Ising, Heisenberg and spin glass model simulations on GPU

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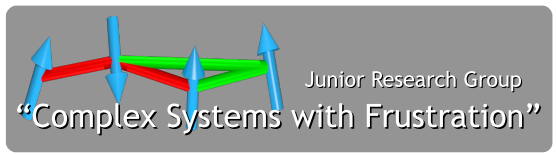


GPU computation frameworks

GPGPU = General Purpose Computation on Graphics Processing Unit

"Old" times: use original graphics primitives

- OpenGL
- DirectX

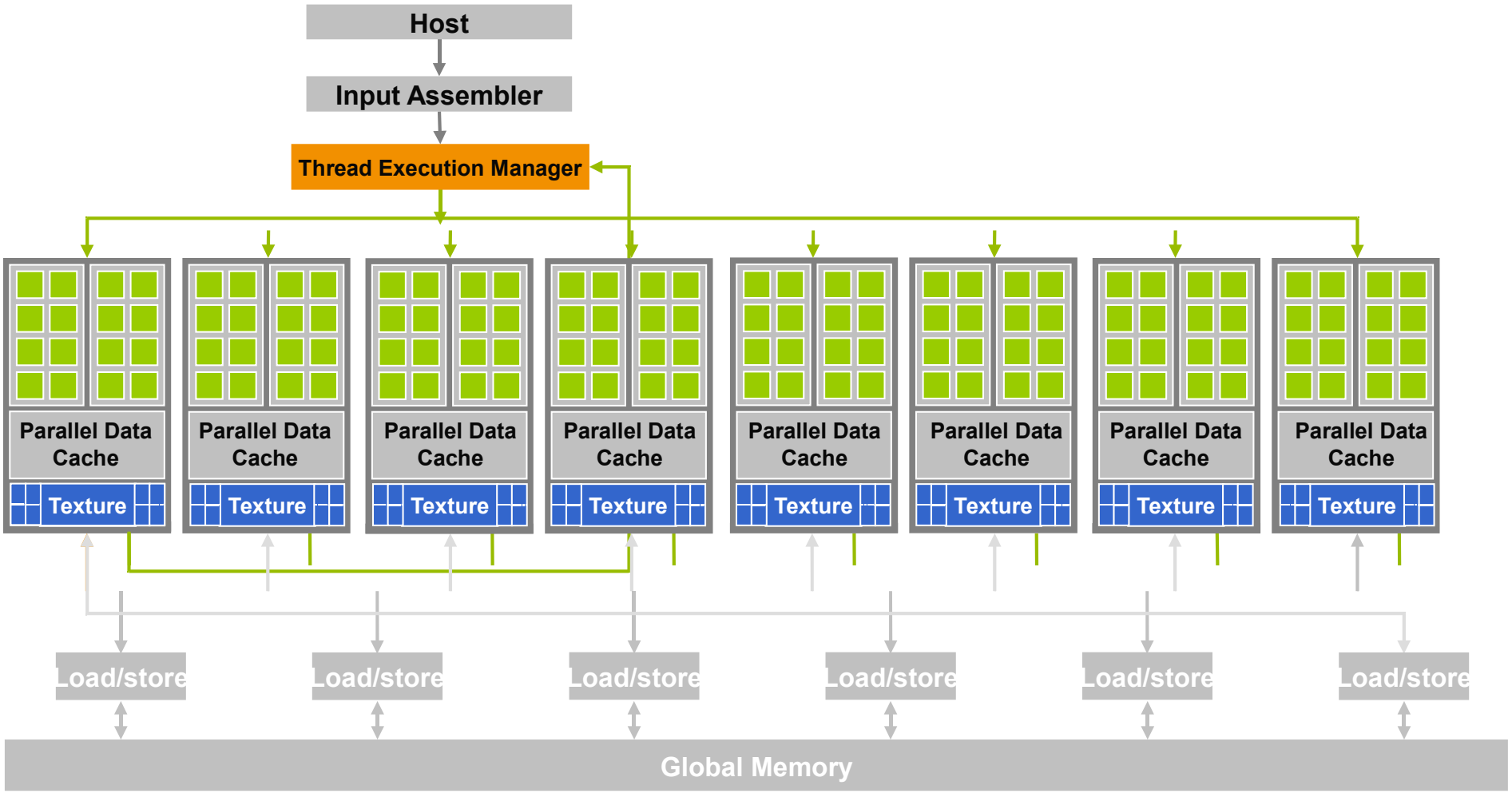
Vendor specific APIs for GPGPU:

- NVIDIA CUDA: library of functions performing computations on GPU (C, C++, Fortran), additional preprocessor with language extensions
- ATI/AMD Stream: similar functionality for ATI GPUs

Device independent schemes:

- BrookGPU (Standford University): compiler for the "Brook stream program language" with backends for different hardware; now merged with AMD Stream
- Sh (University of Waterloo): metaprogramming language for programmable GPUs
- OpenCL (Open Computing Language): open framework for parallel programming across a wide range of devices, ranging from CPUs, Cell processors and GPUs to handheld devices

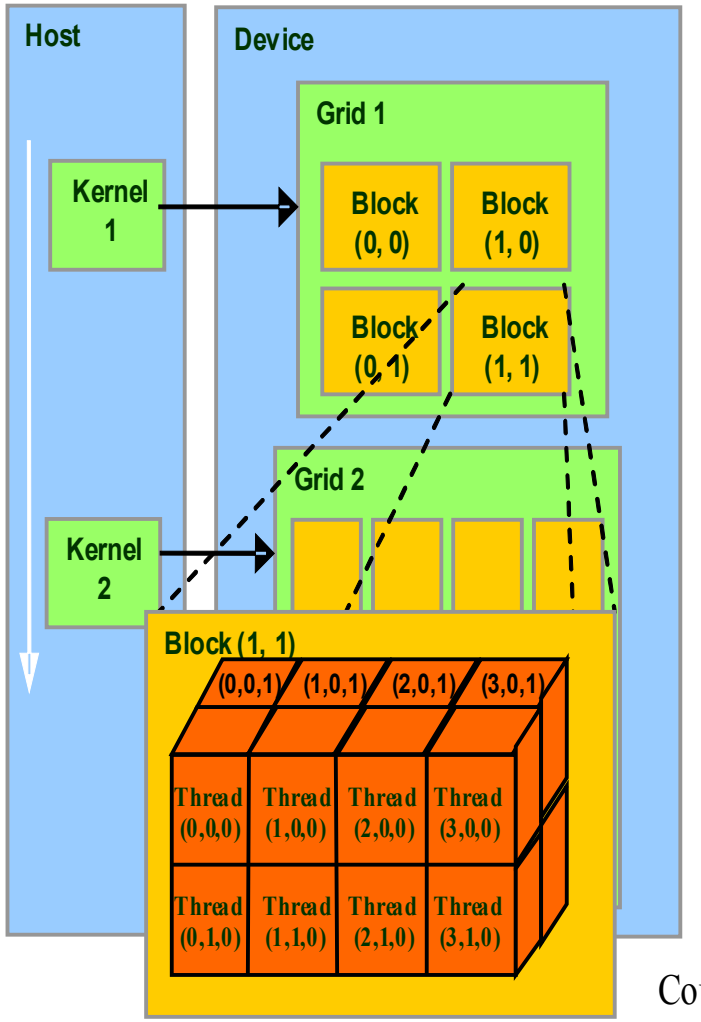
NVIDIA architecture



NVIDIA architecture

Hierarchical organization:

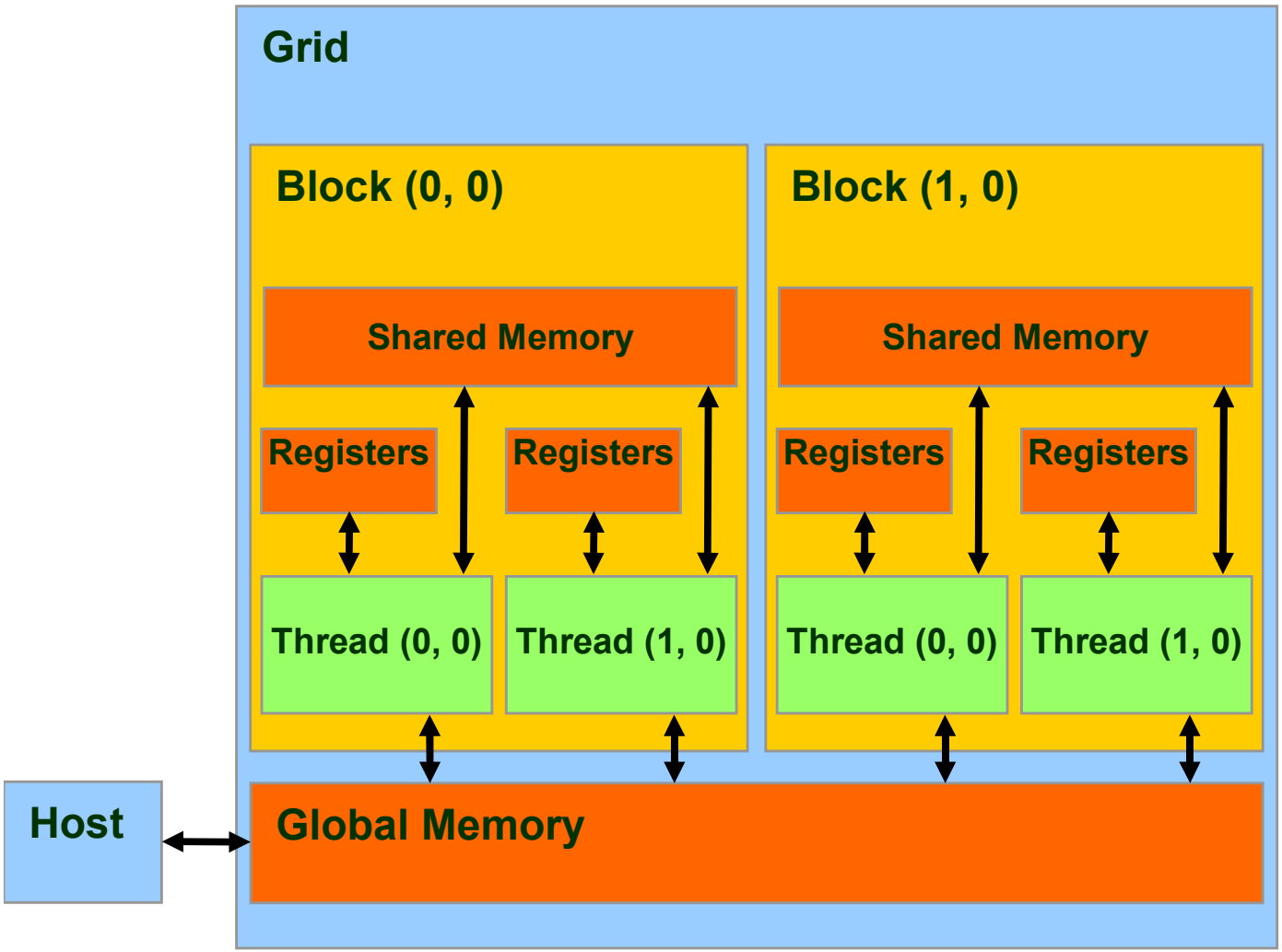
- host code ↔ device code
- grid of blocks are scheduled independently
- each block consists of threads that can synchronize



