TCBG's Workshop on GPU Programming for Molecular Modeling

August 6-8, 2010

Urbana, IL

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My goals I have not achieved yet (my problems):

- Understand how MM algorithms are implemented on the GPU

- Pull the RMSD algorithm into the GPU

- Above all, be comfortable programming the GPU

Root Mean Square Deviation (RMSD)

Who – RMSD

What – $\sqrt{(\Sigma_n |x_n - U\, y_n|^2 / N)}$

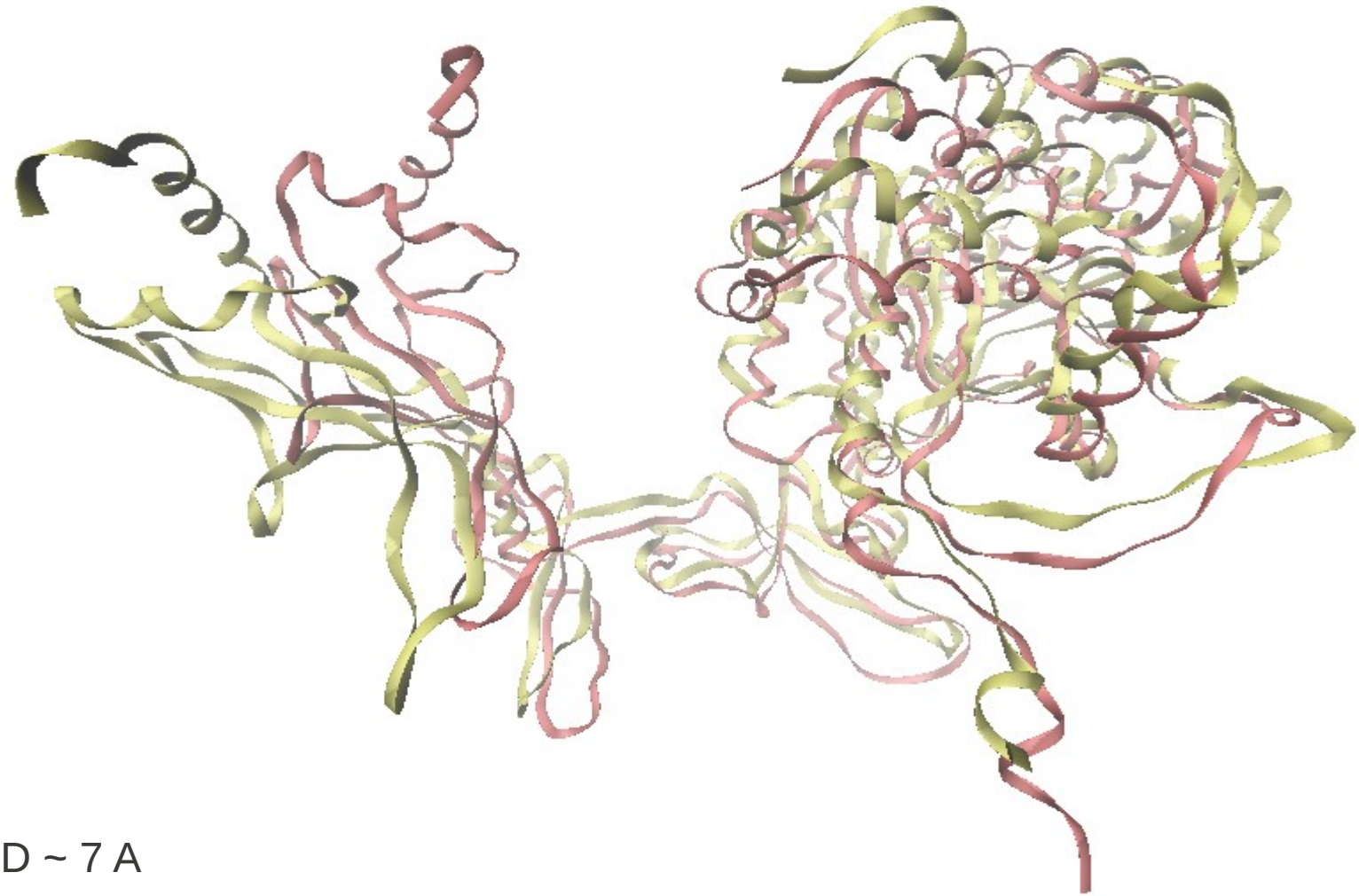
When – Need average offset between two sets

