Konferencja Użytkowników Komputerów Dużej Mocy

15 min

Aleksander Dawid

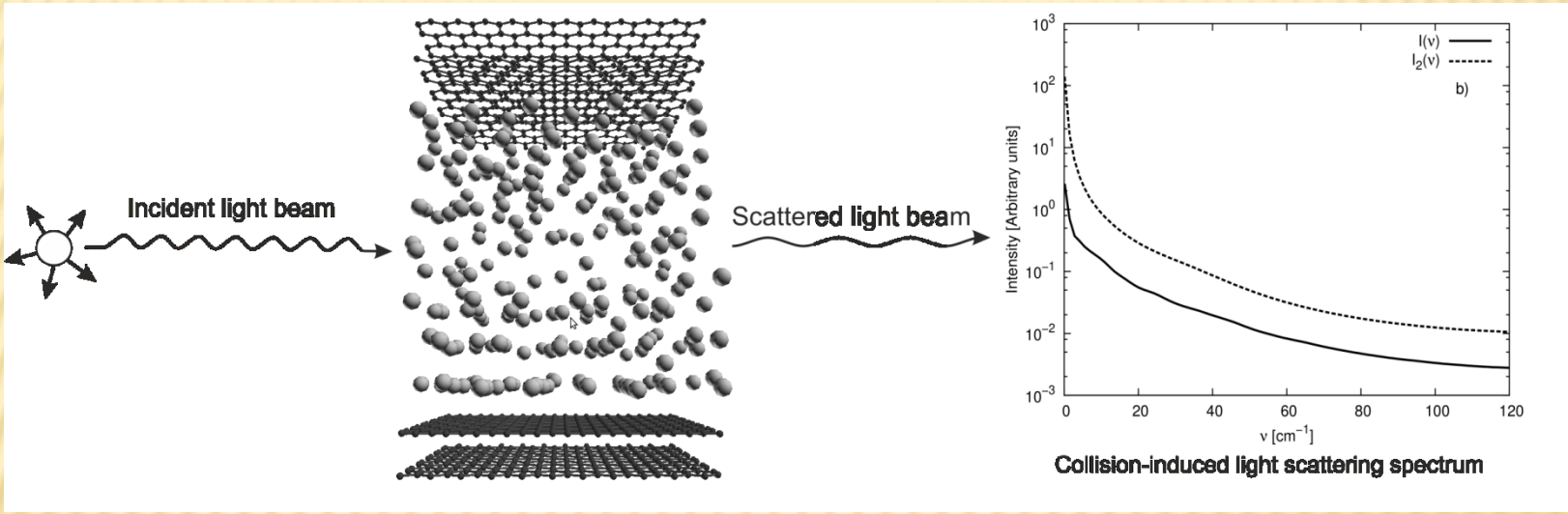
THE CALCULATION OF FOUR BODY CORRELATION FUNCTION USING MASSIVE MULTICORE CUDA TECHNOLOGY

Zakopane 2015

OUTLINE

- Interaction-induced light scattering
- The four-body correlation function
- CUDA algorithm
- Results

INTERACTION-INDUCED LIGHT SCATTERING



When two clouds of electrons overlap on each other the polarizability of such system is no longer isotropic. This anisotropy generates short-time dipole moment that is able to interact with electromagnetic radiation.

Dipol-Induced-Dipol Model

$$\beta_{ij}(t) = \sigma^3[3x_{ij}(t)z_{ij}(t)/r_{ij}^5(t)]$$

INTERACTION-INDUCED LIGHT SCATTERING

The depolarized Rayleigh spectrum is the Fourier transform of the polarizability anisotropy autocorrelation function G(t), which for a monatomic sample of N atoms is

$$G(t) \propto \left\langle \sum_{i,j,k,l=1, i\neq j, k\neq l}^{N} \beta_{ij}(t)\beta_{kl}(0) \right\rangle$$