Courtesy: NDVIA

NVIDIA architecture

Memory layout:



Spin models

Consider classical spin models with nn interactions, in particular

Ising model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j + H \sum_i s_i, \quad s_i = \pm 1$$

Heisenberg model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + \vec{H} \cdot \sum_i \vec{S}_i, \quad |\vec{S}_i| = 1$$

Edwards-Anderson spin glass

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} s_i s_j, \quad s_i = \pm 1$$

Design goals

Computations need to be organized to suit the GPU layout for maximum performance:

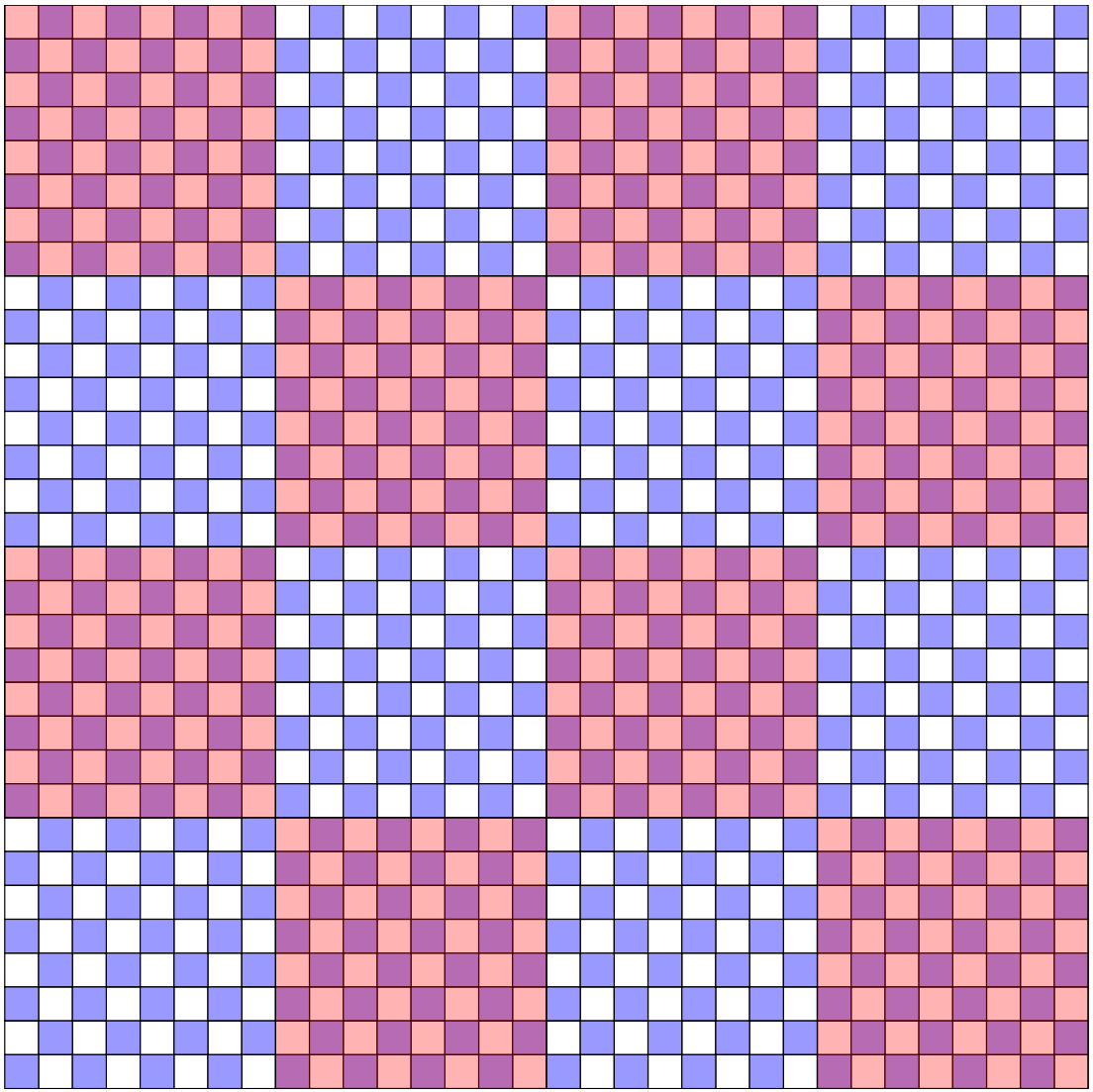
- many threads/blocks required to alleviate memory latencies
- per block shared memory much faster than global memory $\Rightarrow$ define sub-problems that fit in to the (currently 16KB) shared memory
- threads within a block can synchronize and reside on the same processor, blocks must be independent (arbitrary execution order)

Consequences for (Metropolis) simulations:

- best to use an independent RNG per thread $\Rightarrow$ need to make sure that sequences are uncorrelated
- divide system into tiles that can be worked on independently $\Rightarrow$ level-1 checkerboard
- each tile should fit into shared memory
- divide tile (again) in checkboard fashion for parallel update with different threads $\Rightarrow$ level-2 checkerboard

Checkerboard decomposition

- (red) large tiles: thread blocks
- (red) small tiles: individual threads
- load one large tile (plus boundary) into shared memory
- perform several spin updates per tile



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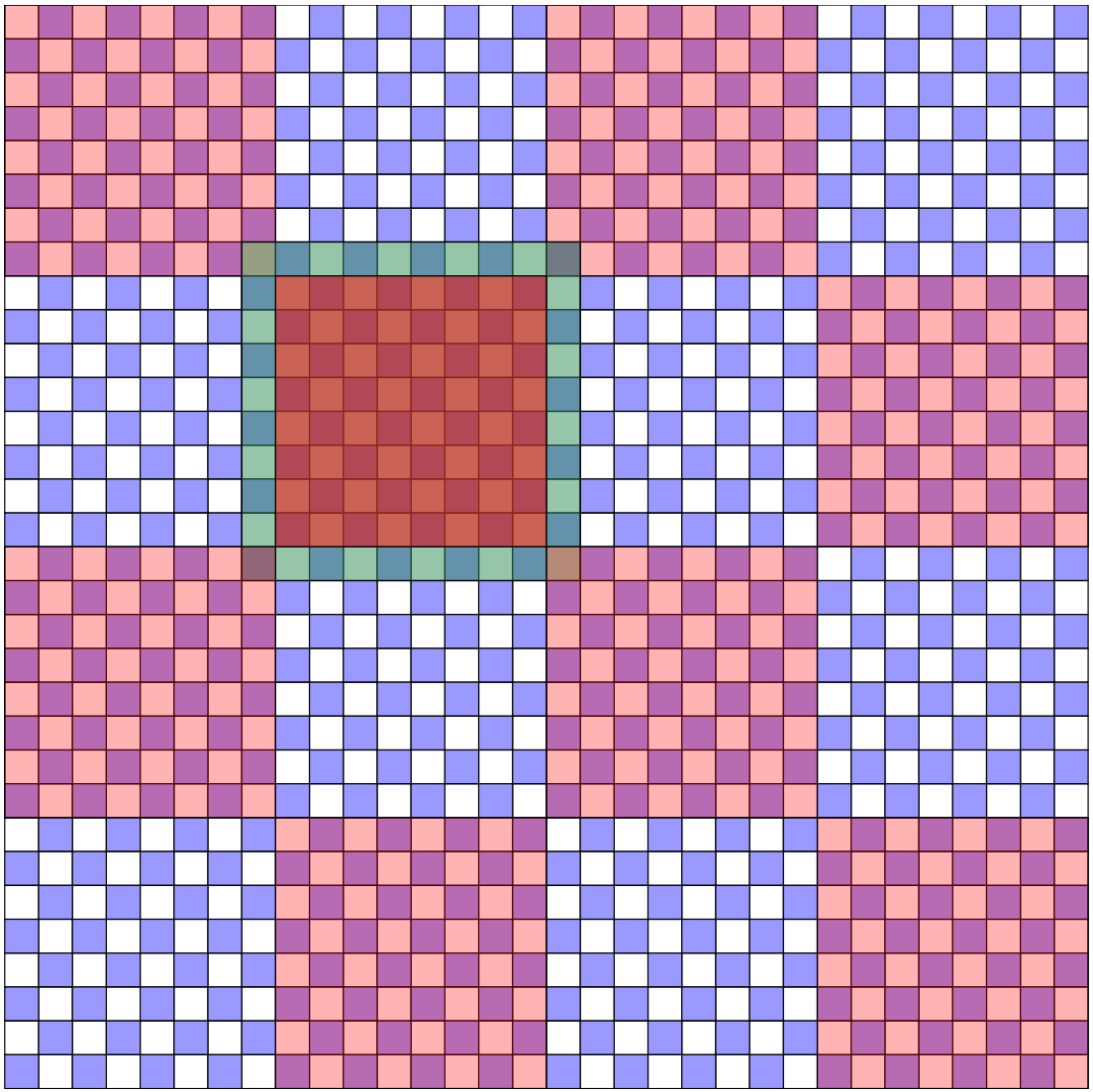

