Rigorous Calculation of the Partition Function for the Finite Number of Ising Spins

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МАРТ

Formalism of the Ising Model

- Hamiltonian

$$H = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{Z} J_{ij} S_i S_j - h\sum_{i}^{N} S_i, \qquad (1)$$

$$Z_N(h,T) = \sum_{S_1}\sum_{S_2}\cdots\sum_{S_N} Exp\left[-\frac{H}{T}\right]. \qquad (2)$$

Partition Function for 4x4

$$
\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Sum}\Big[\mathrm{Exp}\Big[-k\Big(
$$

$$
\begin{aligned}
& S_1 S_2 + S_2 S_3 + S_3 S_4 + S_4 S_1 + \\
& S_5 S_6 + S_6 S_7 + S_7 S_8 + S_8 S_5 + \\
& S_9 S_{10} + S_{10} S_{11} + S_{11} S_{12} + S_{12} S_9 + \\
& S_{13} S_{14} + S_{14} S_{15} + S_{15} S_{16} + S_{16} S_{13} + \\
& \\
& S_1 S_5 + S_5 S_9 + S_9 S_{13} + S_{13} S_1 + \\
& S_2 S_6 + S_6 S_{10} + S_{10} S_{14} + S_{14} S_2 + \\
& S_3 S_7 + S_7 S_{11} + S_{11} S_{15} + S_{15} S_3 + \\
& S_4 S_8 + S_8 S_{12} + S_{12} S_{16} + S_{16} S_4 + \\
& h \sum_{r=1}^{16} S_r \Big)\Big], \{S_1, -1, 1, 2\}\Big], \{S_2, -1, 1, 2\}\Big], \{S_3, -1, 1, 2\}\Big],
\end{aligned}
$$

$$
\{S_4, -1, 1, 2\}\Big], \{S_5, -1, 1, 2\}\Big], \{S_6, -1, 1, 2\}\Big], \{S_7, -1, 1, 2\}\Big],
$$

$$
\{S_8, -1, 1, 2\}\Big], \{S_9, -1, 1, 2\}\Big], \{S_{10}, -1, 1, 2\}\Big], \{S_{11}, -1, 1, 2\}\Big],
$$

$$
\{S_{12}, -1, 1, 2\}\Big], \{S_{13}, -1, 1, 2\}\Big], \{S_{14}, -1, 1, 2\}\Big], \{S_{15}, -1, 1, 2\}\Big], \{S_{16}, -1, 1, 2\}\Big]
$$

Partition Function for 4x4

$$e^{-32k+16hk} +$$
$$16\, e^{-24k+14hk} +$$
$$32\, e^{-20k+12hk} + 88\, e^{-16k+12hk} +$$
$$96\, e^{-16k+10hk} + 256\, e^{-12k+10hk} + 208\, e^{-8k+10hk} +$$
$$24\, e^{-16k+8hk} + 256\, e^{-12k+8hk} + 736\, e^{-8k+8hk} + 576\, e^{-4k+8hk} + 228\, e^{8hk}$$
$$192\, e^{-12k+6hk} + 688\, e^{-8k+6hk} + 1664\, e^{-4k+6hk} + 1248\, e^{6hk} + 448\, e^{4k+6hk} + 128\, e^{8k+6hk} +$$
$$96\, e^{-12k+4hk} + 704\, e^{-8k+4hk} + 1824\, e^{-4k+4hk} + 2928\, e^{4hk} + 1568\, e^{4k+4hk} + 768\, e^{8k+4hk} + 64\, e^{12k+4hk} + 56\, e^{16k+4hk} +$$
$$64\, e^{-12k+2hk} + 624\, e^{-8k+2hk} + 1920\, e^{-4k+2hk} + 3680\, e^{2hk} + 3136\, e^{4k+2hk} + 1392\, e^{8k+2hk} + 512\, e^{12k+2hk} + 96\, e^{16k+2hk} + 16\, e^{24k+2hk} +$$
$$8\, e^{-16k} + 768\, e^{-8k} + 1600\, e^{-4k} + 4356 + 3264\, e^{4k} + 2112\, e^{8k} + 576\, e^{12k} + 120\, e^{16k} + 64\, e^{20k} + 2\, e^{32k} +$$
$$64\, e^{-12k-2hk} + 624\, e^{-8k-2hk} + 1920\, e^{-4k-2hk} + 3680\, e^{-2hk} + 3136\, e^{4k-2hk} + 1392\, e^{8k-2hk} + 512\, e^{12k-2hk} + 96\, e^{16k-2hk} + 16\, e^{24k-2hk} +$$
$$96\, e^{-12k-4hk} + 704\, e^{-8k-4hk} + 1824\, e^{-4k-4hk} + 2928\, e^{-4hk} + 1568\, e^{4k-4hk} + 768\, e^{8k-4hk} + 64\, e^{12k-4hk} + 56\, e^{16k-4hk} +$$
$$192\, e^{-12k-6hk} + 688\, e^{-8k-6hk} + 1664\, e^{-4k-6hk} + 1248\, e^{-6hk} + 448\, e^{4k-6hk} + 128\, e^{8k-6hk} +$$
$$24\, e^{-16k-8hk} + 256\, e^{-12k-8hk} + 736\, e^{-8k-8hk} + 576\, e^{-4k-8hk} + 228\, e^{-8hk}$$
$$96\, e^{-16k-10hk} + 256\, e^{-12k-10hk} + 208\, e^{-8k-10hk} +$$
$$32\, e^{-20k-12hk} + 88\, e^{-16k-12hk} +$$
$$16\, e^{-24k-14hk} +$$
$$e^{-32k-16hk}$$

