza Ódor, R. Juhász, I. Borsos, Gergely Ódor, Máté Nagy Ferenc, Budapest (KFKI)
H. Schulz, N. Schmeisser, J. Kelling, B. Liedke, K-H. Heinig, Dresden (HZDR)

German-Hungarian collaboration supported by DAAD and MÖB: 2010-2011

MFA

Budapest 08/07/2011

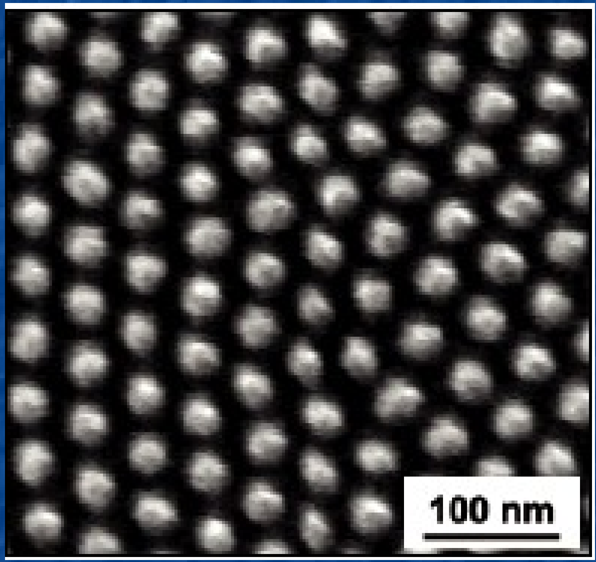
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

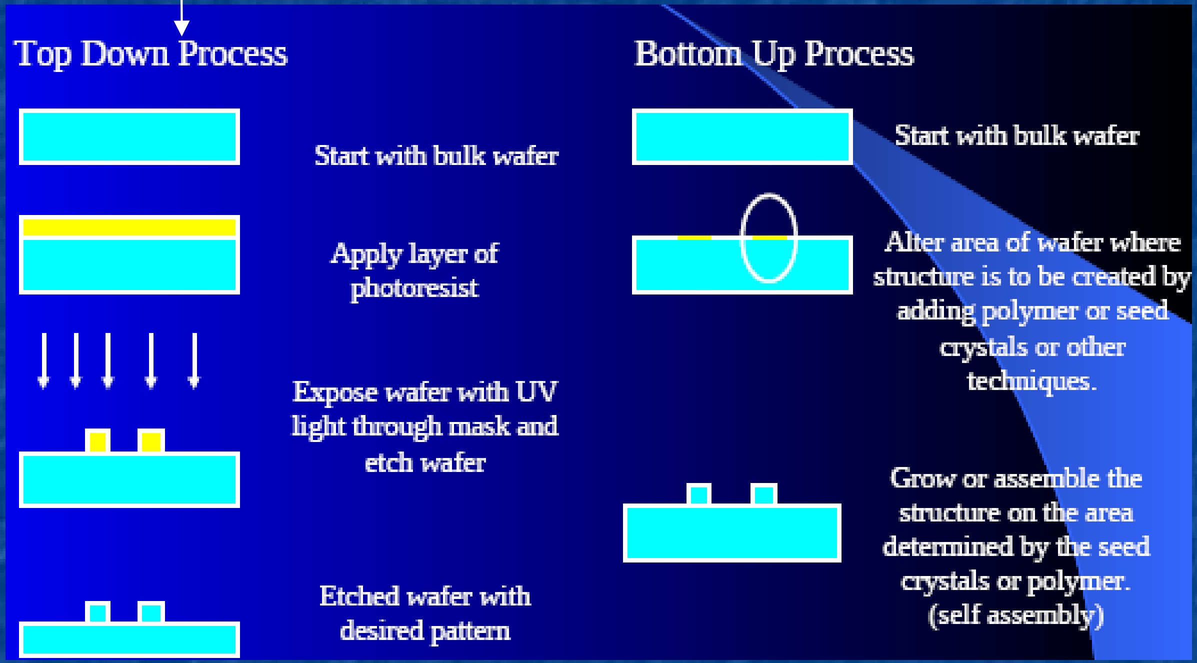
KFKI RMKI

www.mfa.kfki.hu/~odor

Motivation

In nano-technologies large areas of **nano-patterns** are needed, fabricated today by expensive techniques, e.g. electron beam lithography or direct writing with electron and ion beams.