Implementation

```
__global__ void metro_sublattice_shared(spin_t *s, int *ranvec, int offset)
{
  int n = threadIdx.y*(BLOCKL/2)+threadIdx.x;

  int xoffset = (2*blockIdx.x+(blockIdx.y+offset)%2)*BLOCKL;
  int yoffset = blockIdx.y*BLOCKL;

  __shared__ spin_t sS[(BLOCKL+2)*(BLOCKL+2)];

  sS[(threadIdx.y+1)*(BLOCKL+2)+2*threadIdx.x+1] = s[(yoffset+threadIdx.y)*L+xoffset+2*threadIdx.x];
  sS[(threadIdx.y+1)*(BLOCKL+2)+2*threadIdx.x+2] = s[(yoffset+threadIdx.y)*L+xoffset+2*threadIdx.x+1];
  if(threadIdx.y == 0) {
    if(blockIdx.y == 0) {
      sS[2*threadIdx.x+1] = s[(L-1)*L+xoffset+2*threadIdx.x];
      sS[2*threadIdx.x+2] = s[(L-1)*L+xoffset+2*threadIdx.x+1];
    } else {
      sS[2*threadIdx.x+1] = s[(yoffset-1)*L+xoffset+2*threadIdx.x];
      sS[2*threadIdx.x+2] = s[(yoffset-1)*L+xoffset+2*threadIdx.x+1];
    }
  }
  if(threadIdx.y == BLOCKL-1) {
    if(blockIdx.y == GRIDL-1) {
      sS[(BLOCKL+1)*(BLOCKL+2)+2*threadIdx.x+1] = s[xoffset+2*threadIdx.x];
      sS[(BLOCKL+1)*(BLOCKL+2)+2*threadIdx.x+2] = s[xoffset+2*threadIdx.x+1];
    } else {
      sS[(BLOCKL+1)*(BLOCKL+2)+2*threadIdx.x+1] = s[(yoffset+BLOCKL)*L+xoffset+2*threadIdx.x];
      sS[(BLOCKL+1)*(BLOCKL+2)+2*threadIdx.x+2] = s[(yoffset+BLOCKL)*L+xoffset+2*threadIdx.x+1];
    }
  }
  if(threadIdx.x == 0) {
    if(xoffset == 0) sS[(threadIdx.y+1)*(BLOCKL+2)] = s[(yoffset+threadIdx.y)*L+(L-1)];
    else sS[(threadIdx.y+1)*(BLOCKL+2)] = s[(yoffset+threadIdx.y)*L+xoffset-1];
  }
  if(threadIdx.x == BLOCKL/2-1) {
    if(xoffset == L-BLOCKL) sS[(threadIdx.y+1)*(BLOCKL+2)+BLOCKL+1] = s[(yoffset+threadIdx.y)*L];
    else sS[(threadIdx.y+1)*(BLOCKL+2)+BLOCKL+1] = s[(yoffset+threadIdx.y)*L+xoffset+BLOCKL];
  }
```

Implementation

```
  __shared__ int ranvecS[THREADS];
  ranvecS[n] = ranvec[(blockIdx.y*(GRIDL/2)+blockIdx.x)*THREADS+n];

  __syncthreads();

  int x1 = (threadIdx.y%2)+2*threadIdx.x;
  int x2 = ((threadIdx.y+1)%2)+2*threadIdx.x;
  int y = threadIdx.y;

  for(int i = 0; i < SWEEPS_LOCAL; ++i) {
    int ide = sS(x1,y)*(sS(x1-1,y)+sS(x1+1,y)+sS(x1,y-1)+sS(x1,y+1));
    if(ide <= 0 || RAN(ranvecS[n]) < boltzD[ide]) sS(x1,y) = -sS(x1,y);

    __syncthreads();

    ide = sS(x2,y)*(sS(x2-1,y)+sS(x2+1,y)+sS(x2,y-1)+sS(x2,y+1));
    if(ide <= 0 || RAN(ranvecS[n]) < boltzD[ide]) sS(x2,y) = -sS(x2,y);

    __syncthreads();
  }

  s[(yoffset+threadIdx.y)*L+xoffset+2*threadIdx.x] = sS[(threadIdx.y+1)*(BLOCKL+2)+2*threadIdx.x+1];
  s[(yoffset+threadIdx.y)*L+xoffset+2*threadIdx.x+1] = sS[(threadIdx.y+1)*(BLOCKL+2)+2*threadIdx.x+2];
  ranvec[(blockIdx.y*(GRIDL/2)+blockIdx.x)*THREADS+n] = ranvecS[n];
}
```

Performance

How to assess performance?

- what to compare to (one CPU core, whole CPU, SMP system, ...)
- for really fair comparison: optimize CPU code for cache alignment, use SSE instructions etc.
- ignore measurements, since spin flips per μs, (ns, ps) is well-established unit for spin systems

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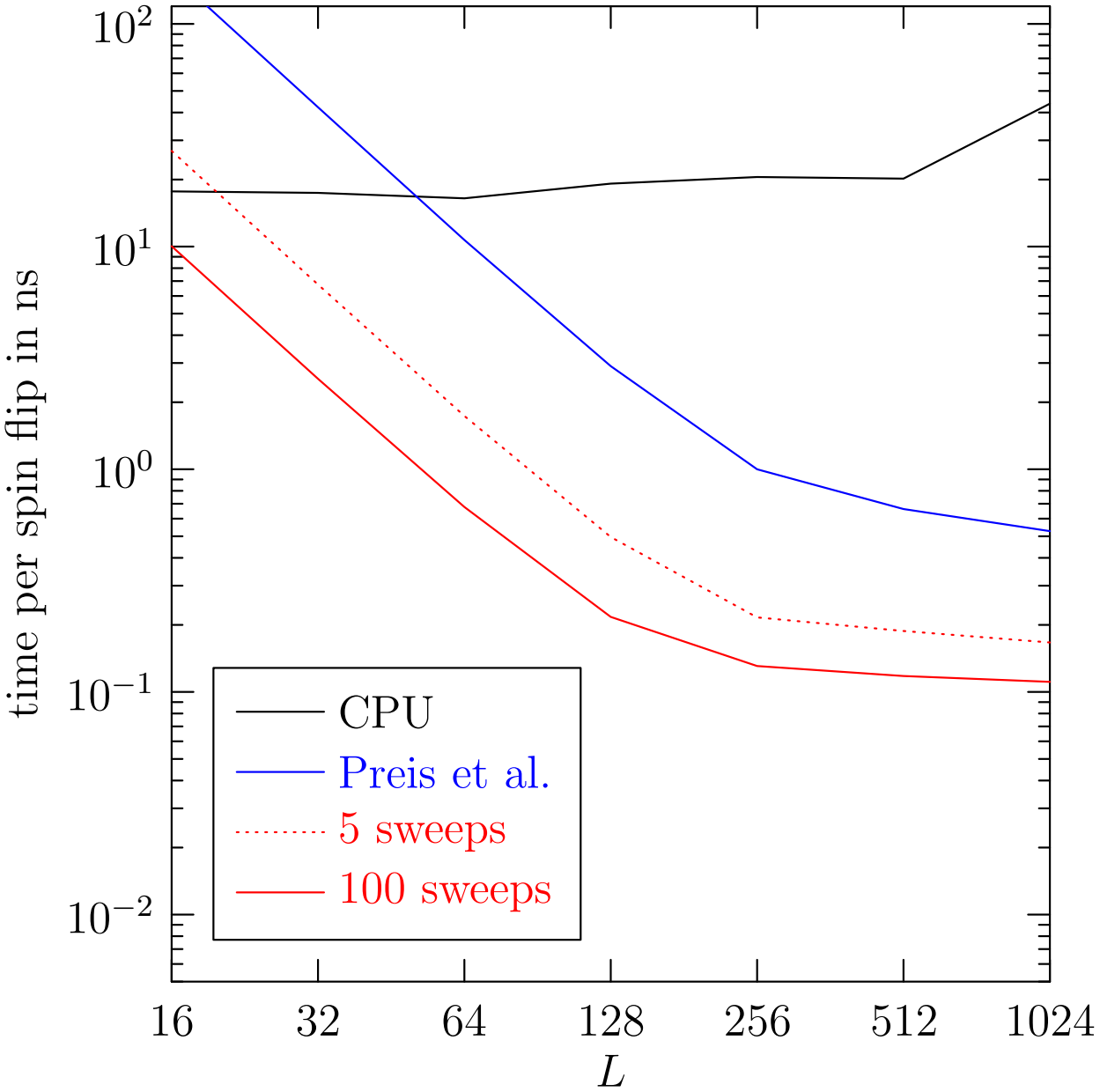
Example: Metropolis simulation of 2D Ising system

- use Knuth's linear congruential RNG
- no neighbor table since integer multiplies and adds are very cheap (4 instructions per clock cycle and processor)
- need to play with tile sizes to achieve best throughput

