A display of GPU implementations in Condensed Matter Physics four distinctive cases

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General Purpose Graphics Processing Units have **shaken up** the computational **scientific community**. In many cases, people **adopted** parallelism with **CUDA**, before even knowing what was exactly MPI or OMP about. As statistical physicists working in condensed matter, with the **aim of accelerating** our **simulations**, we have implemented in the last few years some **massively parallel** codes. We present here **four examples** of *ad-hoc* models that effectively describe the phenomenology of **physical systems** at a given scale. We can classify them in two families: (i) **lattice based Monte Carlo simulations** (for classical spin models and electron glasses); (ii) **overdamped dynamics of scalar systems** (for elastic lines in disordered media and sheared amorphous solids). Dimensionality, interaction range, particular dynamics, and other details of the model, determine the **parallelization strategy** in each case.

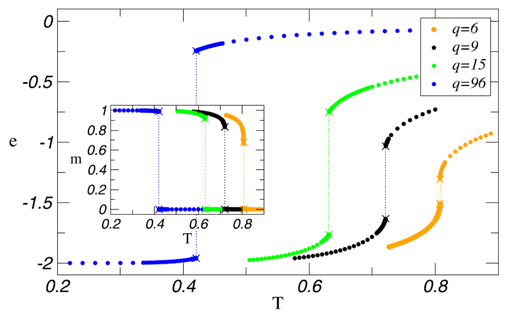
q-state Potts model Monte Carlo (classical spins system)

$$H = -J \sum_{(i,j)} \delta_K(s_i, s_j)$$

$s_i = 1, 2, \ldots, q$
$J > 0$

$$\delta_K(x, x') = \begin{cases} 1 \text{ if } x = x' \\ 0 \text{ otherwise} \end{cases}$$

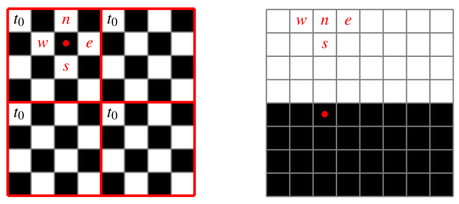
Spin flips are accepted with probability $p = \tau^{-1} e^{-\Delta H / k_B T}$



Equilibrium energy per spin *e* and magnetization *m* versus temperature *T*. Exact values marked as crosses.

Parallelization strategy

Checkerboard scheme (interactions limited to nearest neighbors)



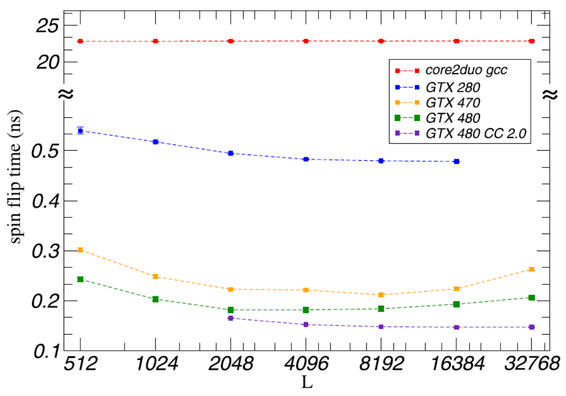
Stencil compaction-- **Left:** an 8×8 checkerboard framed in 4×4 (red marking), the cells updated by thread t_0 are singled out, we also marked the neighbors of cell •. **Right:** packed checkerboard showing first half of whites, neighboring cells *n*, *e*, *s*, *w* are marked, in the second half of black cells • is singled out.

Code features

- Pure **CUDA C**
- **Multiply With Carry RNG** with FRAMExFRAME/2 independent generators.
- **Multiple outputs per thread**. Two consecutive kernels (black/white) of typically 512×512/2 threads.
- **Comprises** the remapping of a two-dimensional **stencil** of four points, **save memory transfers**.
  → **Encodes** each spin in a **byte**.
  → Uses **registers** for **RNG states**.
  → Implements **parallel sums** (butterfly-like) for averages calculations using **shared memory**.

