Accelerate Molecular Dynamics Simulations

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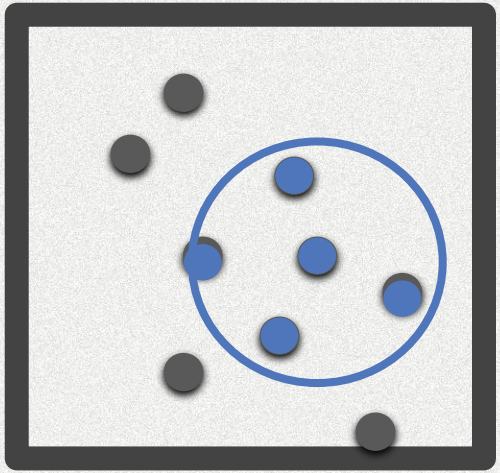
Molecular Dynamics Simulations



Short range forces matter!

Algorithm

t=0
while t<T_final
    for i=1 to N do
        Fi←0
        for j = 1 to N do
            r i , j ← r j − r i
            Fi,j ← compute force(‖ri,j //)
            Fi←fi+fi,j ri,j
        end for
    end for
    t ← t + dt

$O(N^2)$

Molecular Dynamics Simulations

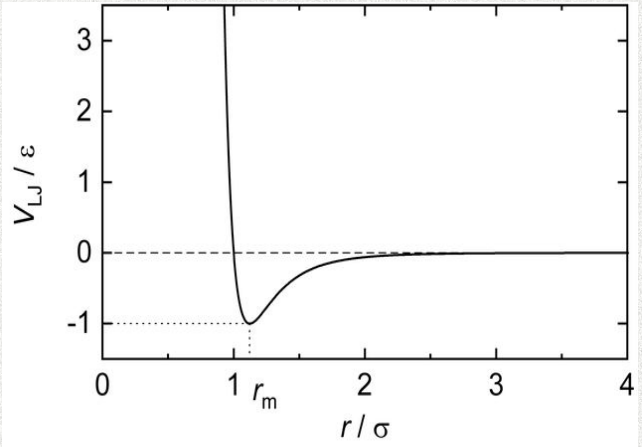
compute force – Verlet method

For the motion of a particle:

$$\begin{aligned} \mathbf{v}(t+\triangle t) &= \mathbf{v}(t)+\mathbf{a}(t)\triangle t+O((\triangle t)^2) \\ \mathbf{r}(t+\triangle t) &= \mathbf{r}(t)+\mathbf{v}(t)\triangle t+\frac{1}{2}\mathbf{a}(t)(\triangle t)^2+O((\triangle t)^3) \end{aligned}$$

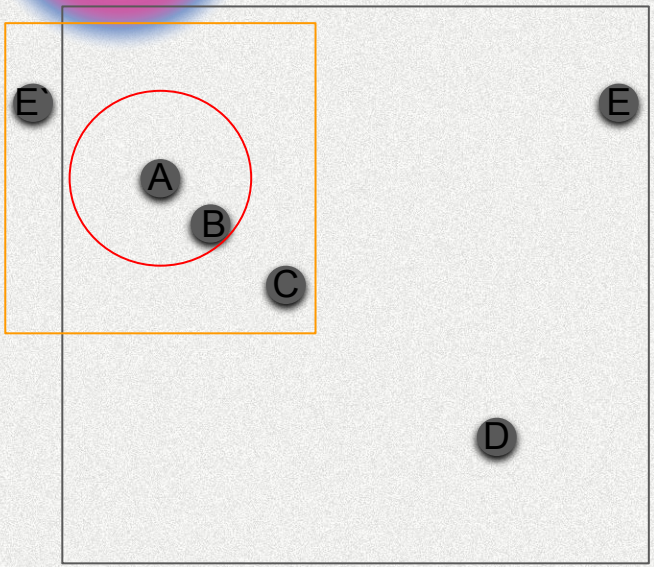
Expressing the speed at mid-interval $v(t+\triangle t/2)$:

$$\begin{cases} \mathbf{v}(t+\triangle t/2)=\mathbf{v}(t)+\mathbf{a}(t)\triangle t/2 \\ \mathbf{r}(t+\triangle t)=\mathbf{r}(t)+\mathbf{v}(t+\triangle t/2)\triangle t \\ \mathbf{a}(t+\triangle t)=\mathbf{F}(\mathbf{r}(t+\triangle t))/m \\ \mathbf{v}(t+\triangle t)=\mathbf{v}(t+\triangle t/2)+\mathbf{a}(t+\triangle t)\triangle t/2 \end{cases}$$