2D Ising ferromagnet



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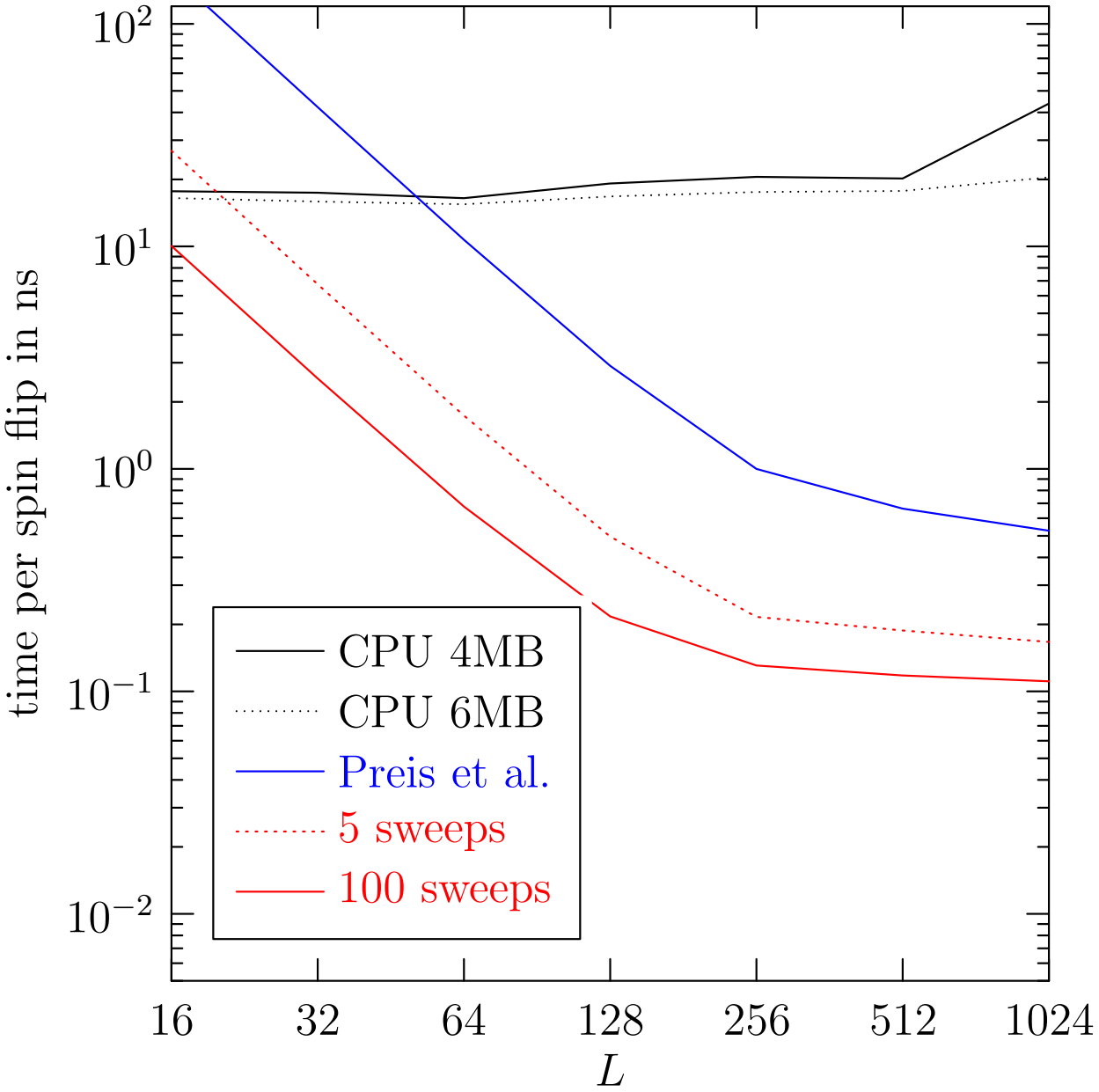

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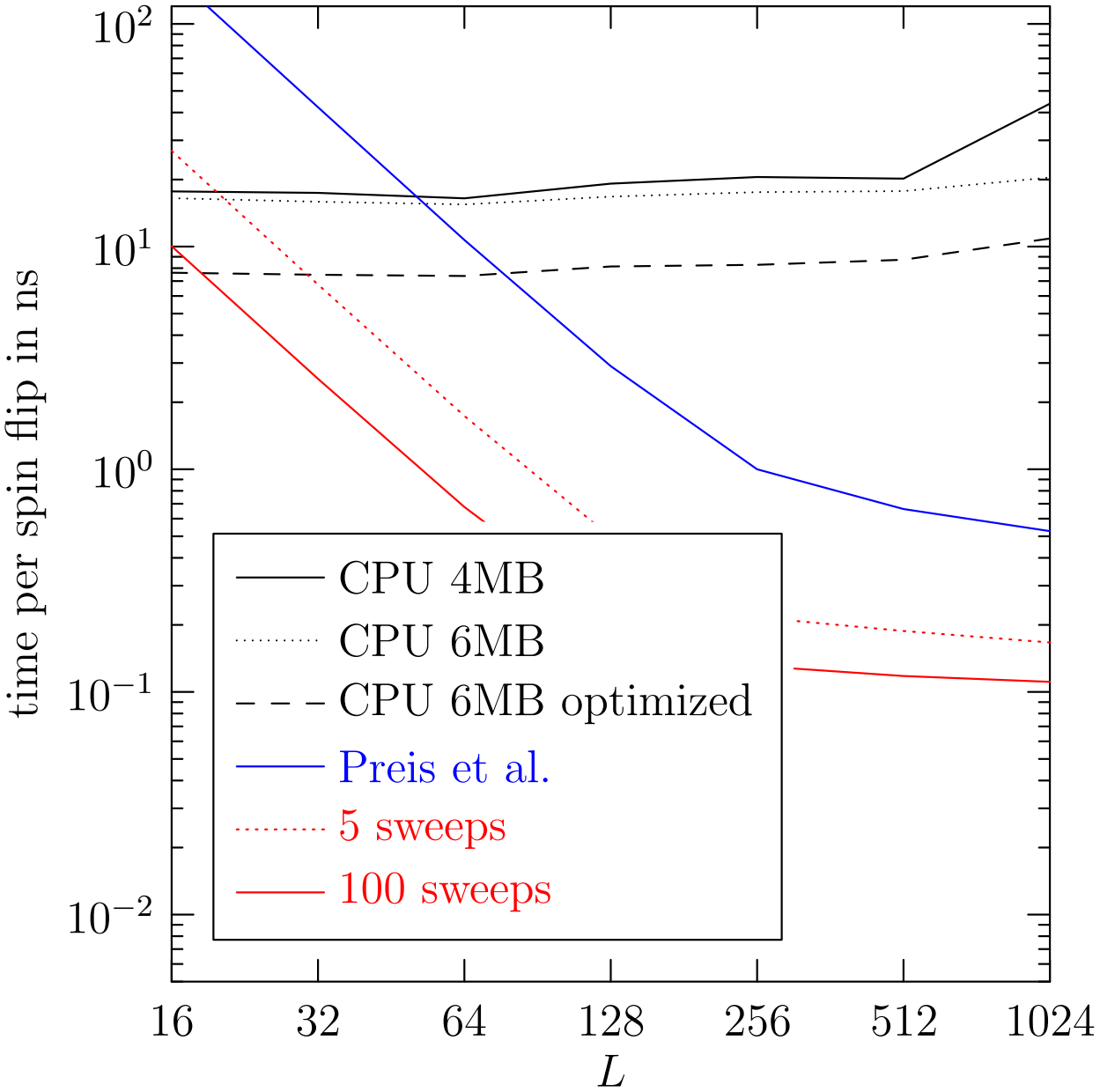

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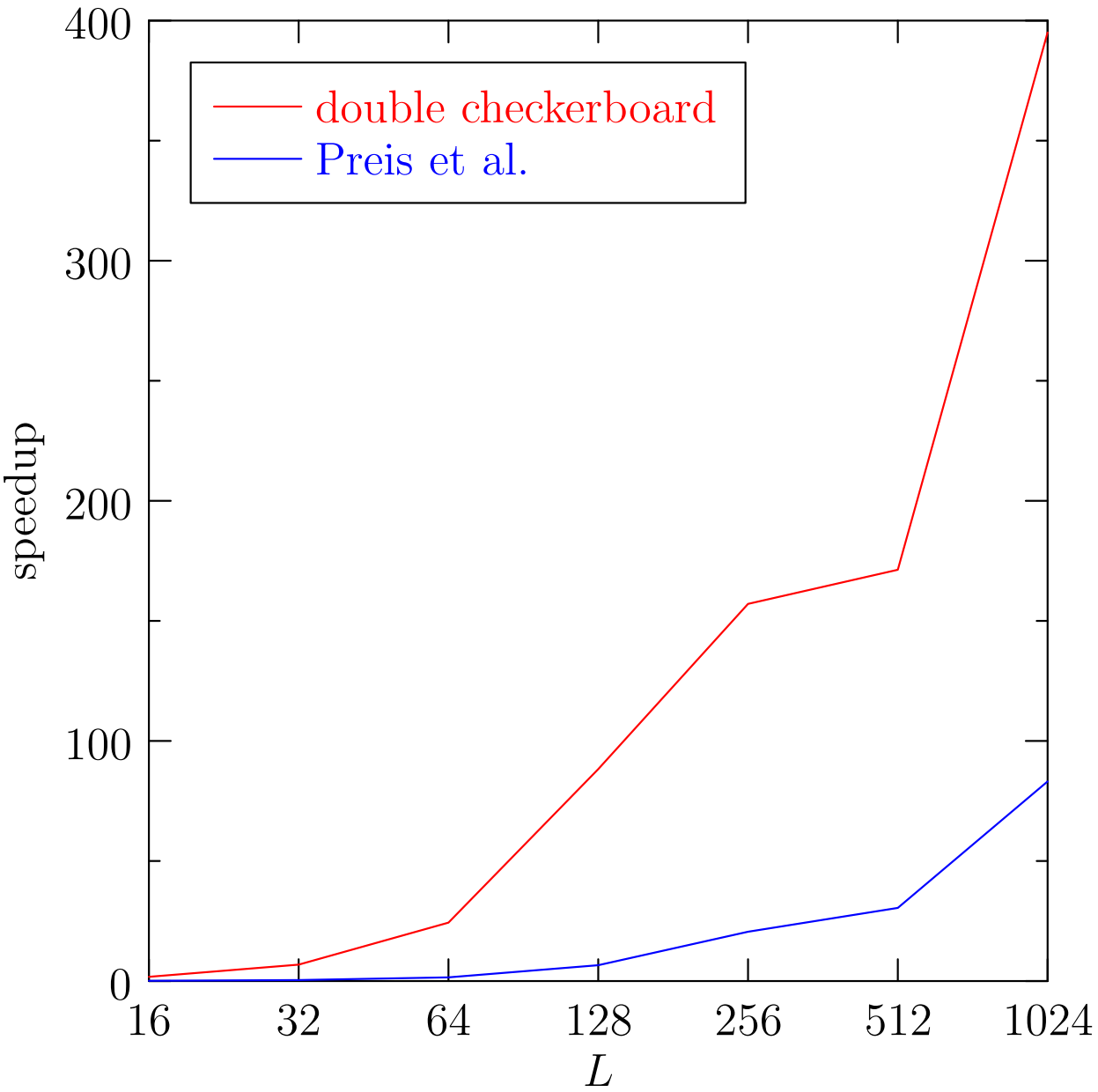