Similar phenomena: sand dunes, chemical reactions … → Universality

Better understanding of basic surface growth phenomena is needed !

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 : local growth velocity, up-down anisotropy
η : roughens the surface by a zero-average, Gaussian noise field with correlator:

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

Characterization of surface growth:

Interface Width:

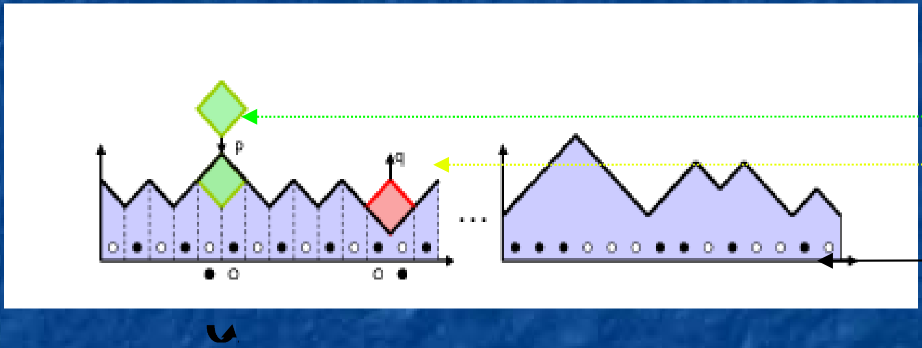
$$W(L,t) = \left[\frac{1}{L^2}\sum_{i,j}^{L} h_{i,j}^2(t) - \left(\frac{1}{L}\sum_{i,j}^{L} h_{i,j}(t)\right)^2\right]^{1/2}$$

Family-Vicsek scaling:

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

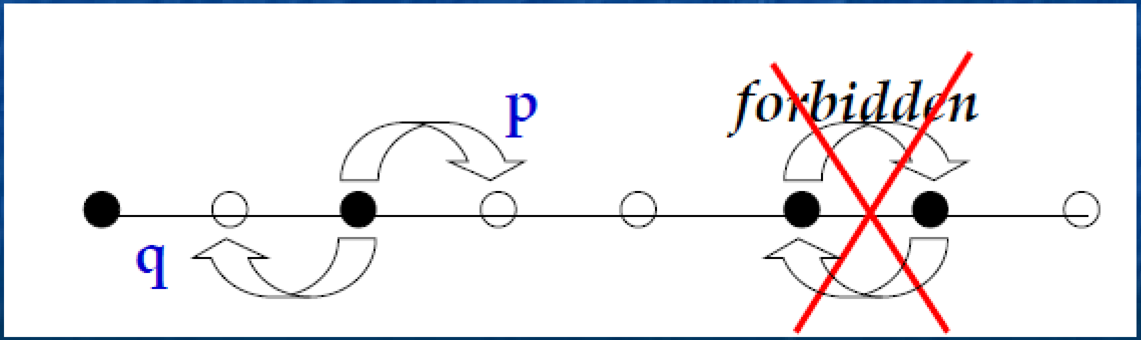
$$z = \alpha/\beta$$

Mapping of KPZ onto ASEP 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)*)

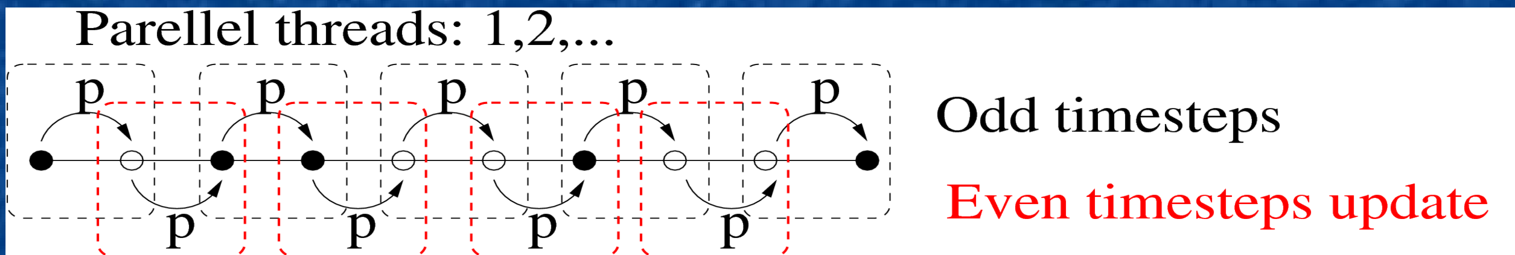


The simple ***ASEP*** (Ligget '95) is an **exactly solved 1d lattice gas**

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

Parallel update algorithms for 1d ASEP/KPZ

Parallel updates on a ring of size *L*:



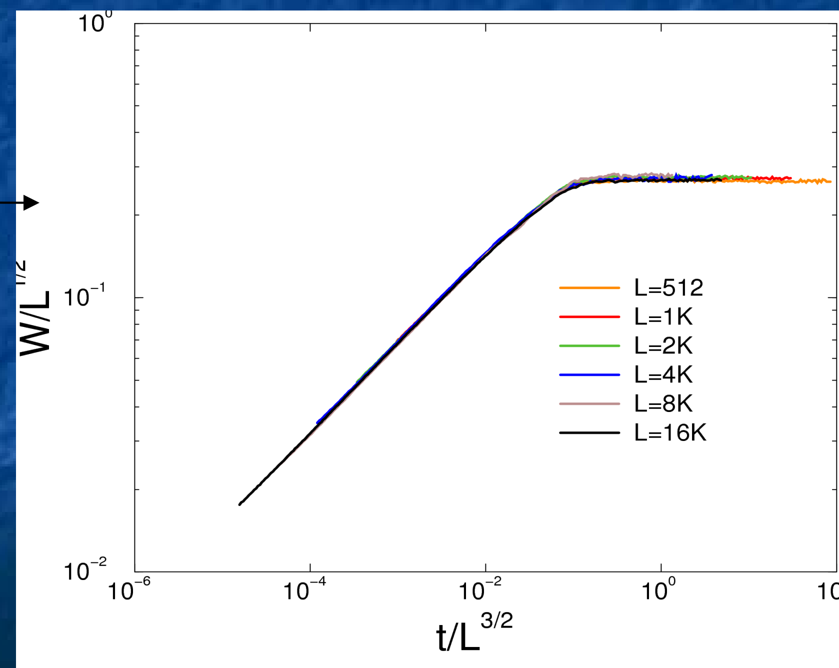
with probability *p* (**TASEP**)

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

L < 32K chains fit into shared memory of Tesla multiprocessor blocks

→ **no communication losses,**

maximal speedup & scaling:
240 cores GPU:
100 x of a CPU (2.8 GHz)

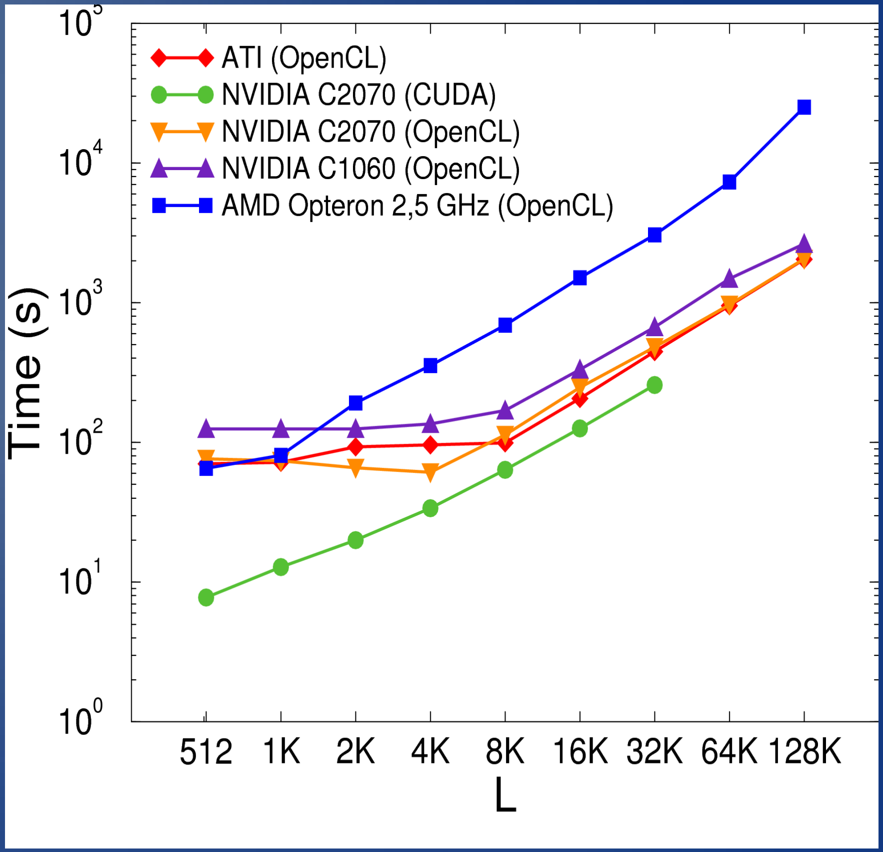


General OpenCL code

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

Portable for “any” parallel computers

- 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:

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

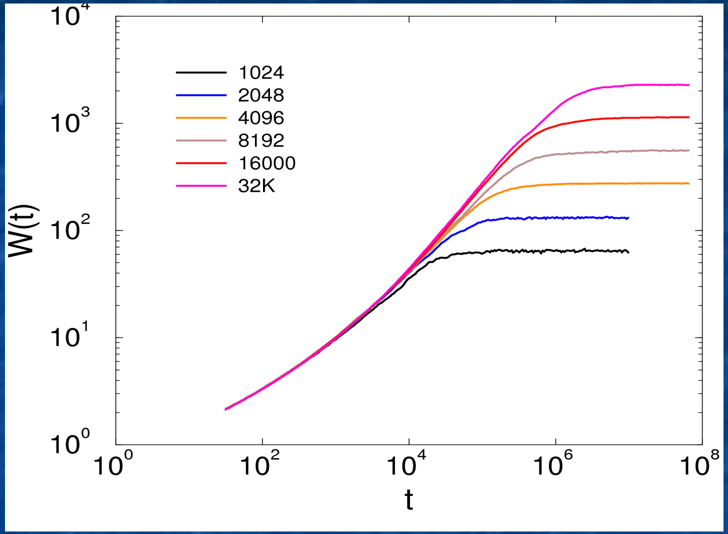
- Corresponds to KPZ + columnar disorder:

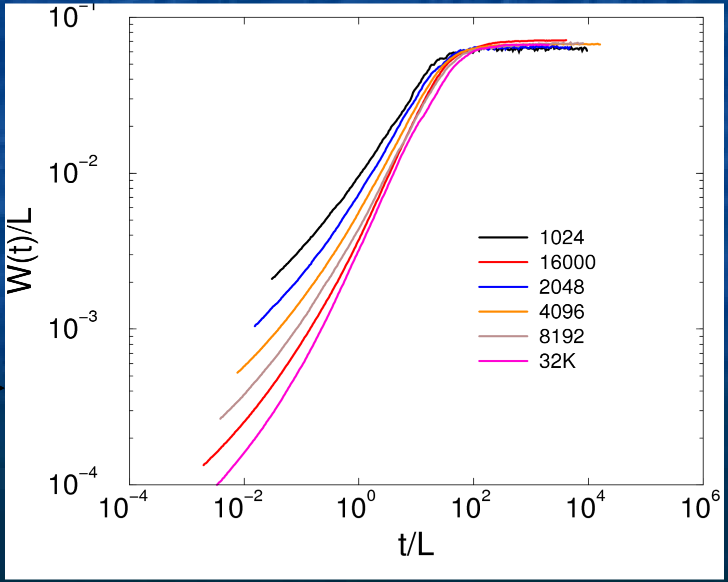
$$\partial_t h(\mathbf{x},t) = v + \sigma\nabla^2 h(\mathbf{x},t) + \lambda(\nabla h(\mathbf{x},t))^2 + \eta(\mathbf{x})$$

- Q-TASEP: *p_i=0.8 or 0.2, q_i=0*
  L=1024, 2048, ... 14000
  t_{max} = 10^8 MCs

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

- *Studied by Krug 1999: Stinchcombe et al. 2008: $\beta<1$*
- *Data collapse with **$\alpha=\beta=z=1$** faster than KPZ growth !*
- *Log. corrections are confirmed*