Lennard-Jones Potential $V_{LJ}(r_{ij}) = 4\varepsilon[(\frac{\sigma}{r_{ij}})^{12} - (\frac{\sigma}{r_{ij}})^{6}]$

Neighborhood Table



Array Version

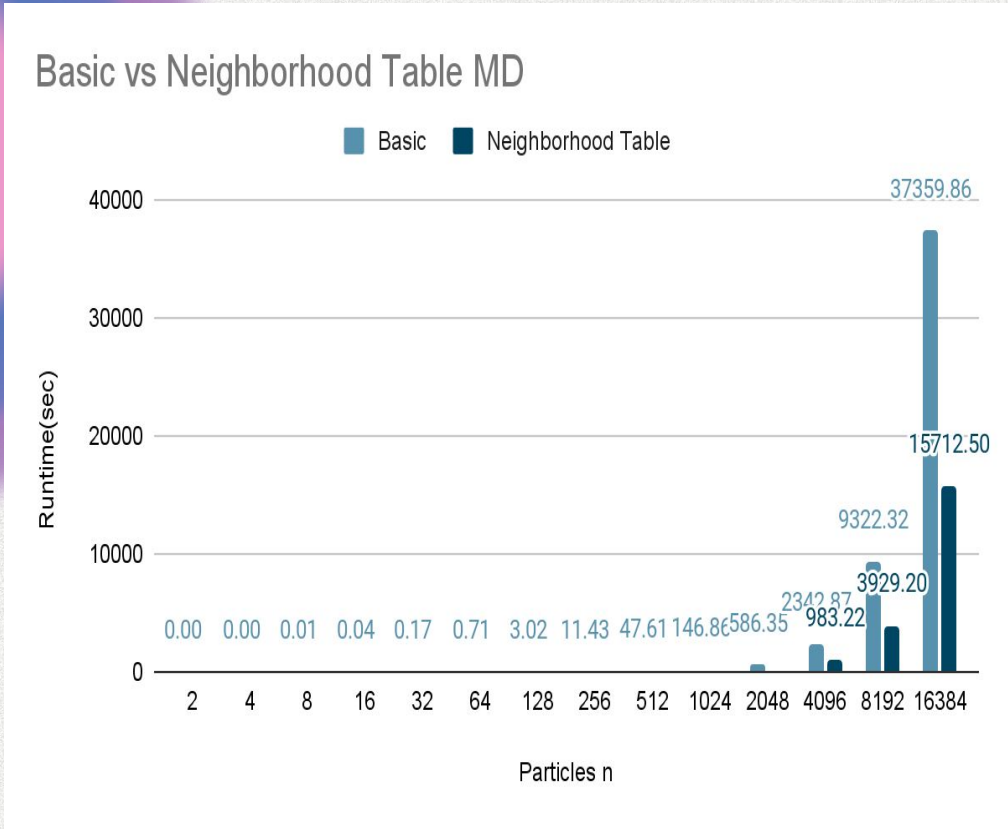
A	0
B	3
C	5
D	D
E	E

B	0
C	1
E	2
A	3
C	4
B	5
A	6
A	7
-1	8

Vector Version

A	B	C	E
B	A	C	
C	A	B	
D			
E	A		