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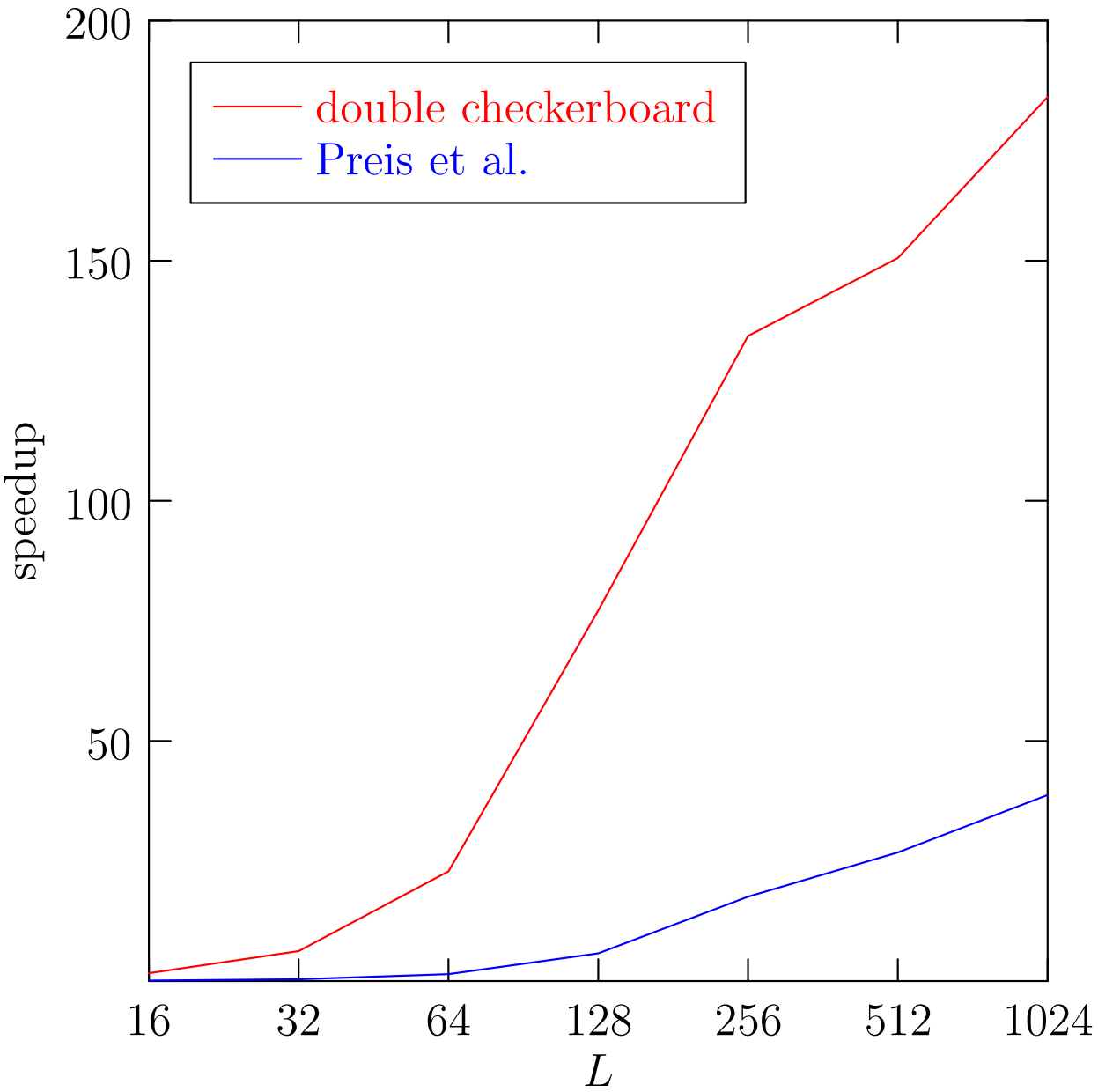

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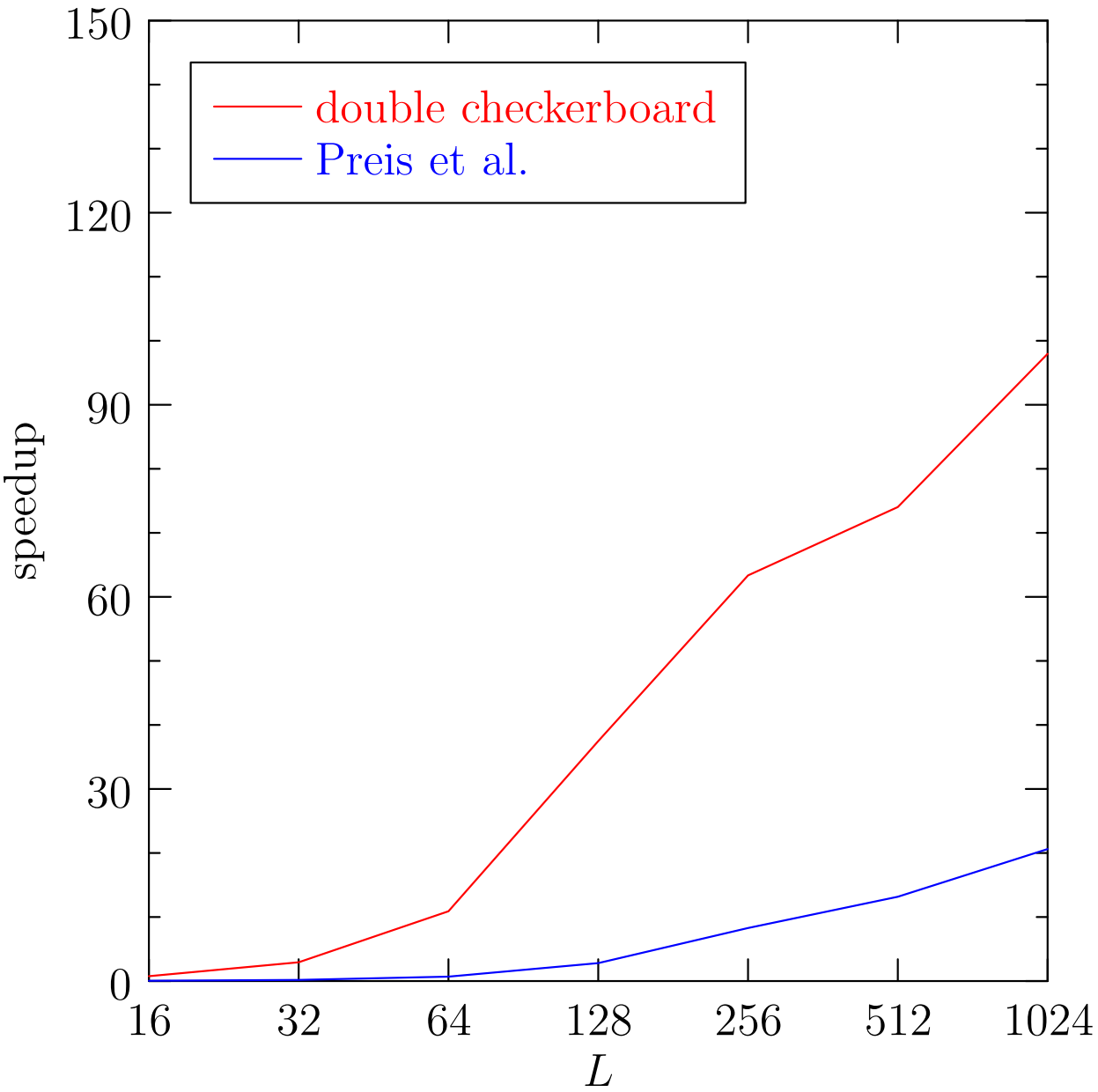

Heisenberg model

Maximum performance around 100 ps per spin flip for Ising model (vs. around 10 ns on CPU). What about continuous spins, i.e., float instead of int variables?

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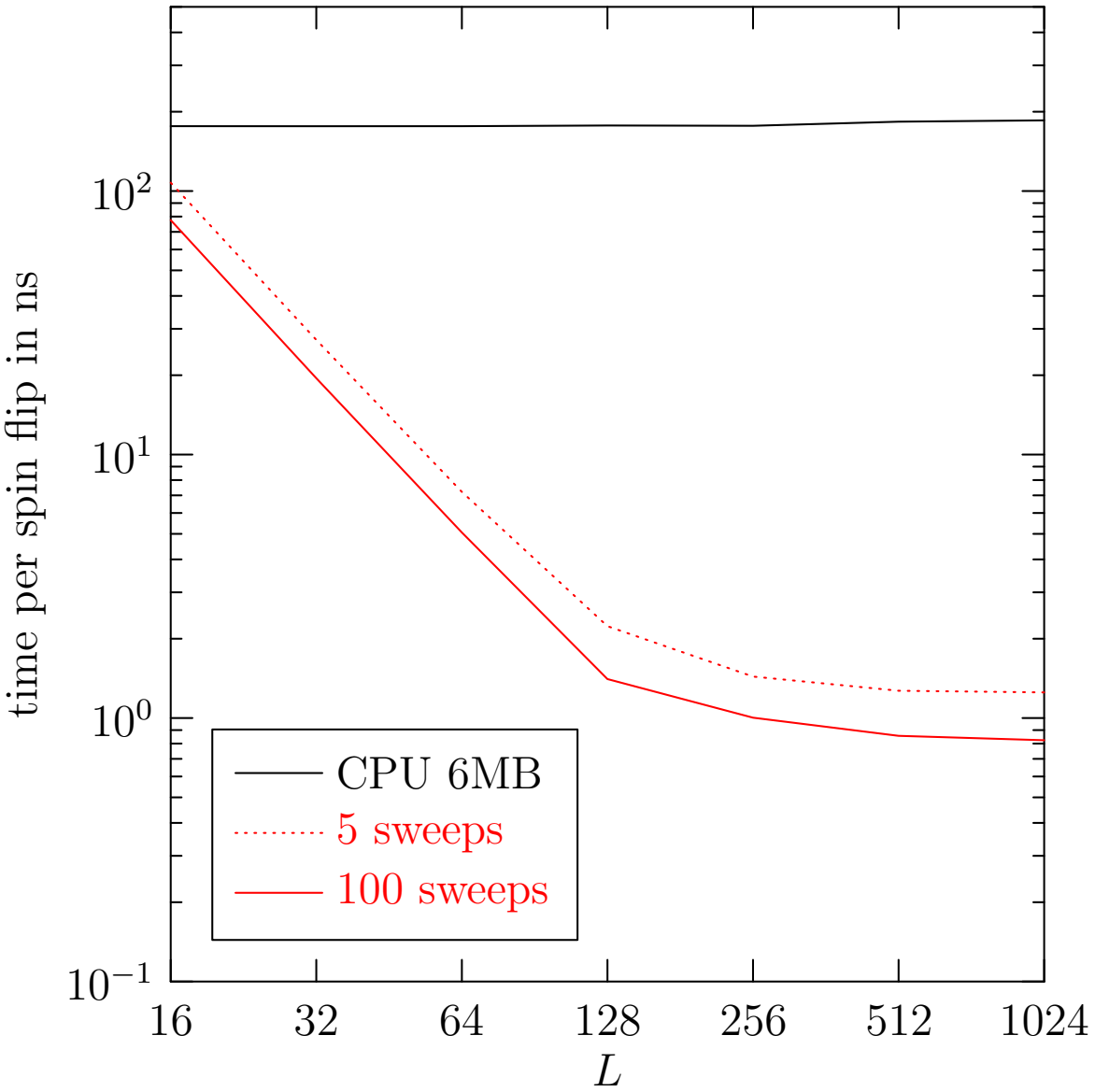
$\Rightarrow$ use same decomposition, but now floating-point computations are dominant:

- CUDA is not 100% IEEE compliant
- single-precision computations are supposed to be fast, double precision (supported since recently) much slower
- for single precision, normal ("high precision") and extra-fast, device-specific versions of sin, cos, exp etc. are provided

Heisenberg model: performance



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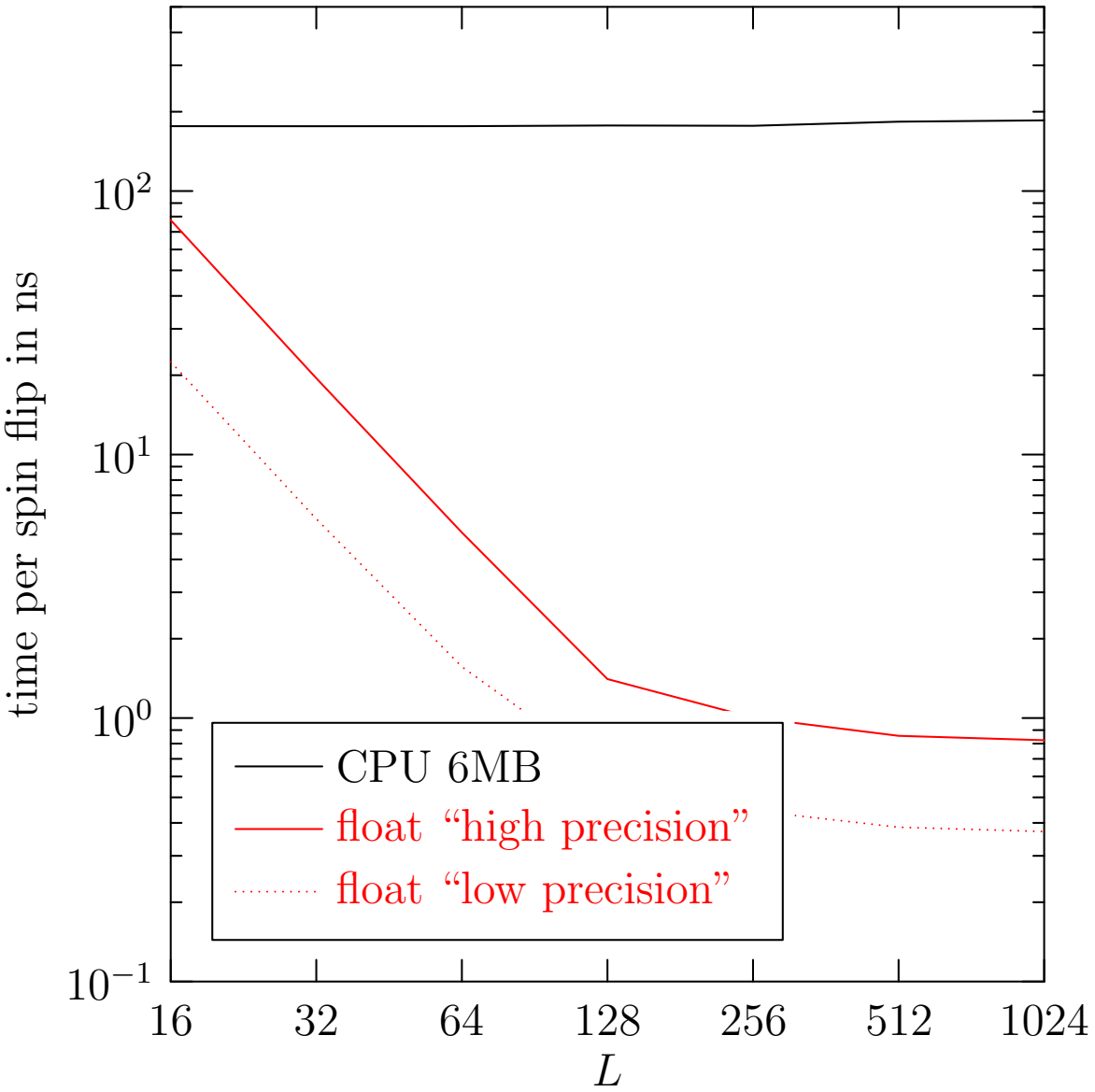

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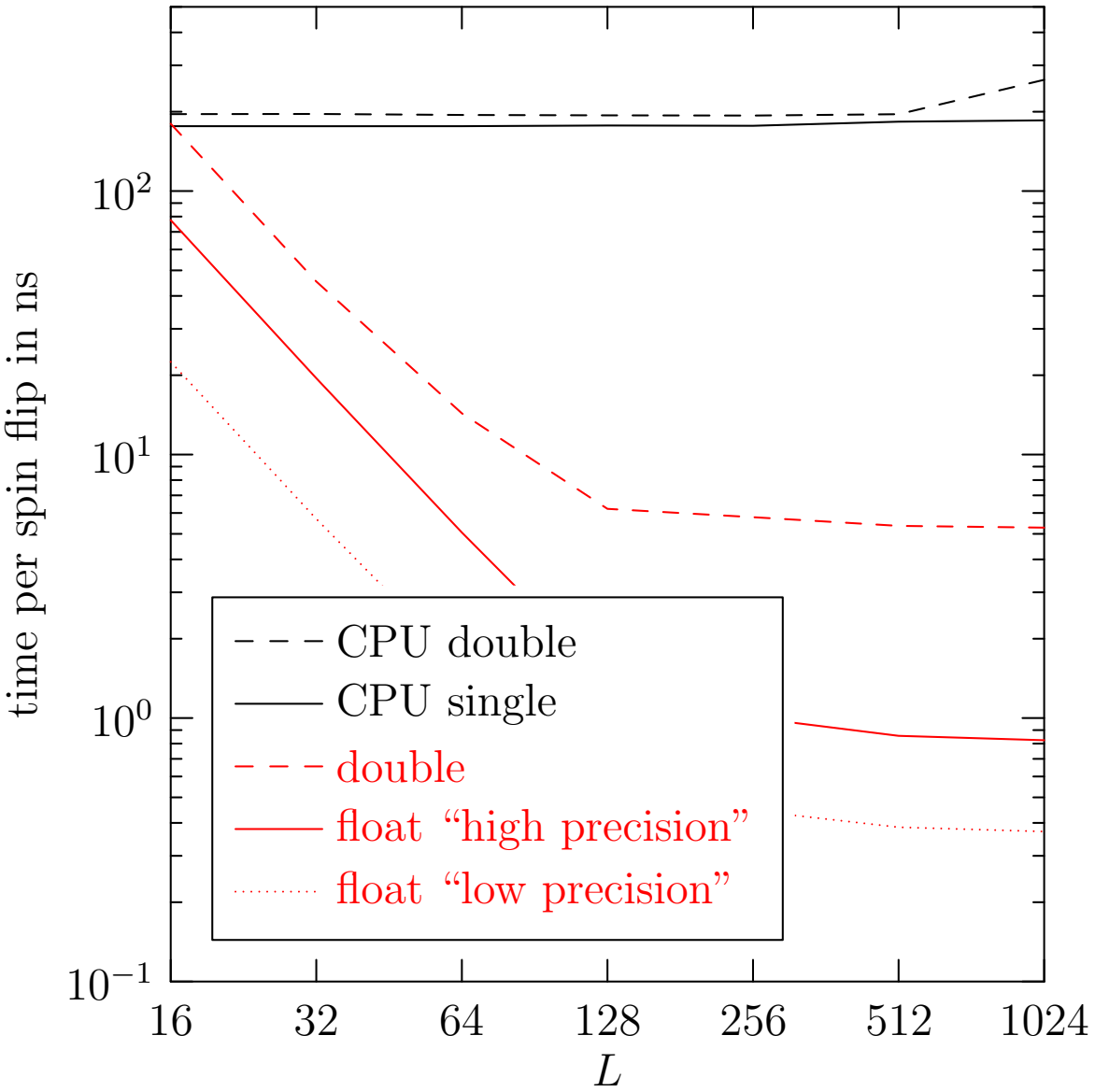