$2^{16}=65536$

Massively Parallel Processing

unsigned short int a[4]={a_1 , a_2 , a_3 , a_4};

a_1	a_2	a_3	a_4
S_1	S_2	S_3	S_4
S_5	S_6	S_7	S_8
S_9	S_{10}	S_{11}	S_{12}
S_{13}	S_{14}	S_{15}	S_{16}

S_i={1,0}

2	4	7	15
0	0	0	1
0	1	1	1
1	0	1	1
0	0	1	1
0	0	0	0
…	…	…	…

Spin Excess

2	4	7	15
0	**0**	**0**	**1**
0	**1**	**1**	**1**
1	**0**	**1**	**1**
0	**0**	**1**	**1**

Kernighan algorithm

```
int q_units(unsigned short int i)
        {
         int j = 0;
         while (i)
         {i&=i-1; ++j;}
          return j;
        }
```

Brian W. Kernighan, Dennis M. Ritchie, "C Programming Language", Published by Prentice-Hall in 1988, ISBN 0-13-110362-81988.

$\mathbf{M_i}$+=q_units(2);

$\mathbf{M_i}$+=q_units(4);

$\mathbf{M_i}$+=q_units(7);

$\mathbf{M_i}$+=q_units(15);

Spin Excess=2$\mathbf{M_i}$-N

usigned int units[2^4]={0,1,1,2,1,…}

Energy of Columns and Strings. Parallelism

	2 ^	4 ^	7 ^	15	2^4=6	~6-(0^0-N))=9
	0	0	0	1	0	1
^	0	1	1	1	1	0
^	1	0	1	1	1	0
^	0	0	1	1	0	1
					…	

Pairs of zeros

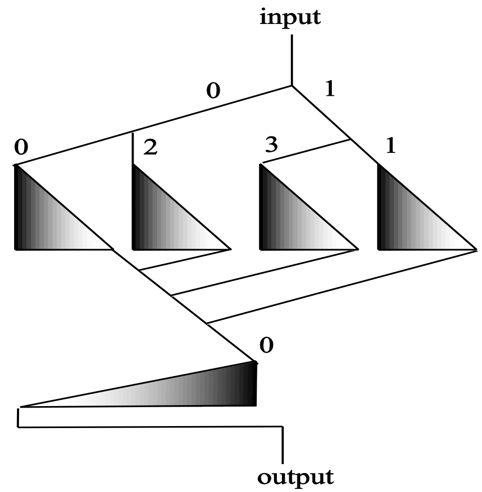
$$E_{tot}=2(-En+N)$$

if a[i]<7

0 ^	0
0	1
1	0
0	0
2 ^	4

if a[i]>7

1 ^	0
0	0
0	0
0	1
8 ^	1 (9^3)



The logical scheme of the parallel algorithm with dynamical generation of two processes by two.