Result - Brute force and Neighborhood Table



N particles in 4096*4096 2D box
dt=0.005
5000 time steps
m=1

Neighborhood Table save
~60% computation time

Result - Open ACC

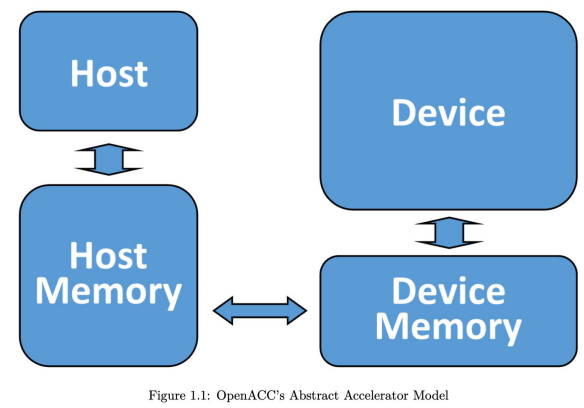
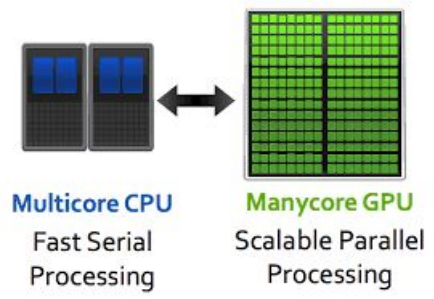


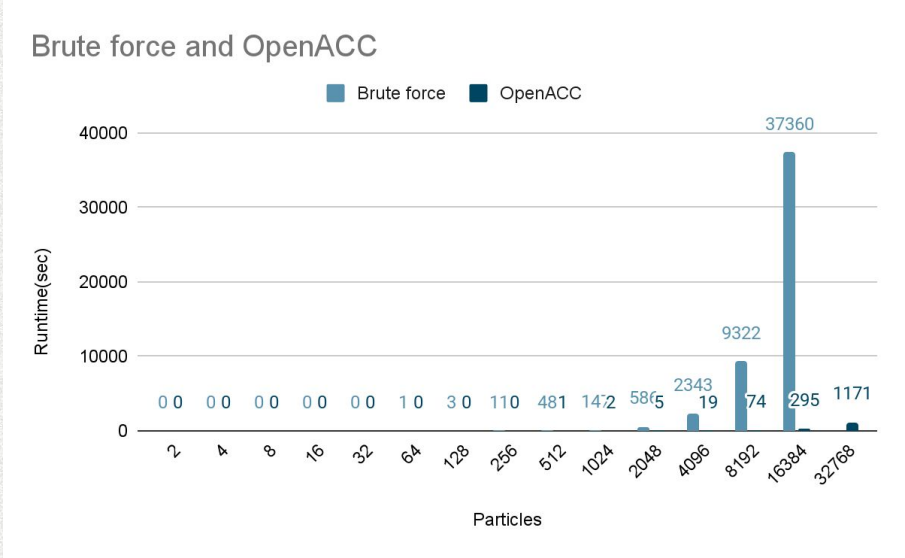
Figure 1.1: OpenACC's Abstract Accelerator Model