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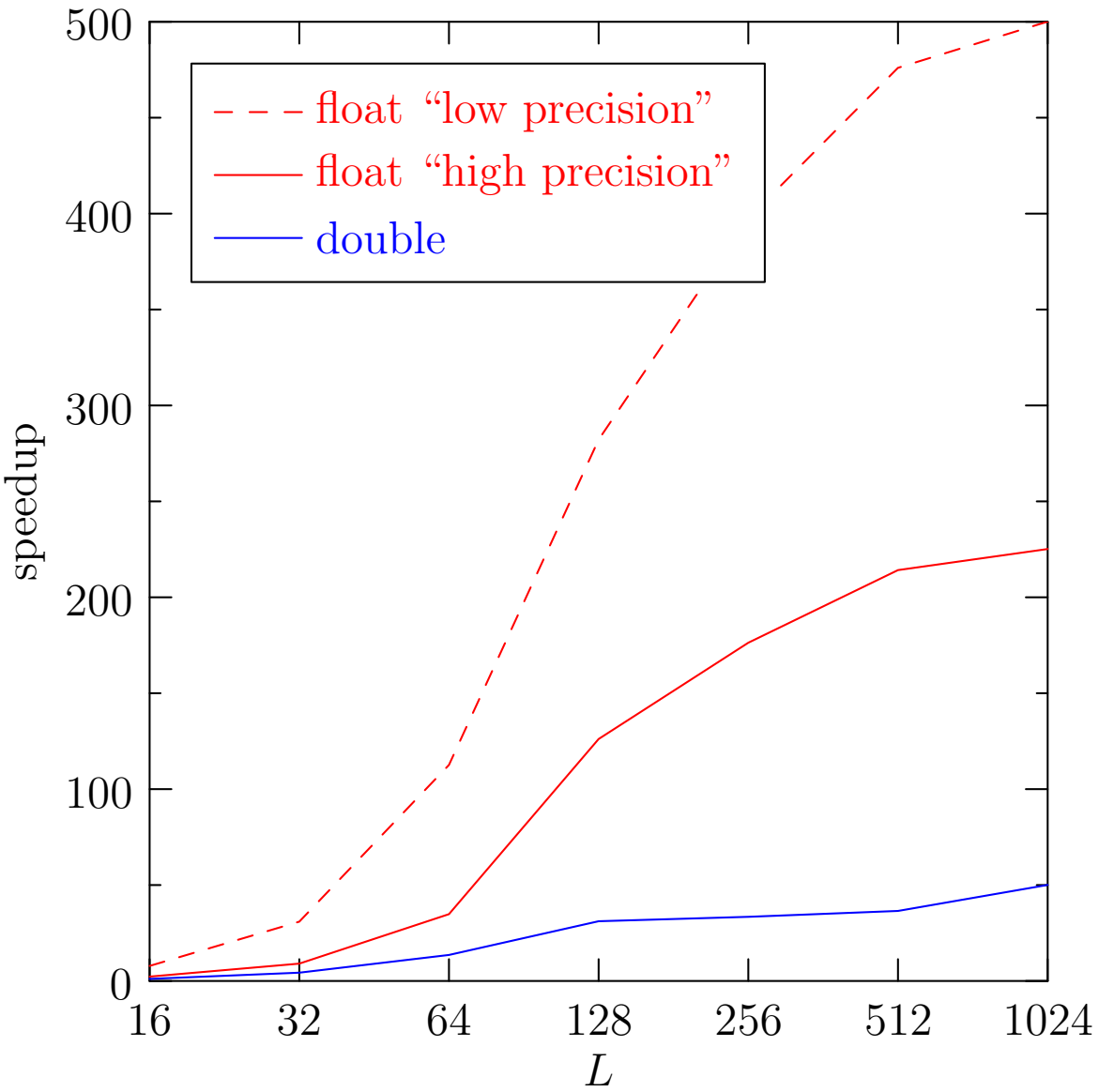

Heisenberg model: stability

Performance results:

- CPU: 185 ns (single) resp. 264 (double) per spin flip
- GPU: 0.8 ns (single), 0.4 ns (fast single) resp. 5.3 ns (double) per spin flip

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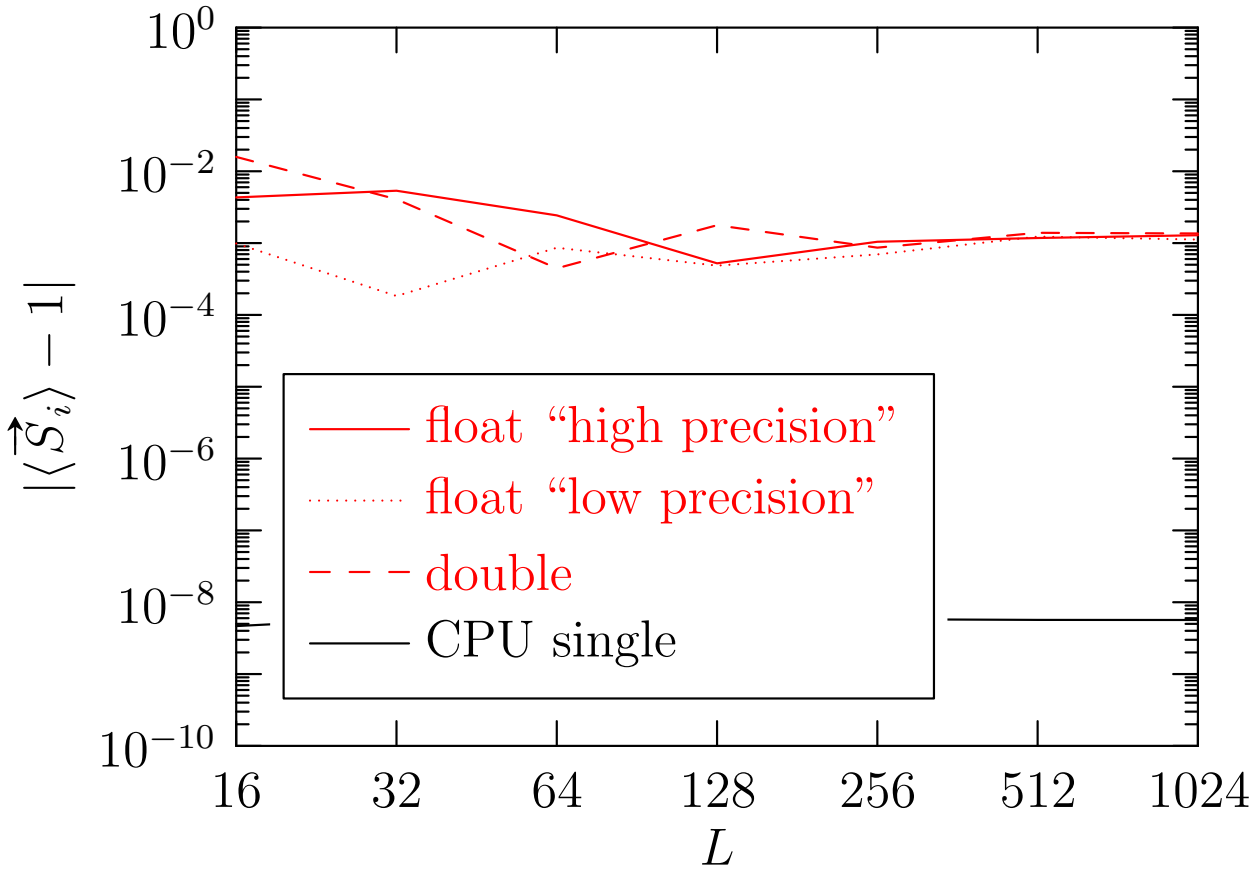

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- CPU: 185 ns (single) resp. 264 (double) per spin flip
- GPU: 0.8 ns (single), 0.4 ns (fast single) resp. 5.3 ns (double) per spin flip

How about stability?

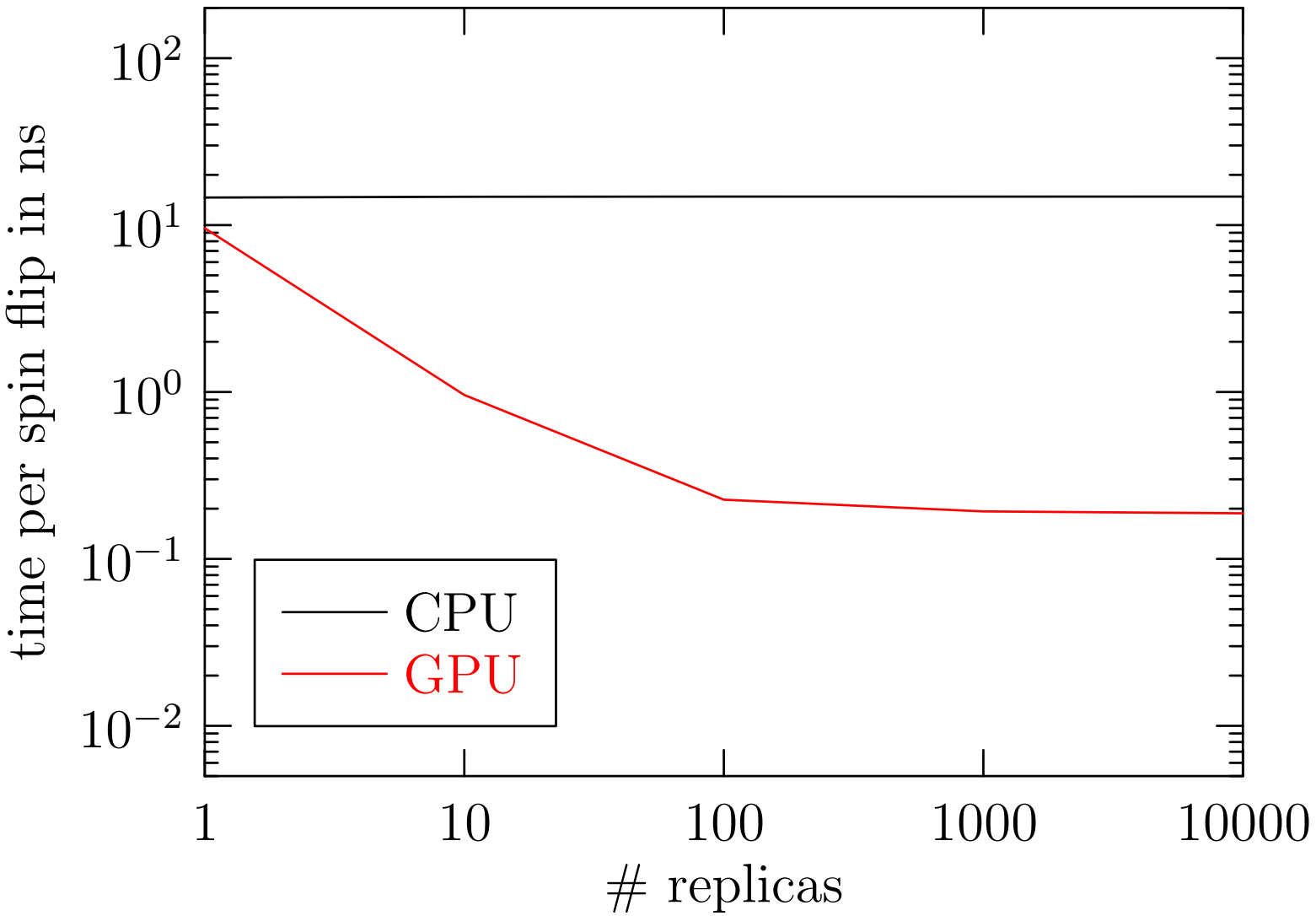
- no drift of spin normalization
- no deviations in averages from reference implementation (at least at low precision)
- more subtle effects: non-uniform trial vectors etc.
- needs closer look