Performance

- Largely dominated by the **update routine** (with 2 RNG calls/site).
- **Two competing factors** in the loop of the update kernel:
  - 1) The global memory for the RNG state of each thread is retrieved one time at the beginning and stored at the end. **The larger the L**, the load/store **latency is better distributed.**
  - 2) The **inherent overhead** incurred by a loop (comparison and branching), **increases with L.**
- Practical **speedups respect to a single-core CPU:**
  - GTX 280: 42x to **47x**
  - GTX 470: 76x to **108x**
  - GTX 480: 95x to **155x**



Spin flip time in nanoseconds vs. lattice size running on an Intel Core 2 Duo E8400@3.0 GHz CPU, and running on GTX 280, GTX 470 and GTX 480 NVIDIA GPUs.

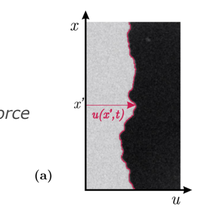
[1] E.E. Ferrero, J.P. De Francesco, N. Wolovick, S. A. Cannas, *Comp. Phys. Commun.* **183** 1578 (2012)
[2] E.E. Ferrero, F. Romá, S. Bustingorry, P.M. Gleiser, *Phys. Rev. E* **86** 031121 (2012)

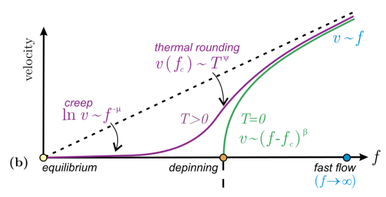
https://bitbucket.org/ezeferrero/potts
https://bitbucket.org/ezeferrero/potts-glass

Quenched Edwards-Wilkinson model (elastic manifolds in disordered media)

$$\eta \partial_t u(x,t) = c \partial_x^2 u(x,t) + F_p(u,x) + f$$

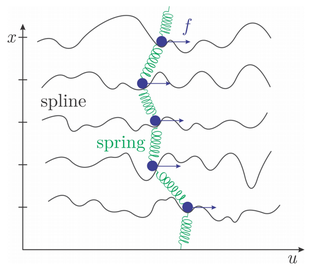
interface velocity — *elastic interactions* — *pinning potential* — *external force*





Implementation

Euler integration in discretized time



- Line of **size *L***
  - **discrete *x*=0...(*L*-1)**
  - keep ***u(x,t)*** as a **real** variable
  - **p**eriodic **b**oundary **c**onditions (*u*[0] coupled with *u*[*L*-1])
- Alternative **disorder schemes**
  - **Spline** from a presorted array *LxM*
  - **Step-like** dynamically generated

Code features

- **C++** and **CUDA C**
- Massively **parallel dynamics evolution** (alternating even and odd sites), L/2 threads.
- **Intensive use** of **Thrust** transforms and reductions (e.g.: velocity averages).
- **Coexisting** CUDA **kernels and Thrust** functions.
- Uses alternatively two **different RNGs**:
  → **Multiply With Carry**
  → **Philox** (**counter based**), Random123 library.
- Uses **cuFFT** to compute structure factor.

Benchmarking

Mean update time execution and their related GPU vs. (single-core) CPU practical speedups.
In tables: system size L=65536.

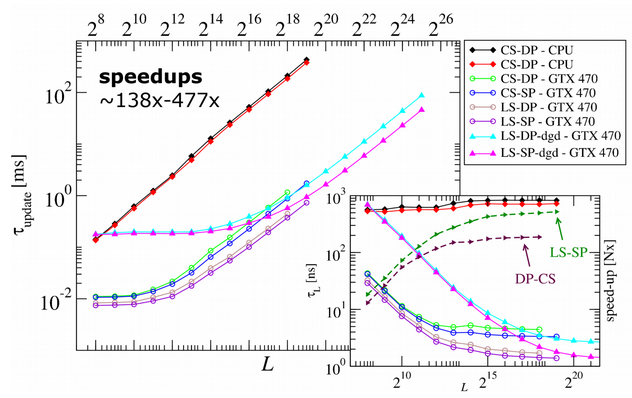
Case	single-core CPU	CPU + GTX 470		CPU + Tesla C2075	
	time[ms]	*time[ms]*	*psu*	*time[ms]*	*psu*
CS DP	54.49	0.301	181	0.396	138
CS SP	~ 54	0.227	238	0.298	181
LS DP	46.46	0.123	377	0.152	305
LS SP	~ 46	0.101	455	0.128	359

Platform: AMD Phenom II X4 955 Processor @3.2GHz, NVIDIA Tesla C2075, NVIDIA GTX 470.