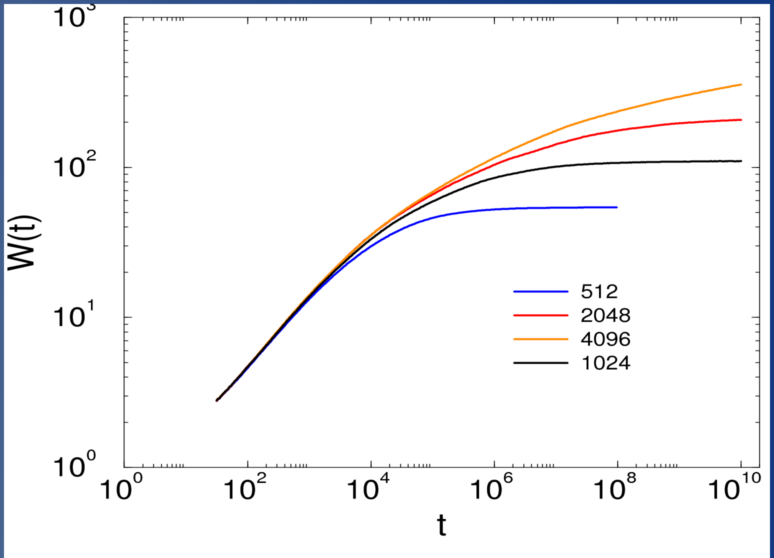




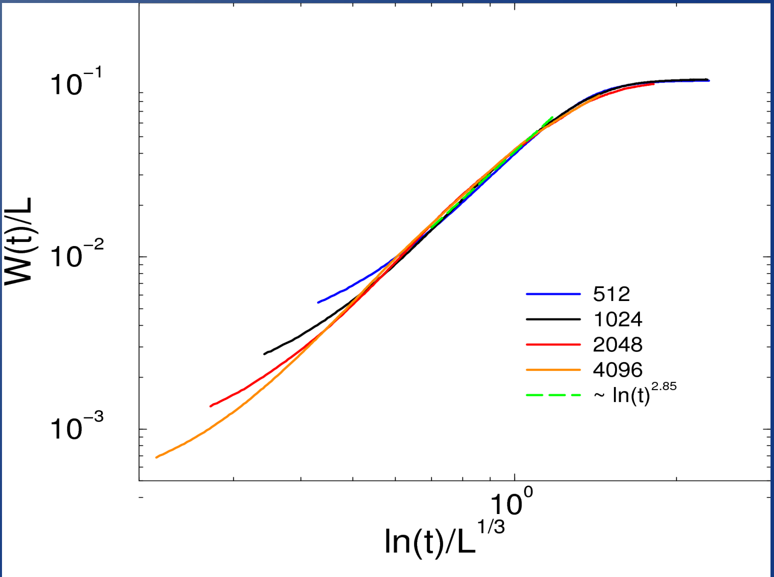
Disordered model (Q-SSEP)

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

$$W(t,L) \propto \ln(t)^{\bar{\beta}} \qquad \ln(\tau) \propto \xi^{\psi}$$

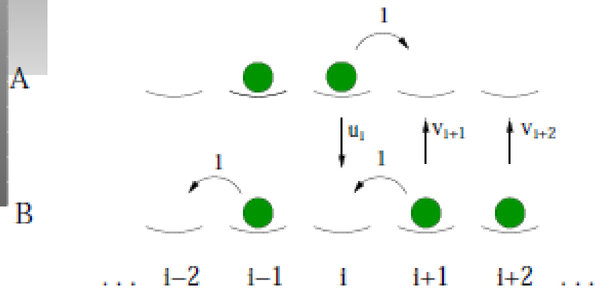


- Studied by *R. Juhász et al.* analytically (RG)



- Agreement, but due to wide distributions the typical values scale ($\psi = 1/3$) differently than mean values ($\psi = ½$)

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**

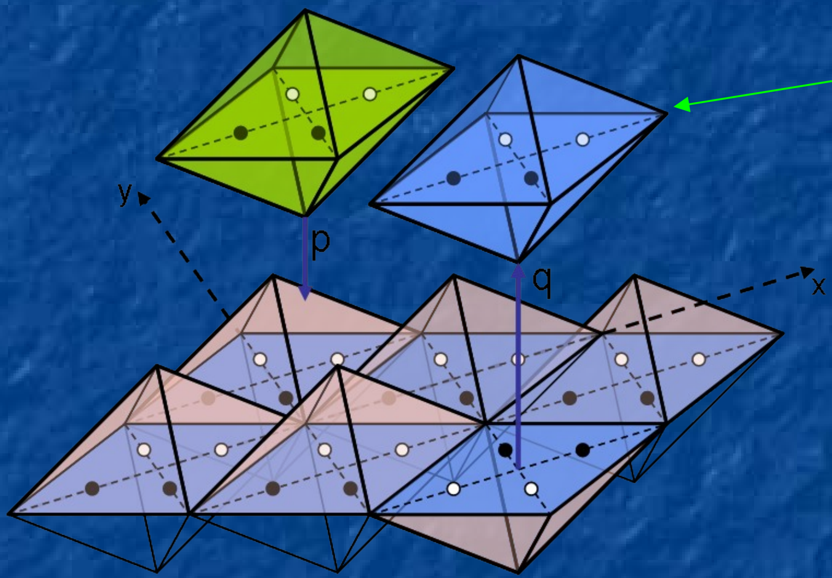
Preliminary results: *H. Schulz et al:* ***arXiv:0166093***