Spin glasses

Simulate Edwards-Anderson model on GPU:

- same domain decomposition (checkerboard)
- slightly bigger effort due to non-constant couplings
- higher performance due to larger independence?
- very simple to combine with parallel tempering

Spin glass: performance



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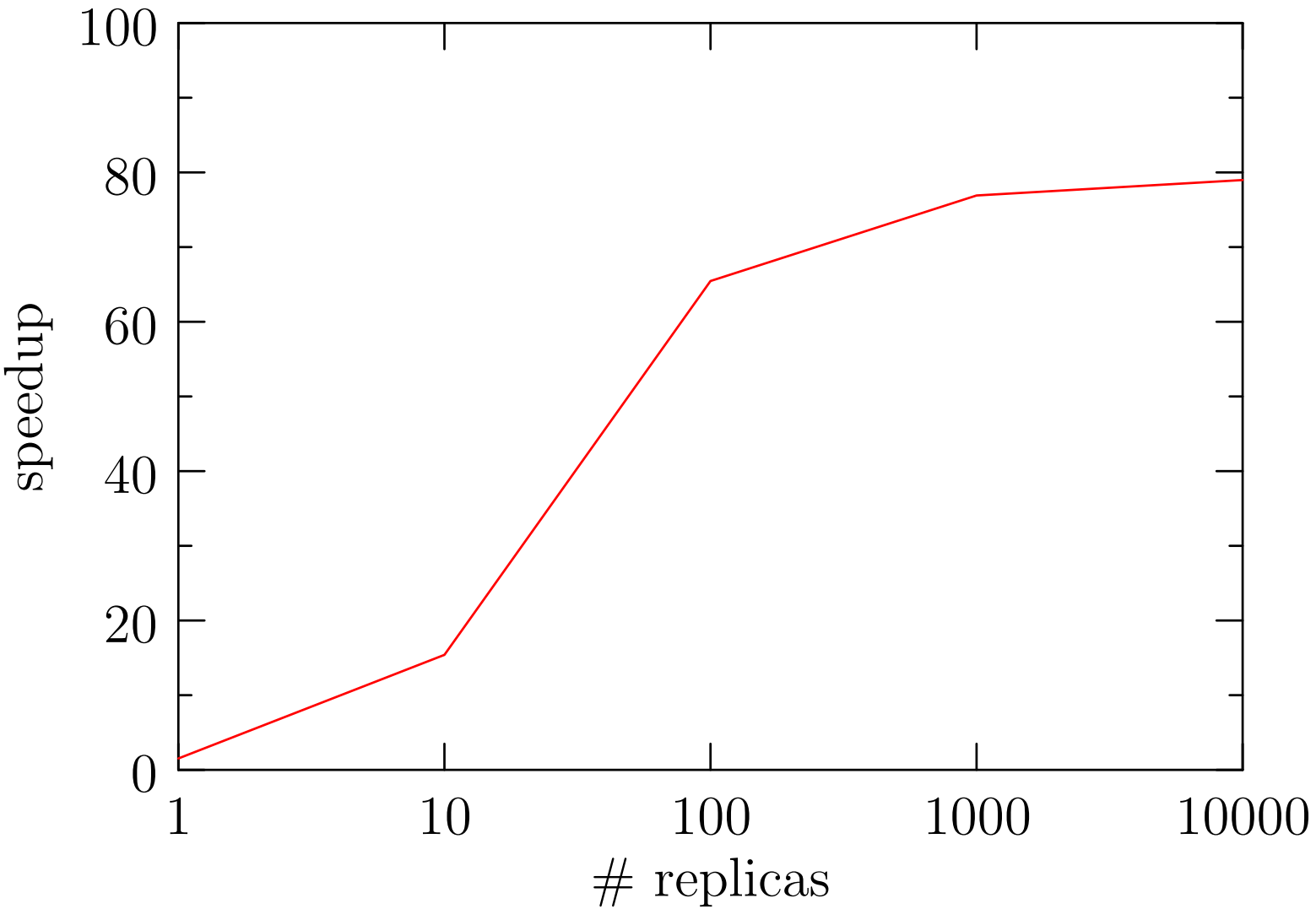

Spin glasses: continued

Seems to work well with

- 15 ns per spin flip on CPU
- 180 ps per spin flip on GPU

but not better than ferromagnetic Ising model.

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Further improvement: use multi-spin coding

- Synchronous multi-spin coding: different spins in a single configurations in one word
- Asynchronous multi-spin coding: spins from different realizations in one word

Implementation

```
for(int i = 0; i < SWEEPS_LOCAL; ++i) {
  float r = RAN(ranvecS[n]);
  if(r < boltzD[4]) sS(x1,y) = ~sS(x1,y);
  else {
    p1 = JSx(x1m,y) ^ sS(x1,y) ^ sS(x1m,y); p2 = JSx(x1,y) ^ sS(x1,y) ^ sS(x1p,y);
    p3 = JSy(x1,ym) ^ sS(x1,y) ^ sS(x1,ym); p4 = JSy(x1,y) ^ sS(x1,y) ^ sS(x1,yp);
    if(r < boltzD[2]) {
      ido = p1 | p2 | p3 | p4;
      sS(x1,y) = ido ^ sS(x1,y);
    } else {
      ido1 = p1 & p2; ido2 = p1 ^ p2;
      ido3 = p3 & p4; ido4 = p3 ^ p4;
      ido = ido1 | ido3 | (ido2 & ido4);
      sS(x1,y) = ido ^ sS(x1,y);
    }
  }

  __syncthreads();

  r = RAN(ranvecS[n]);
  if(r < boltzD[4]) sS(x2,y) = ~sS(x2,y);
  else {
    p1 = JSx(x2m,y) ^ sS(x2,y) ^ sS(x2m,y); p2 = JSx(x2,y) ^ sS(x2,y) ^ sS(x2p,y);
    p3 = JSy(x2,ym) ^ sS(x2,y) ^ sS(x2,ym); p4 = JSy(x2,y) ^ sS(x2,y) ^ sS(x2,yp);
    if(r < boltzD[2]) {
      ido = p1 | p2 | p3 | p4;
      sS(x2,y) = ido ^ sS(x2,y);
    } else {
      ido1 = p1 & p2; ido2 = p1 ^ p2;
      ido3 = p3 & p4; ido4 = p3 ^ p4;
      ido = ido1 | ido3 | (ido2 & ido4);
      sS(x2,y) = ido ^ sS(x2,y);
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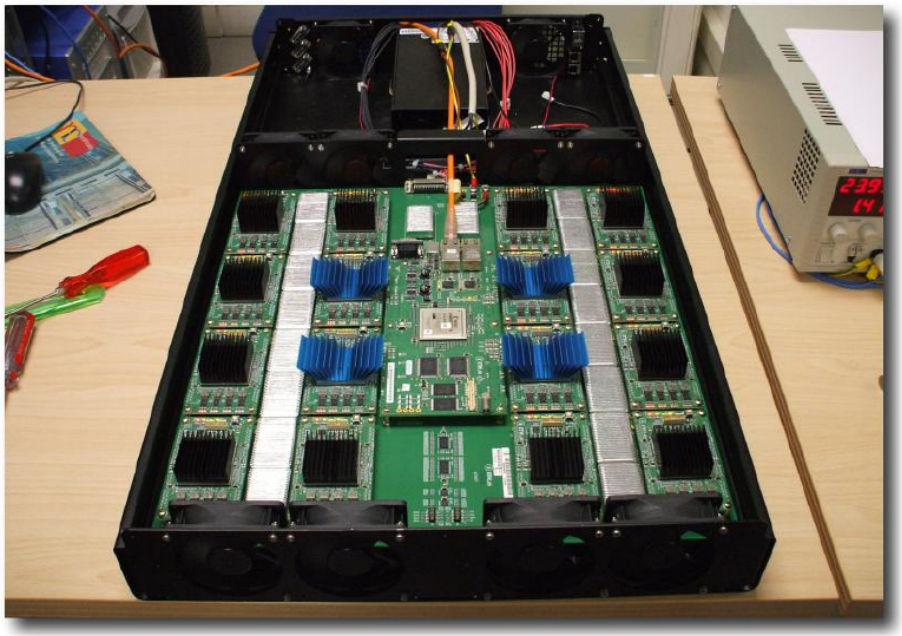
$\Rightarrow$ brings us down to about 15 ps per spin flip

Janus

JANUS, a modular massively parallel and reconfigurable FPGA-based computing system.



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		JANUS		PC		
MODEL	Algorithm	Max size	perfs	AMSC	SMSC	NO MSC
3D Ising EA	Metropolis	96^3	16 ps	45×	190×	
3D Ising EA	Heat Bath	96^3	16 ps	60×		
$Q = 4$ 3D Glassy Potts	Metropolis	16^3	64 ps	1250×	1900×	
$Q = 4$ 3D disordered Potts	Metropolis	88^3	32 ps	125×		1800×
$Q = 4$, $C_m = 4$ random graph	Metropolis	24000	2.5 ns	2.4×		10×

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Costs:

- Janus: 256 units, total cost about $700,000$ Euros
- Same performance with GPU: 64 PCs (2000 Euros) with 2 GTX 295 cards (500 Euros) $\Rightarrow 200,000$ Euros
- Same performance with CPU only (assuming a speedup of ~ 50): 800 blade servers with two dual Quadcore sub-units (3500 Euros) $\Rightarrow 2,800,000$ Euros

Outlook

Conclusions:

- GPGPU promises significant speedups at moderate coding effort
- need to find appropriate domain decomposition to leverage shared memory efficiency
- especially promising for problems with continous variables, but need to study precision effects
- effort significantly smaller than for (design and programming of) special-purpose machines
- GPGPU might be a fashion, but CPU computing goes the same way

Outlook:

- cluster algorithm is possible and looks promising
- parallel tempering no problem
- generalized-ensemble techniques might be more of a challenge