Case	single-core CPU	CPU + GTX 480	
	time[ms]	*time[ms]*	*psu*
CS DP	42.22	0.238	186
CS SP	~ 42	0.179	235
LS DP	36.55	0.098	373
LS SP	~ 36	0.076	477

Platform: Intel Core 2 Quad CPU Q9550 @2.83GHz, NVIDIA GTX 480.

Acronyms: **CS**: Cubic Spline, **LS**: Linear Spline, **DP**: Double Precision, **SP**: Single Precision, **psu**: practical speed-up.



Update step mean-computing time in ms.
Platform: AMD Phenom II X4 955 Processor @3.2GHz, NVIDIA GTX 470

[1] E.E. Ferrero, S. Bustingorry, A.B. Kolton, *Phys. Rev. E* **87** 032122 (2013)
[2] A.B. Kolton, S. Bustingorry, E.E. Ferrero, A. Rosso, JSTAT **P12**004 (2013)

https://bitbucket.org/ezeferrero/qew

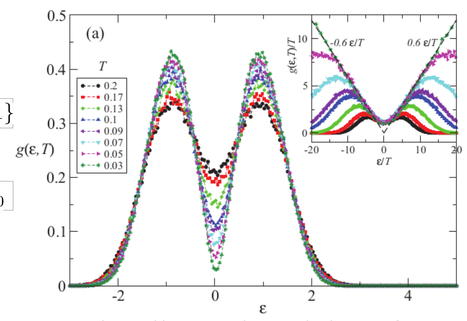
Coulomb glass Kinetic Monte Carlo (electrons glass system)

$$H = \sum_{i=0}^{N-1} \phi_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{(n_i - \nu)(n_j - \nu)}{r_{ij}} - E \sum_{i=0}^{N-1} n_i x_i \qquad n_i \in \{0,1\}$$

random potential

Kinetics $\Gamma_{ij} = \tau_0^{-1} \theta_{ij} e^{-2 r_{ij}/\xi} \min[1, e^{-\epsilon_{ij}/k_B T}]$ $\quad \theta_{ij} = \delta_{n_i,1} \delta_{n_j,0}$

$$\epsilon_{ij} = \epsilon_i - \epsilon_j - \frac{1}{r_{ij}} - E_{ij} \qquad \epsilon_i = \phi_i + \sum_j \frac{1}{r_{ij}} (n_j - \nu)$$

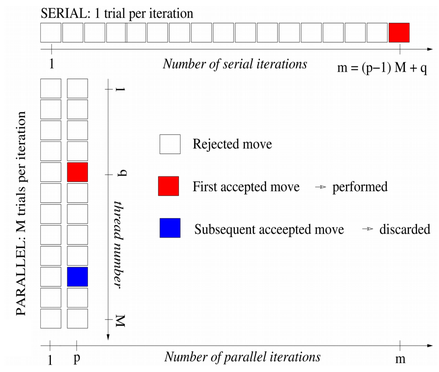


Pseudo-equilibrium single-particle density of states

Parallel Kinetic Monte Carlo

Markov-chain **MC** with proposal matrix $Q_{\alpha\beta}$ and acceptance $P_{\alpha\beta}$ between conf. α and β.

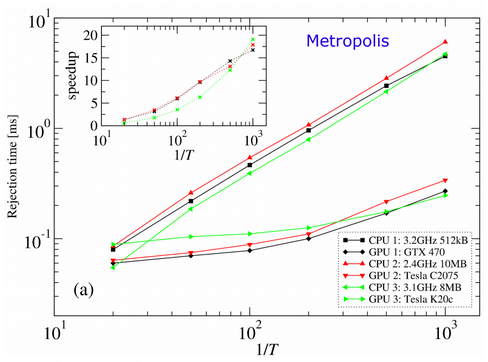
1. Propose with **independent threads** (k=1,...,M), moves $\alpha \to \beta_k$.
2. Accept the move $\alpha \to \beta_k$ **independently** with prob $P_{\alpha\beta_k}$ (without updating)
3. If **at least** one thread has accepted a move, update the conf. to β_q, where *q* is the **lowest label** among the threads accepting.