The total correlation function G(t) can be decomposed into pair, triplet, and quadruplet contributions

$$G(t) = G_2(t) + G_3(t) + G_4(t)$$

INTERACTION-INDUCED LIGHT SCATTERING

The component functions can be written as follow

1:1 $$G_2(t) \propto \left\langle \sum_{\substack{i,j=1,\\ i\neq j}}^{N} \beta_{ij}(t)\beta_{ij}(0) \right\rangle$$ Two-body function

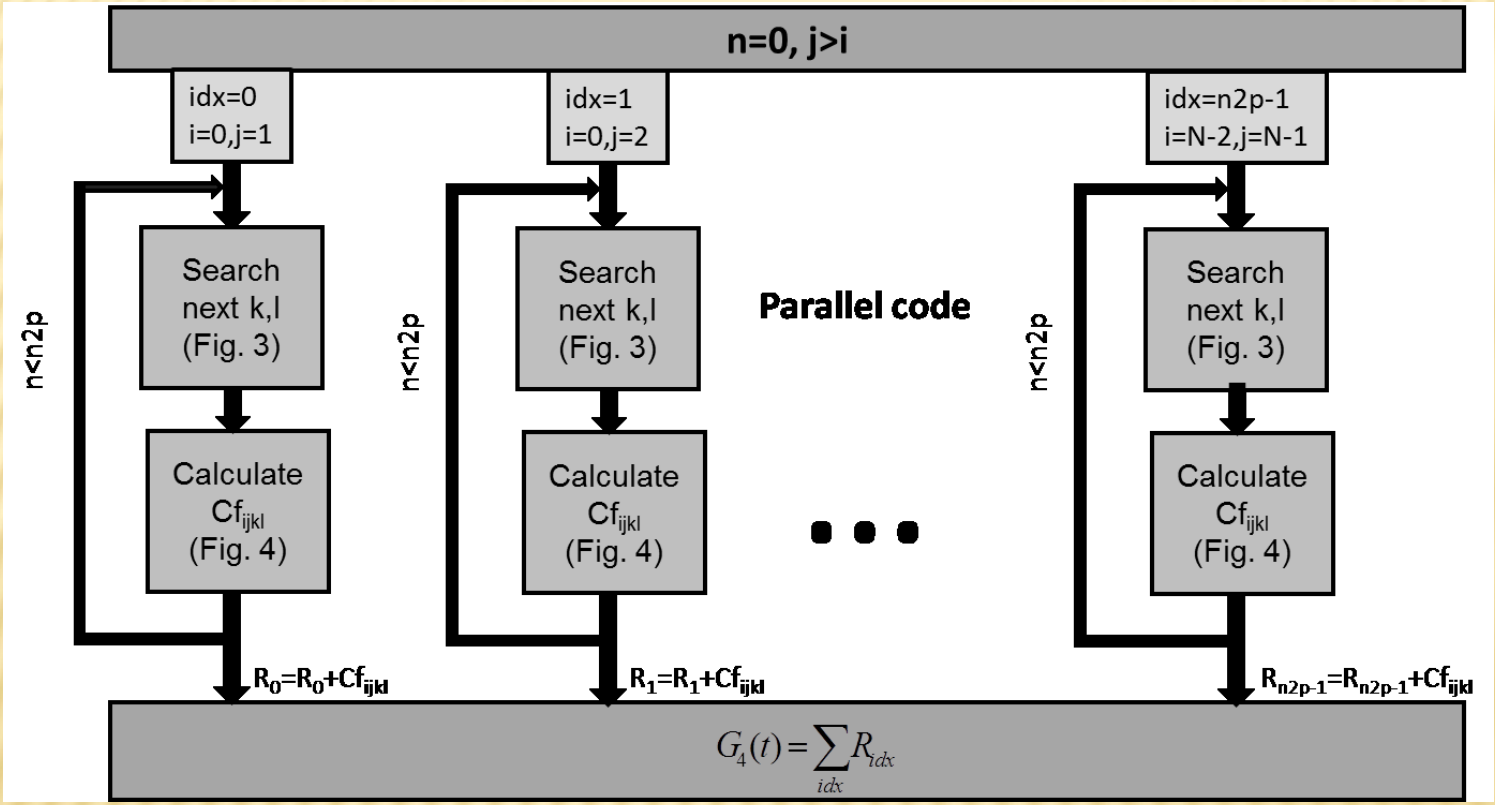
~495:1 $$G_3(t) \propto \left\langle \sum_{\substack{i,j,k=1,\\ i<j,i\neq k,j\neq k}}^{N} \beta_{ij}(t)\beta_{ik}(0) \right\rangle$$ Three-body function