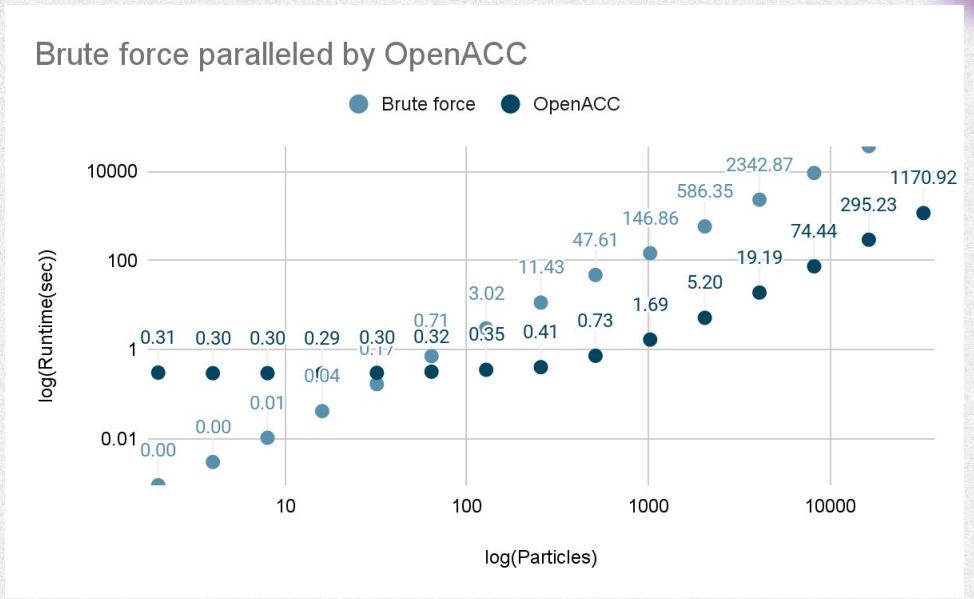


Result - Open ACC

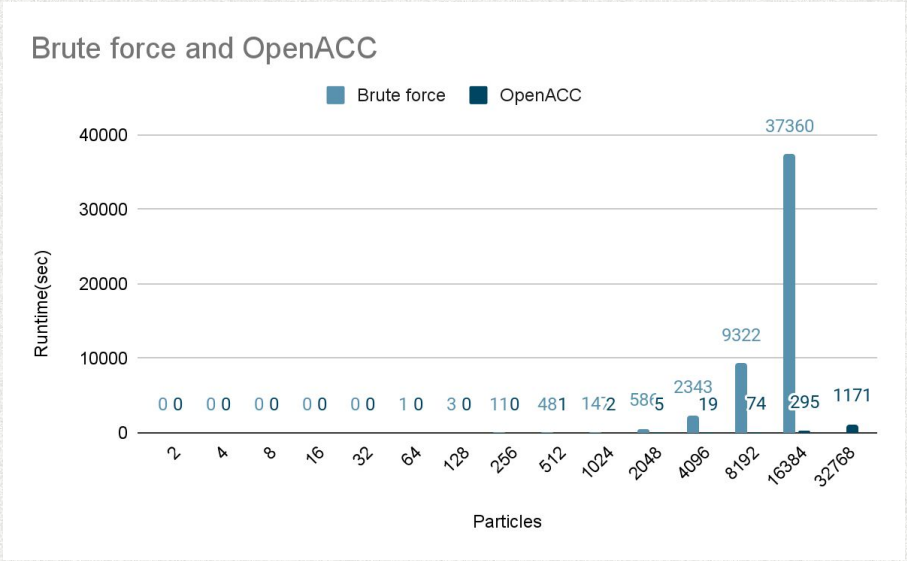
```
sign(double, double):
    205, Generating implicit acc routine seq
         Generating acc routine seq
         Generating Tesla code
calcVerlet(int, int, double, double, double, double, double, double *, double *, double *):
    336, Generating copy(pos[:nd*np],vel[:nd*np],acc[:nd*np])
         Generating Tesla code
        336, #pragma acc loop gang /* blockIdx.x */
        339, #pragma acc loop vector(128) /* threadIdx.x */
             Generating reduction(+:Ekin,Epot)
        343, #pragma acc loop seq
    339, Loop is parallelizable
```