Code features

- **CUDA C**
- Trial hop (*i* → *j*): **tower sampling** with **vectorized** binary search.
- Metropolis: **parallel rejection**
- Update Local Energies: **embarrassingly parallel** kernel.
- Global observables: **parallel reductions with Thrust**.

Performance



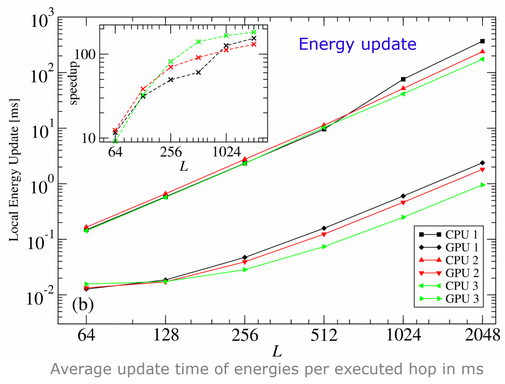
Average rejection time per executed hop in ms

- At large N=L^2, energy update **scales as O(N)** (in both CPU, GPU). An **optimal number** of concurrent threads yields **speedups over 100x**.
- This speedup **dominates** the **total** computation **time** at large N.

Overall speedup

(respect to 1 CPU core)
~100x for $T<10^{-2}$, $L>2^{10}$

Platforms:
1. Phenom II X4 955 @3.2GHz 512kB, GTX 470
2. Xeon E5-2609 @2.4GHz 10M, Tesla c2075
3. Core i7-950 @3.1GHz 8M, Tesla K20c



Average update time of energies per executed hop in ms

- Speedup per accepted hop **monotonically increases** with **decreasing temperature** (acceptance), roughly independent on L.
- **No signs of saturation** for the speedup.

[1] E. E. Ferrero, A. B. Kolton, M. Palassini, *AIP Conf. Proc.* **1610** 71 (2014)

https://bitbucket.org/ezeferrero/coulomb_glass

Athermal elasto-plastic model (sheared amorphous solids)

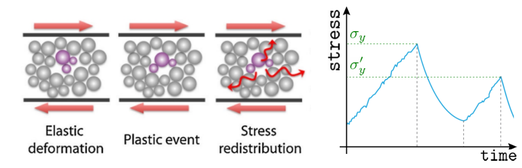
$$\partial_t \sigma(\mathbf{r},t) = \mu \dot{\gamma}^{\text{ext}} + \mu \int d\mathbf{r}' G(\mathbf{r},\mathbf{r}') \dot{\gamma}^{\text{plast}}(\mathbf{r}',t)$$

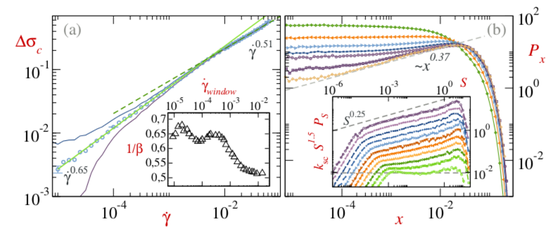
stress change — *shear-rate*

plastic strain rate: $\dot{\gamma}^{\text{plast}}(\mathbf{r},t) = n(\mathbf{r},t) \dfrac{\sigma(\mathbf{r},t)}{\mu\tau}$

elastic propagator **long-range!** $G(r,\theta) = cos(4\theta)/\pi r^d \qquad r = |\mathbf{r}' - \mathbf{r}|$

$$n(\mathbf{r},t): \begin{cases} 0 \to 1 & \text{if} \quad \sigma > \sigma_y \quad \leftarrow \textit{randomly taken from } P(\sigma_y) \\ 0 \leftarrow 1 & \text{when} \quad \int dt' |\partial_t \sigma(t')/\mu + \dot{\gamma}^{pl}(t')| \geq \gamma_c \end{cases}$$