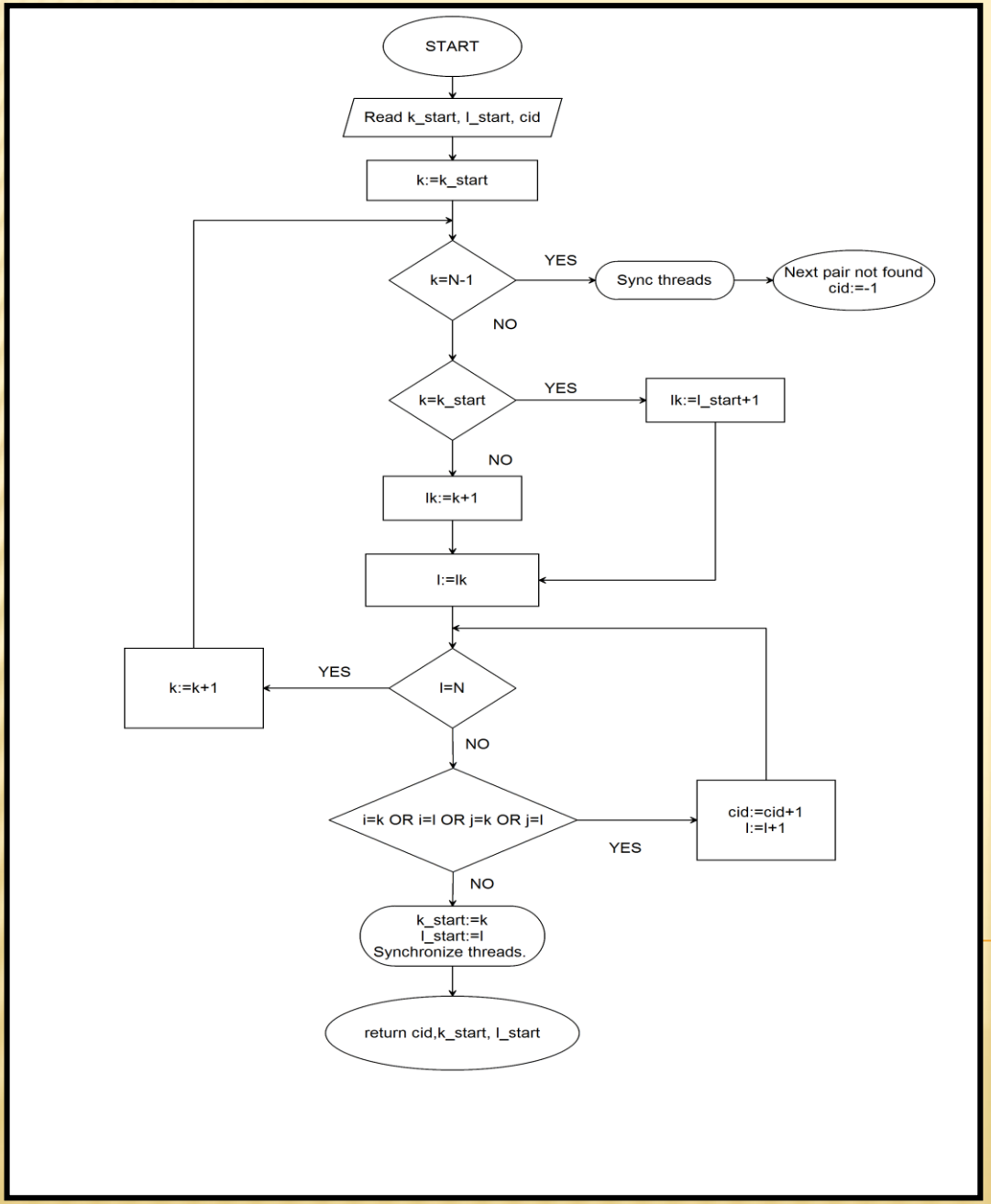
~10597:1 $$G_4(t) \propto \left\langle \sum_{\substack{i,j,k,l=1,i<j,i\neq k,\\ k<l,i\neq l,j\neq l,j\neq k}}^{N} \beta_{ij}(t)\beta_{kl}(0) \right\rangle$$ Four-body function