Results of Calculation for 4x4 System

Nc	M_i	E_i
1	16	-32
16	14	-24
32	12	-20
88	12	-16
96	10	-16
256	10	-12
208	10	-8
24	8	-16
256	8	-12
736	8	-8
228	8	0
576	8	-4
192	6	-12
688	6	-8
1664	6	-4
1248	6	0
448	6	4
128	6	8

Nc	M_i	E_i
96	4	-12
704	4	-8
1824	4	-4
2928	4	0
1568	4	4
768	4	8
56	4	16
64	4	12
64	2	-12
624	2	-8
1920	2	-4
3680	2	0
3136	2	4
1392	2	8
512	2	12
96	2	16
16	2	24

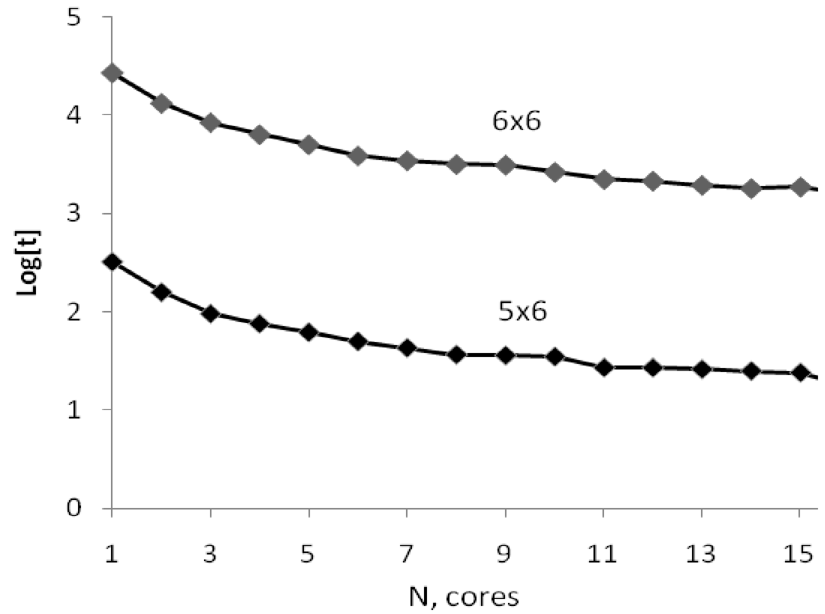
Nc	M_i	E_i
8	0	-16
768	0	-8
1600	0	-4
4356	0	0
2112	0	8
3264	0	4
576	0	12
120	0	16
64	0	20
2	0	32

Nc	M_i	E_i
64	-2	-12
624	-2	-8
1920	-2	-4
3680	-2	0
3136	-2	4
1392	-2	8
512	-2	12
96	-2	16
16	-2	24
96	-4	-12
704	-4	-8
1824	-4	-4
2928	-4	0
1568	-4	4
768	-4	8
64	-4	12
56	-4	16

Nc	M_i	E_i
192	-6	-12
688	-6	-8
1664	-6	-4
1248	-6	0
448	-6	4
128	-6	8
24	-8	-16
256	-8	-12
736	-8	-8
576	-8	-4
228	-8	0
96	-10	-16
256	-10	-12
208	-10	-8
32	-12	-20
88	-12	-16
16	-14	-24
1	-16	-32

HP Cluster

HP cluster Intel Xeon E5410 @ 2.33GHz.



The dependence on logarithm of time from number of the cores for deferent number of spins.
time.h and the function *MPI_Wtime()*

Gordon Bell's Expectation

Table. 1 The measuring of process duration by means of different methods for 5x5 lattice system. Time in sec.

N	**clock();**	**MPI_Wtime();**	**ftime();**	**System Command "time"**	**Duration open-closing datafile**
0	37.530	**37.9297**	**38.662**	real **38.613**s	**37.478**
1	37.460	37.4688	37.468		
2	37.710	37.7188	37.66		
3	**37.910**	37.918	38.612		
Single process	**156.280**	**156.312**	**156.315**	real **156.536**	**156.286**
Speedup 4	**4.122**	**4.121**	**4.043**	**4.054**	**4.170**
Speedup 8	**8.068**	**8.064**	**8.062**	**7.714**	**8.08**
Speedup 16	**15.947**	**8.279**	**8.279**	**7.529**	**8.116**

Conclusions

1) The using of massive bit-parallelism allows cut the time of calculations, but to get the solution for tasks with large lattice it demand the enhancement of algorithm (for example, to take into account the symmetry of task)

2) The exceeding of experimental speedup values under predicted by Amdahl low values could be in connection with inquiry processing form the cache.

Thank You!