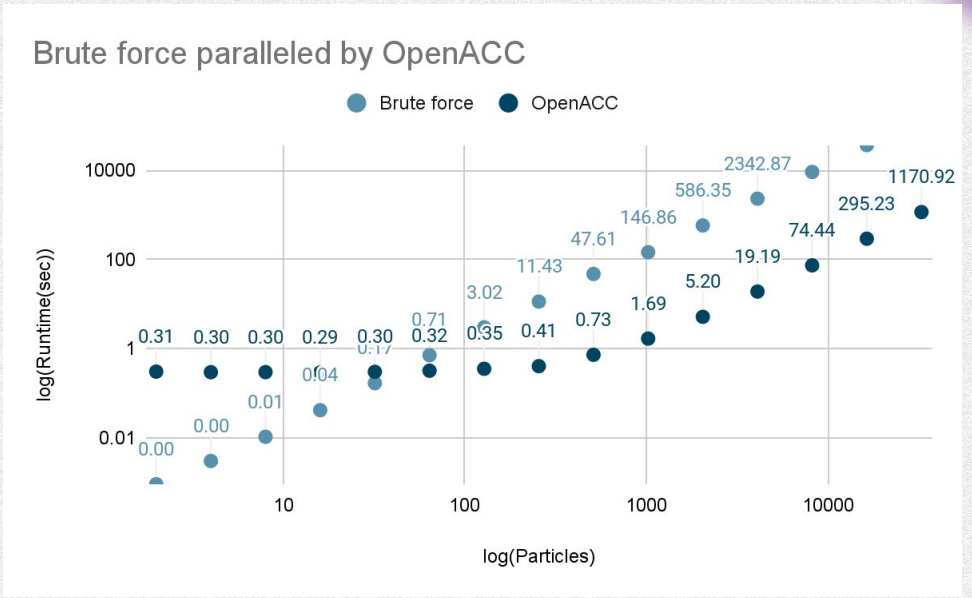
Result - Open ACC



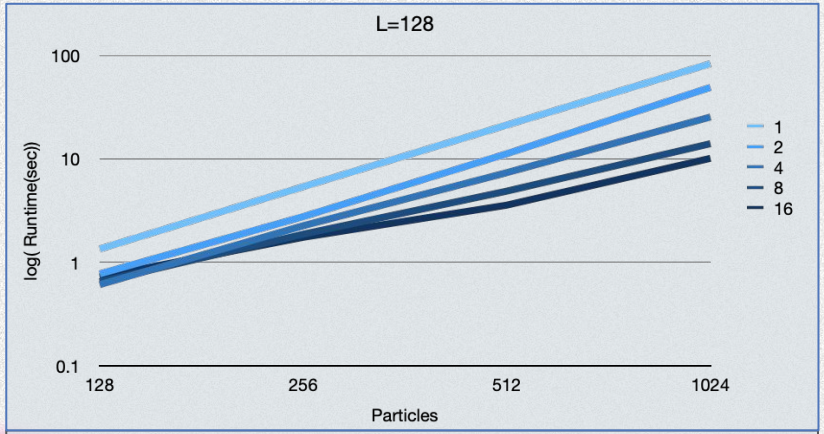


Result - OpenMP

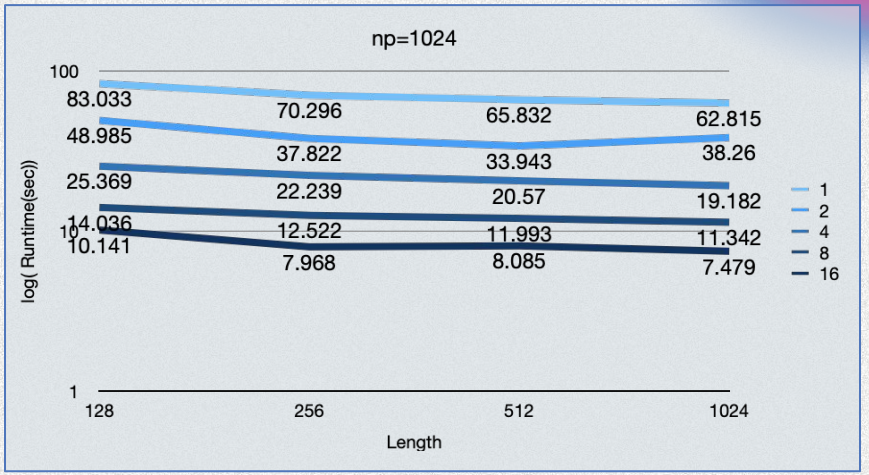


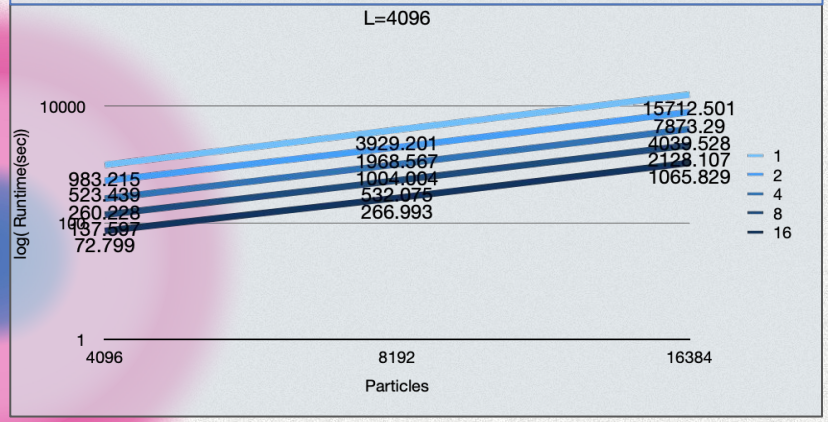


Result - OpenMP



For Small Area





For Large Area

Animation

Discussion

What is this error mean?

```
[imhaoyu@scc-c13 openacc]$ ./openACC 10
Failing in Thread:1
call to cuCtxCreate returned error 101: Invalid device
```

Thank You