Critical flow-curve, stability and avalanche distributions

Parallelization strategy

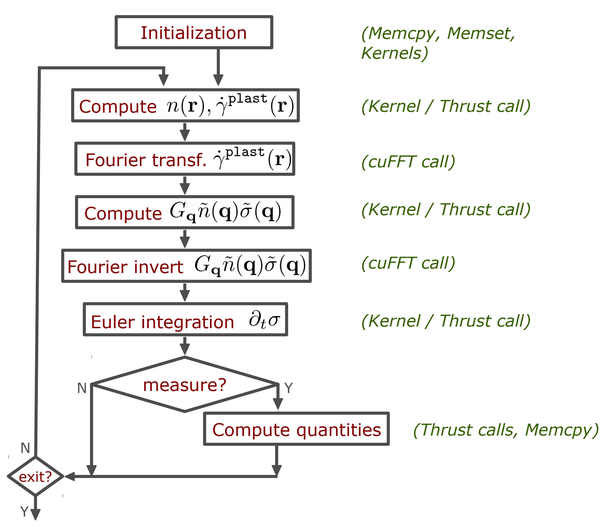
"Pseudo-spectral" method: transform Fourier, compute and anti-transform at each step

$$\int d\mathbf{r}' G(|\mathbf{r} - \mathbf{r}'|) n(\mathbf{r}') \sigma(\mathbf{r}') \longrightarrow G_{\mathbf{q}} \tilde{n}(\mathbf{q}) \tilde{\sigma}(\mathbf{q})$$

$$G(r,\theta) = cos(4\theta)/\pi r^d \longrightarrow \hat{G} = -4 \frac{q_x q_y}{q^2}$$

Embarrassingly **parallel in Fourier** space, local in (q_x, q_y)

General work-flow

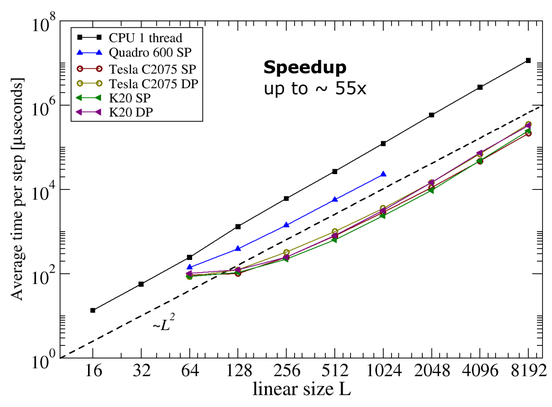


Code features

- **C++** and **CUDA C**
- Intensive use of **cuFFT**
- Uses **Thrust** for averages and extrema finding
- Uses **Philox RNG**

Performance

Just a fast benchmark so far...



Platforms:
- Xeon E5-2609 @2.4GHz 10M, Quadro 600 & Tesla c2075
- Xeon EP E5-2670 @2.6GHz 20M, NVIDIA K20

[1] E. E. Ferrero, K. Martens, J.-L. Barrat, *Phys. Rev. Lett.* **113**, 248301 (2014)
[2] C.Liu, E.E. Ferrero, F. Puosi, J.-L. Barrat, K. Martens, arXiv 1506.08161 (2015)

https://bitbucket.org/ezeferrero/ep

General considerations:

We have **adopted** the the **GPGPU approach** to address different problems in Condensed Matter physics. The **goal** in each case was to **implement and verify a code** to **produce valid physical results**. Very good **practical speedups** have been attained respect to what people have been using before for the same kind of problems (**single-core CPU programs**), even when optimization is not seriously considered. Present **challenges** include: *i)* exploit better the hardware, starting with CPU-GPU **concurrency** and multi-GPU approaches; *ii)* deal better with **I/O operations**, sometimes they drain all the obtained performance, dilemma "output raw vs compute on-the-fly"; *iii)* migrate from ad-hoc CUDA kernels to library calls for better **portability**; *iv)* make the switch to OpenCL.