Where – Anywhere

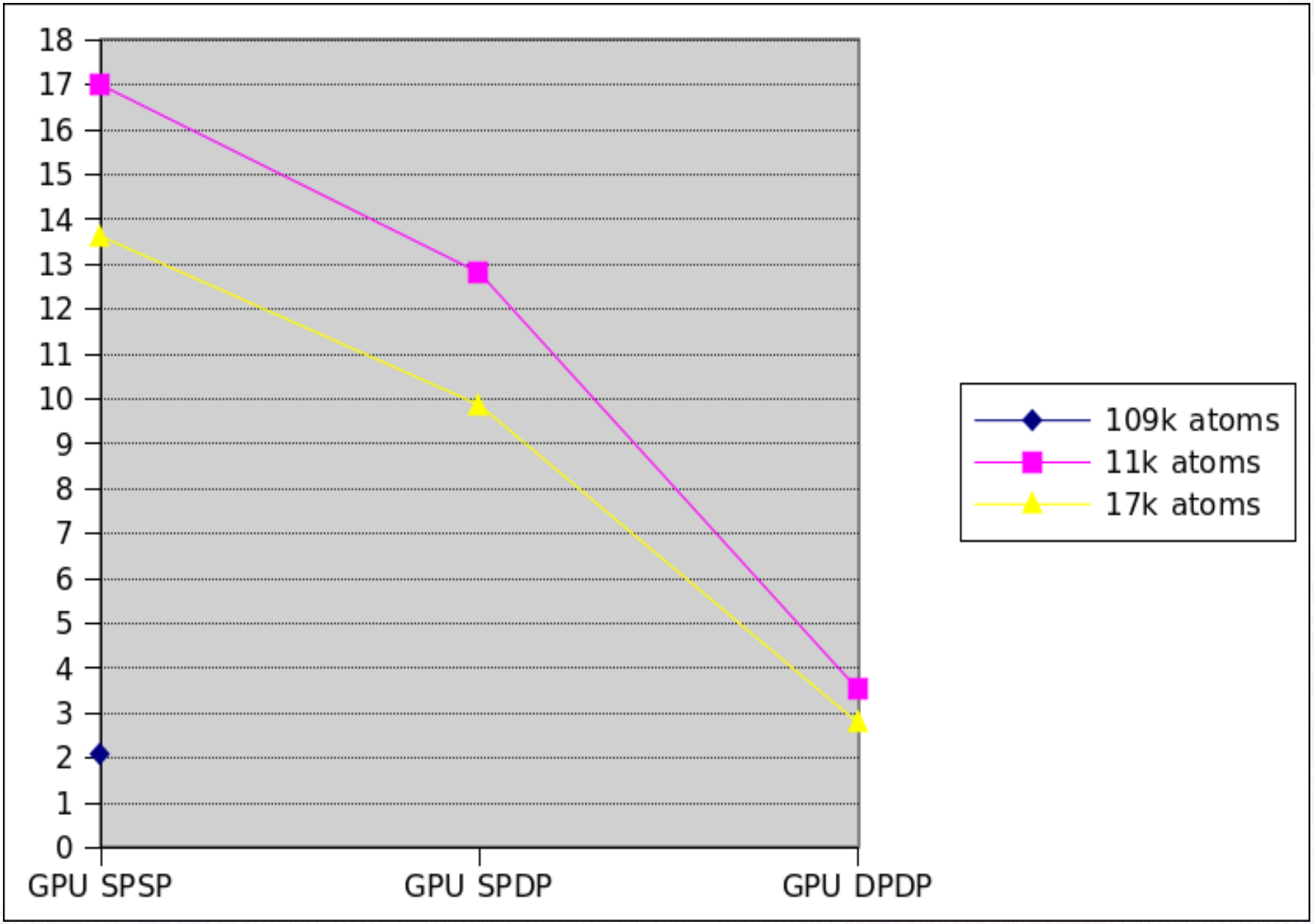
Why – In my case, protein conformation analysis