CPU SOLUTION FOR 4-BODY FUNCTION

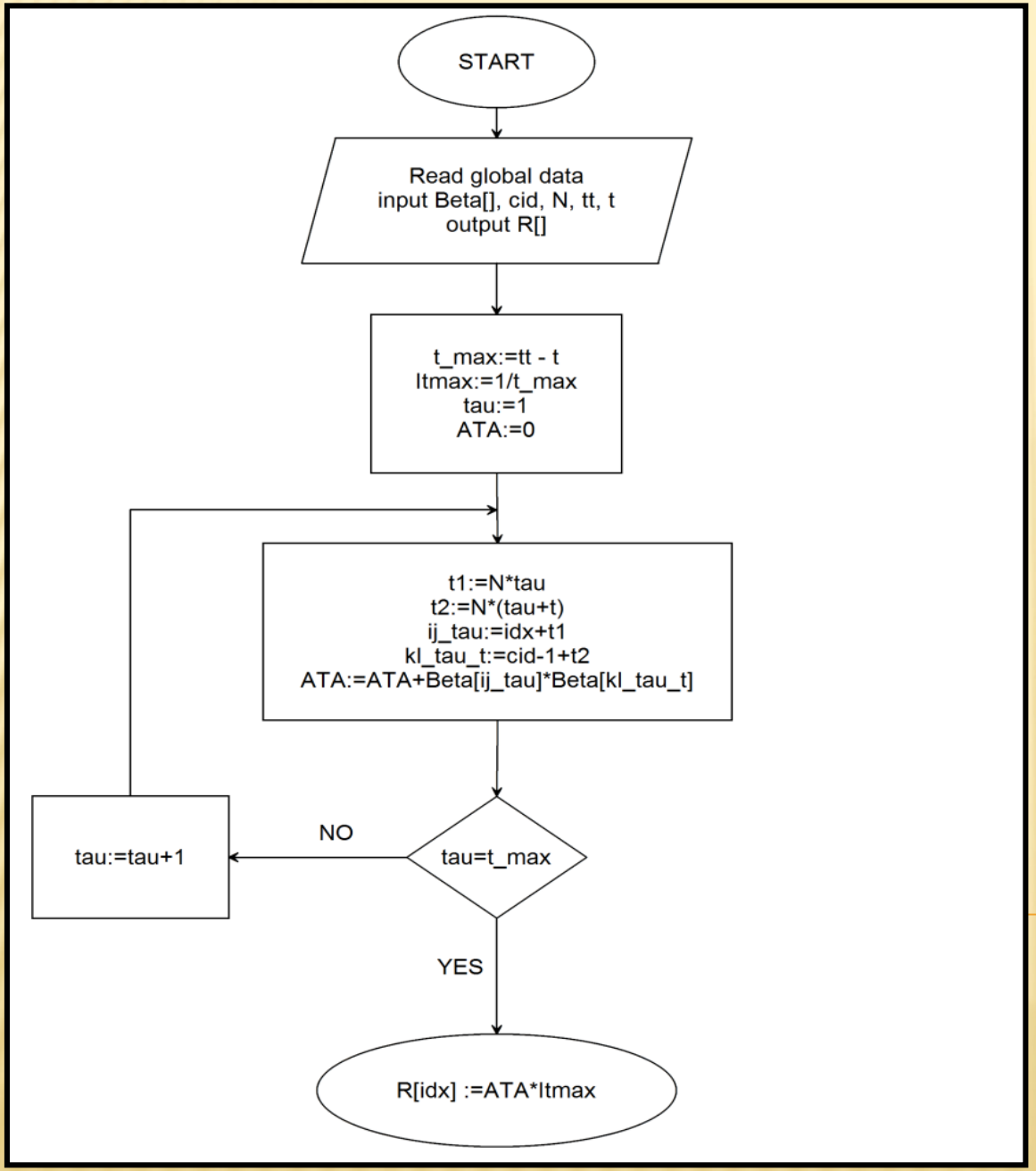
```
1. SET N to be equal to number of atoms
2. SET TMAX to be the total simulation time
3. SET input beta to be the polariazability anisotropy 3D matrix of dimensions N,N,TMAX
4. FOR t=1 to TMAX
5. SET output AVER to zero
6. SET TORIG = TMAX - t
7.     FOR i=1 to N
8.        FOR j=i+1 to N
9.          FOR k=1 to N
10.           FOR l=k+1 to N
11.               IF i≠k AND j≠k AND i≠l AND j≠l THEN
12.                   SET ATA to zero
13.                 FOR tau=1 to TORIG
14.                   ATA = ATA + beta[i][j][tau]*beta[k][l][tau+t]
15.                 END FOR
16.                 ATA = ATA / TORIG
17.                 AVER = AVER + ATA
18.               END IF
19.           END FOR
20.         END FOR
21.       END FOR
22.     END FOR
23. print t, AVER
24. END FOR
```

