Extremely Large Scale Simulation of Surface Growth and Lattice Gases

Géza Ódor, Budapest (MTA-TTK-MFA), Gergely Ódor, (MIT Boston)
Jeffrey Kelling, Henrik Schulz, Karl-Heinz Heinig, Dresden (HZDR),
Ferenc Maté Nagy-Egri, Róbert Juhász, Budapest (Wigner FKK)

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

GTC2013 21/03/2013

www.mfa.kfki.hu/~odor
Grand challenges in science

- Understanding of physics far from equilibrium is recognized to be one of the ‘grand challenges’ of our time, by both the US National Academy of Sciences [1] and the US Department of Energy [2].


- Furthermore, these studies point out the importance of non-equilibrium systems and their impact far beyond physics, including areas such as computer science, biology, public health, civil infrastructure, sociology, and finance.

- Striking new example: string theory (quantum gravity) ↔ non-equilibrium physics.
In nanotechnologies 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 & Nonequilibrium physics**

Better understanding of basic surface growth phenomena is needed!
The Kardar-Parisi-Zhang (KPZ) equation

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

\( \sigma \): (smoothing) surface tension coefficient
\( \lambda \): local growth velocity, up-down anisotropy
\( \eta \): roughens the surface by a zero-average, Gaussian noise field with correlator:

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

Characterization of surface growth:

Interface Width:

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

Most fundamental model of non-equilibrium surface physics

Surface growth power-laws:

\[ W(L,t) \propto \begin{cases} t^\beta & \text{for } t_0 \ll t \ll t_s, \\ L^\alpha & \text{for } t \gg t_s. \end{cases} \]
Grand challenges in Statistical Physics and Surface Science

- Solution of KPZ equation in $d>1$ dimensions
  Even for 2d controversial results!
- Existence of the upper critical dimension, beyond which fluctuations are irrelevant (smooth surfaces)?
  Most simulations predict: $d = \infty$
  $\leftrightarrow$ analytical studies
- Determination of universal scaling functions ($P(W)$, $P(h)$ ... etc.)
  Description of universal self-organized ripple/dot pattern formation
- Foundation of nonequilibrium statistical physics via understanding lattice gas models
Mapping of KPZ onto ASEP in 1d

- Attachment (with probability $p$) and
- Detachment (with probability $q$)

Corresponds to anisotropic diffusion of particles (bullets) along the 1d base space (Racz et al 1987)

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

Widespread application in biology
Parallel update algorithms for 1d ASEP/KPZ

Parallel updates on a ring of size $L$:

with probability $p$ (TASEP)

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

$L < 64K$ chains fit into the shared memories of multiprocessor blocks

- no communication losses

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

OpenCL Implementation

No size limitation by shared memory

Uses vectorization of AMD

Portable for “any” parallel computers (in principle)

Tested by ASEP (KPZ) on ATI, NVIDIA, CPU clusters

Multi-GPU program using Message Passing Interface
Run-time analysis

For larger system OCL speed is comparable to the CUDA code.

MPI parallelization efficiency varies non-monotonically with no. of cards → possibility for optimization.
Disordered ASEP model simulations

- Site-wise binary quenched disorder:
  \[ P(p_i) = (1 - D)\delta(p_i - p) + D\delta(p_i - \tau p) \]

- Q-TASEP: \( p = 0.8 \) or \( 0.2 \), \( q_i = 0 \)
  \( L = 1024, 2048, \ldots, 16000 \)
  \( t_{\text{max}} = 10^8 \text{ MCs} \)

- Studied by: Krug 1999, Stinchcombe et al. 2008: \( \beta < 1 \)

- Data collapse with \( \alpha = \beta = z = 1 \)
  Precise form of log. corrections are derived

- + Q-PASEP and 2-lane TASEP:

Mapping of KPZ growth in $2+1$ dimensions

Octahedron model

- Generalized Kawasaki update:
  \[
  \begin{bmatrix}
  -1 & 1 \\
  -1 & 1
  \end{bmatrix}
  \Rightarrow
  \begin{bmatrix}
  1 & -1 \\
  1 & -1
  \end{bmatrix}
  \]

- Driven diffusive gas of pairs (dimers)

- Surface pattern formation via dimer model

CUDA code for 2d KPZ

- Each 32-bit word stores the slopes of 4x4 sites
- Speedup 430 x (Fermi) with respect a CPU core of 2.8 GHz on: 131072 x 131972 size
- Field theory: growth exponent $\beta = 1/4$?

Domain decomposition methods

- dead border decomposition at device level (active sites \((n-1) \times (n-1)\))
- randomly moving origin (word-wise)
- every MCS at device layer
  \[\Rightarrow\] avoids accumulation of errors at borders

Fig. 3: Decomposition of the whole system into work-groups at device layer, with gray areas indicating dead borders. Further decomposition at work-group layer using double tiling is indicated for work-group 1: Each work-item executes four virtual threads using VLIW vector operations. The virtual threads are denoted by their corresponding vector components \((x, y, z, w)\). A single-hit double tiling scheme is employed to distribute the work-group among all virtual threads. The cells of the four sets of domains are indicated for virtual thread 1.x.
OpenCL and Optimizations

- HD6970 provides 128-bit registers (Very Long Instruction Word)
- Even with OpenCL different architectures require different code

Conclusions & outlook

- Fast parallel simulations due to mapping onto stochastic cellular automata (lattice gases)
- Important scaling results in 1d disordered ASEP models with **ultra-slow dynamics**
- **Extremely large scale** \((2^{\text{17}} \times 2^{\text{17}})\) **results** in 2d KPZ clarified long lasting debate: ruling out rational \((\frac{1}{4}, \ldots)\) scaling exponents of a field theory
  + determination of **Universal Scaling Functions**

Double Tiling is more efficient than Dead Border domain decomposition

OpenCl performs almost as good as CUDA on NVIDIA devices,
  **but it could not fulfill it’s promise on platform independence**

Extension for studying Surface pattern formation would be very efficient

- **Acknowledgements:** DAAD-MÖB, OTKA, OSIRIS FP7, NVIDIA, FuturICT.hu

**Publications:**