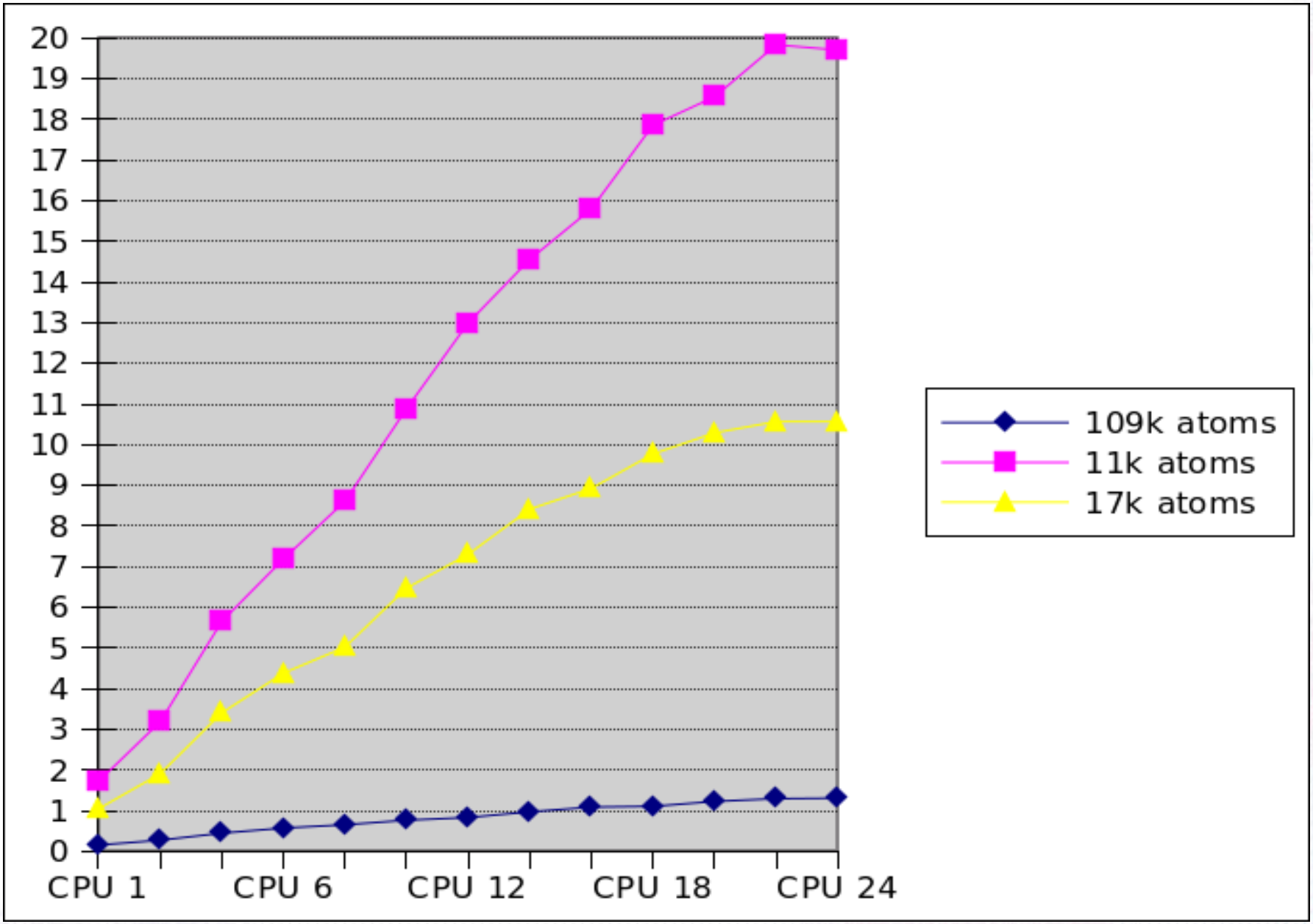
How – For the GPU... good question!

PDB 2QSG ~11,000 atoms, ~109,000 atoms w/ TIP3P
8 ns comparison



RMSD ~ 7 A


18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
GPU SPSP
GPU SPDP
GPU DPDP
109k atoms
11k atoms
17k atoms


20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
CPU 1
CPU 6
CPU 12
CPU 18
CPU 24
109k atoms
11k atoms
17k atoms

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