GPU ACCELERATION



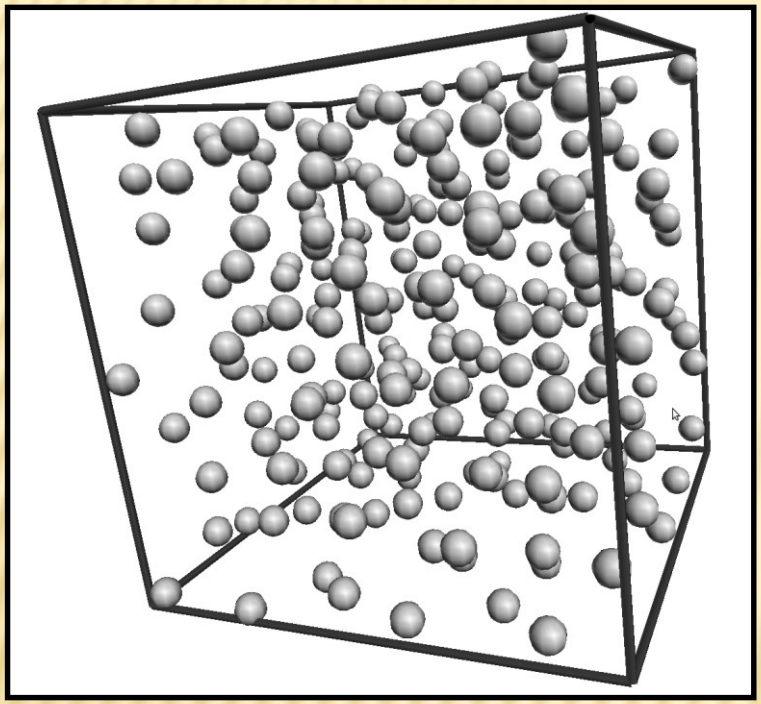


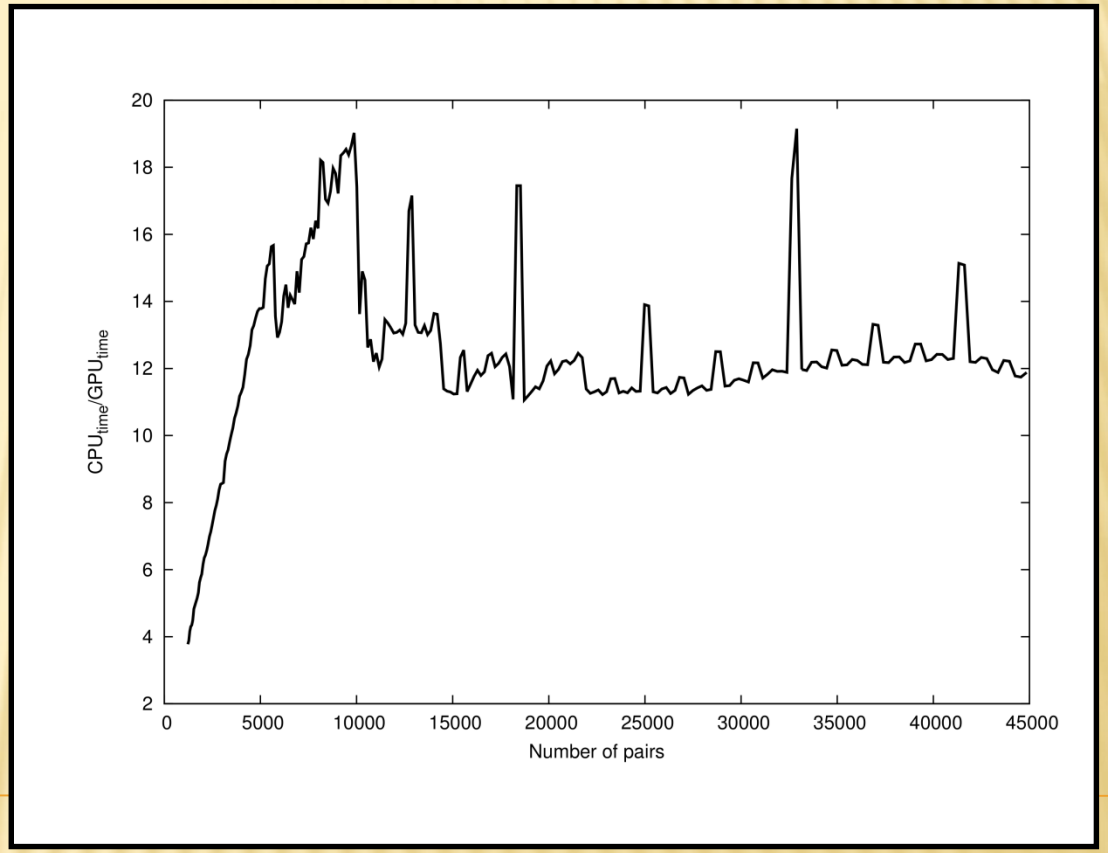
GPU ACCELERATION



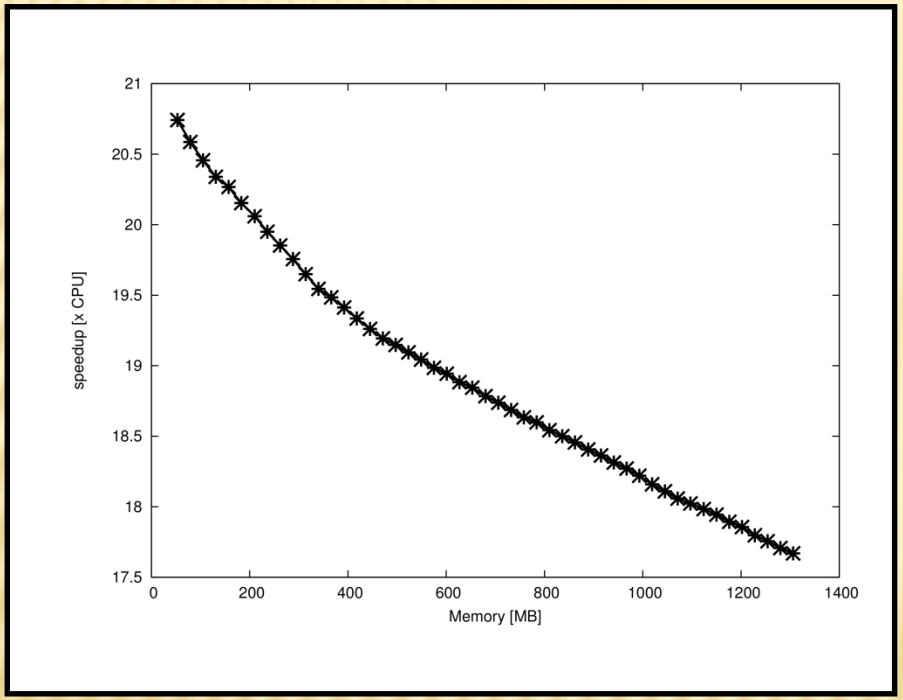
GPU ACCELERATION

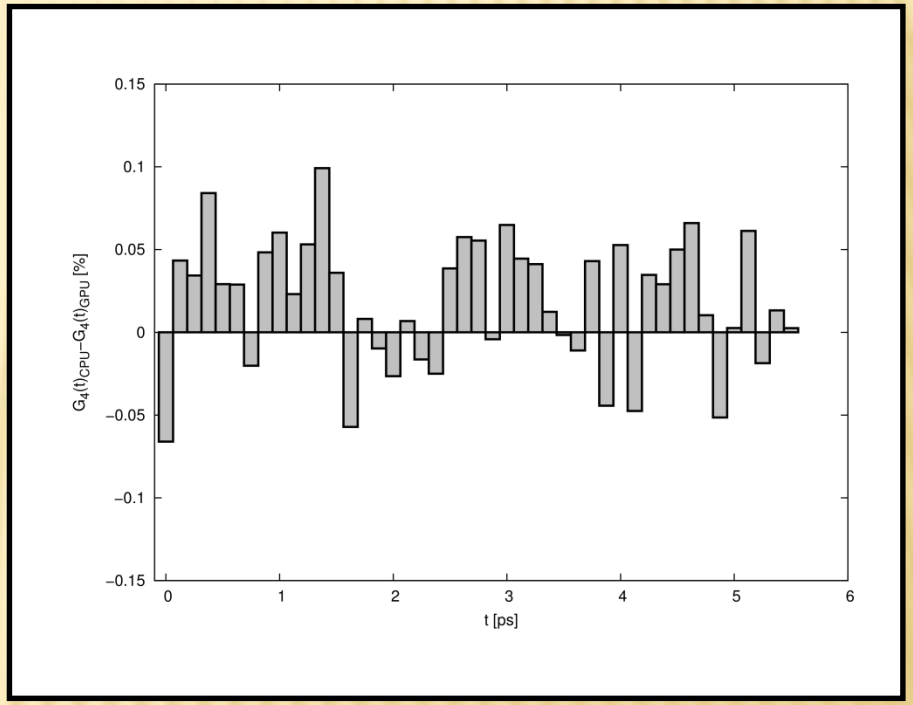
RESULTS




20
18
16
14
12
10
8
6
4
2
0
5000
10000
15000
20000
25000
30000
35000
40000
45000
CPU$_{time}$/GPU$_{time}$
Number of pairs

RESULTS


speedup [x CPU]
Memory [MB]
21
20.5
20
19.5
19
18.5
18
17.5
0
200
400
600
800
1000
1200
1400


$G_4(t)_{CPU}-G_4(t)_{GPU}$ [%]
t [ps]
0.15
0.1
0.05
0
−0.05
−0.1
−0.15
0
1
2
3
4
5
6

SUMMARY

- *The correlation functions are not a good subject for parallelizing.*
- *The peak performance of GPU shows that calculations of 4-body correlation function are 21 times faster than calculations performed on single core CPU.*
- *The acceleration of calculation depends on number of particles.*
- *The relative error lies within 0.1 %*

Thank you for your attention