Comp. Phys. Comm. 182 (2011) 1467

Mapping of KPZ growth in *2+1* dimensions

- Generalized Kawasaki update:

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



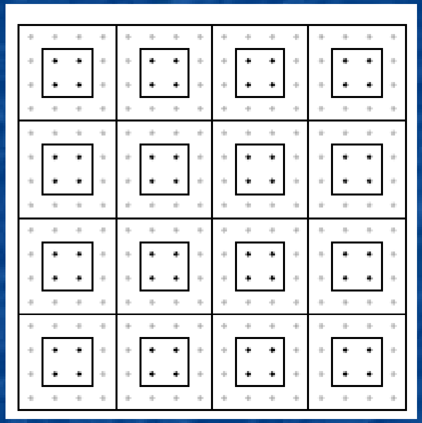
- **Octahedron model**

  Driven diffusive gas of pairs (dimers)

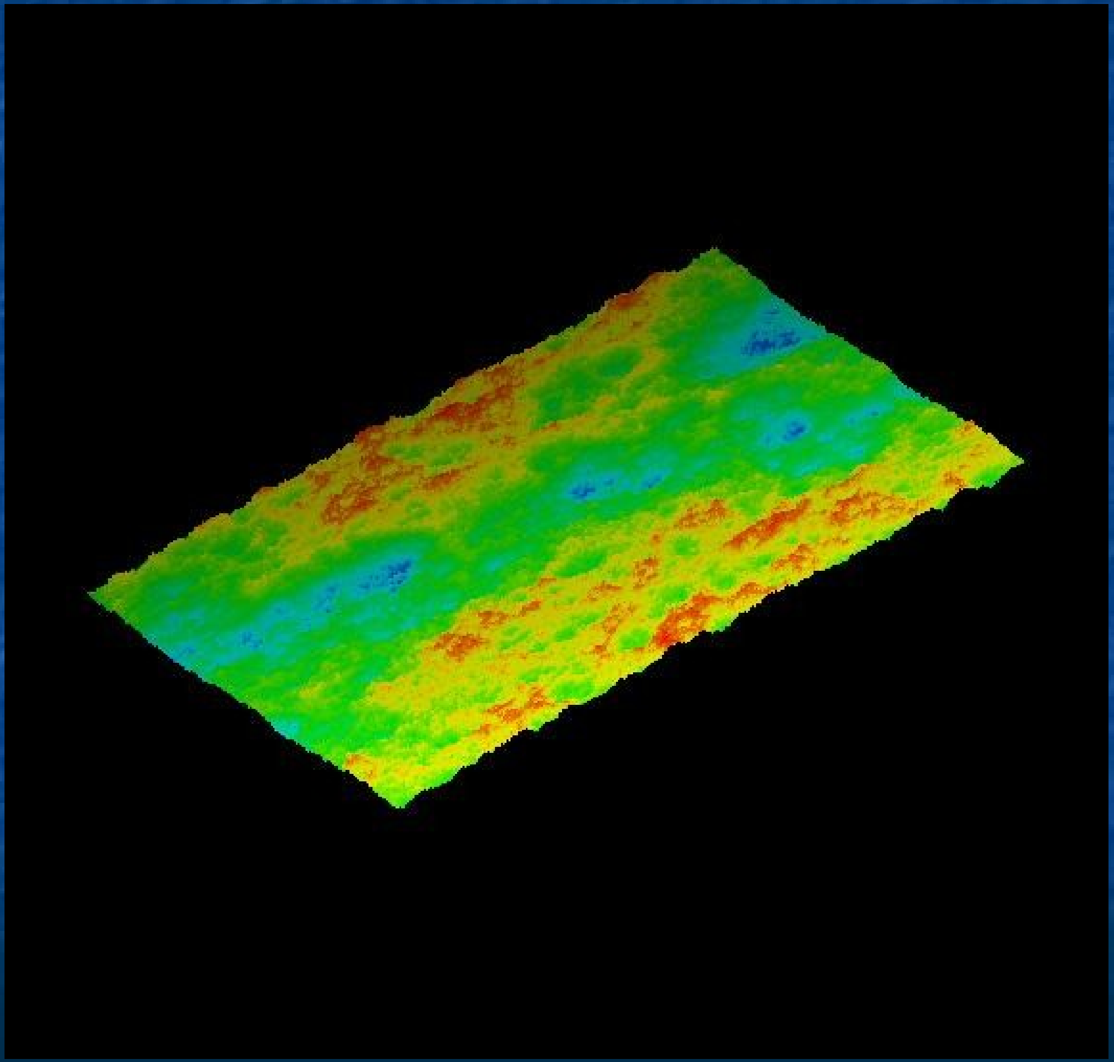
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 021125 (2009)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 031112 (2010)*
- *G. Ódor, B. Liedke and K.-H. Heinig, PRE79, 051114 (2010)*

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 a CPU of 2.8 GHz 131072 x 131972 size**



The hardware

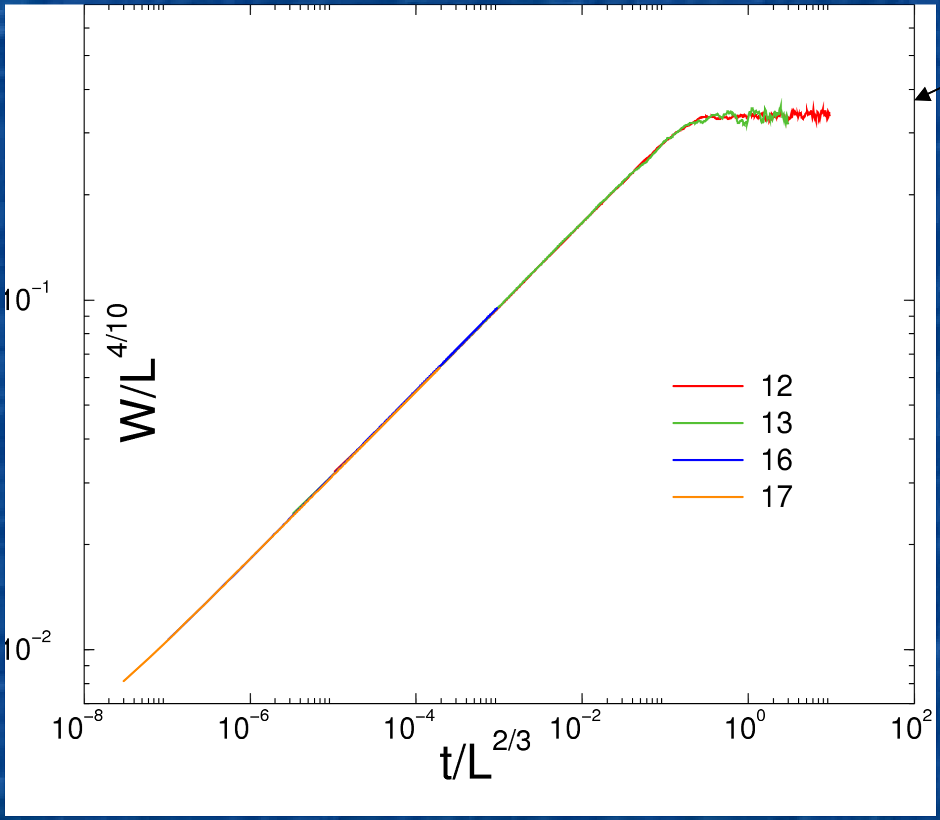
- Local supercomputer
  thanks to NVIDIA
  Professor Partnership*:*

  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 !

Conclusions



Preliminary results with the 2d KPZ CUDA simulations

Henrik Schulz, Géza Ódor, Gergely Ódor, Máté Ferenc Nagy,
Simulation of 1+1 dimensional surface growth and lattices gases using GPUs,
Comp. Phys. Comm. 182 (2011) 1467

Further studies in 2d : probability distribution scaling, disorder, surface diffusion, pattern formation…

Supported from:

DAAD-MÖB 2010-2011,
OTKA 77629 (Hungary),
NVIDIA Professor Partnership
OSIRIS FP7