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CONTACT NAME
Hamidreza Soltani: hsoltani@uclan.ac.uk

GPU TECHNOLOGY CONFERENCE

uclan University of Central Lancashire

Accelerating Cell Dynamic Simulation For 3D Diblock Copolymer Sphere Morphology Using GPU

Hamidreza Soltani, Dung Ly, Waqar Ahmed
School of Computing, Engineering and Physical Sciences
University of Central Lancashire, Preston, PR1 2HE, UK

uclan University of Central Lancashire

INTRODUCTION

Cell dynamic simulation (CDS) is one of the well-known techniques to demonstrate the order structure in block copolymer systems and to consider different effects of simulation parameters. In additions, cell dynamic simulation helps to understand different aspects of morphological topographies and dynamic process of particle tracking. But because it is expensive to develop and implement a complex technique and real time system such as cell dynamic simulation with a sequential algorithm in central processing unit (CPU), it is a need to consider a parallel algorithm and programming model to solve time-consuming and massive computational processing issues.

In order to overcome of the mentioned problems a new algorithm is implemented to accelerate cell dynamic simulation (CDS) for presenting the order structure of 3D diblock copolymer in ultra-thin films under shear. A new achievements is based on a commodity NVIDIA Quadro K5000 graphic card , where results illustrate that GPU-CUDA based processing are approximately 8~9 times faster than sequential processing on CPU with C programming language and typically 5~6 times faster than sequential running on CPU with FORTRAN programming language.

PURPOSE AND HYPOTHESIS

The current study presents a new approach to accelerate computational processing of cell dynamic simulation for 3D diblock copolymer in the form of spheres . This new approach is implemented specifically to utilise CUDA as a parallel computing platform and programming model for solving time-consuming and massive computer processing issues for new material science specifically cell dynamic simulation.

METHODOLOGY

This work is focused on cell dynamic simulation for diblock copolymer in ultra-thin films under shear. In order to achieve formation of sphere diblock copolymer, CDS simulation method is developed using Euler numerical scheme of finite differences. Partial Differential Equation is solved on lattice with the appropriate and accurate boundary conditions on pore surface.

For differences in local and global volume fractions of blocks following equation is used [1].

$$\psi = \phi_A - \phi_B + (1-2f) \qquad (1)$$

Where ϕ_A and ϕ_B are local volume fractions of monomers A and B respectively and ψ is an order parameter.

For the time evolution of order parameter Cahn-Hilliard-Cook (CHC) equation is used [2, 3].

$$\frac{\partial \psi}{\partial t} = \nabla^2 \left(\frac{\delta F[\psi]}{\delta \psi} \right) \qquad (2)$$

Where $F(\psi)$ is free energy function.

The evolution of ψ in time can provide essential information about morphology and shape evolution of a diblock copolymer.

Computer Unified Device Architecture (CUDA) as a data parallel computing device is used to solve the issues of expensive calculations and to manage computations.

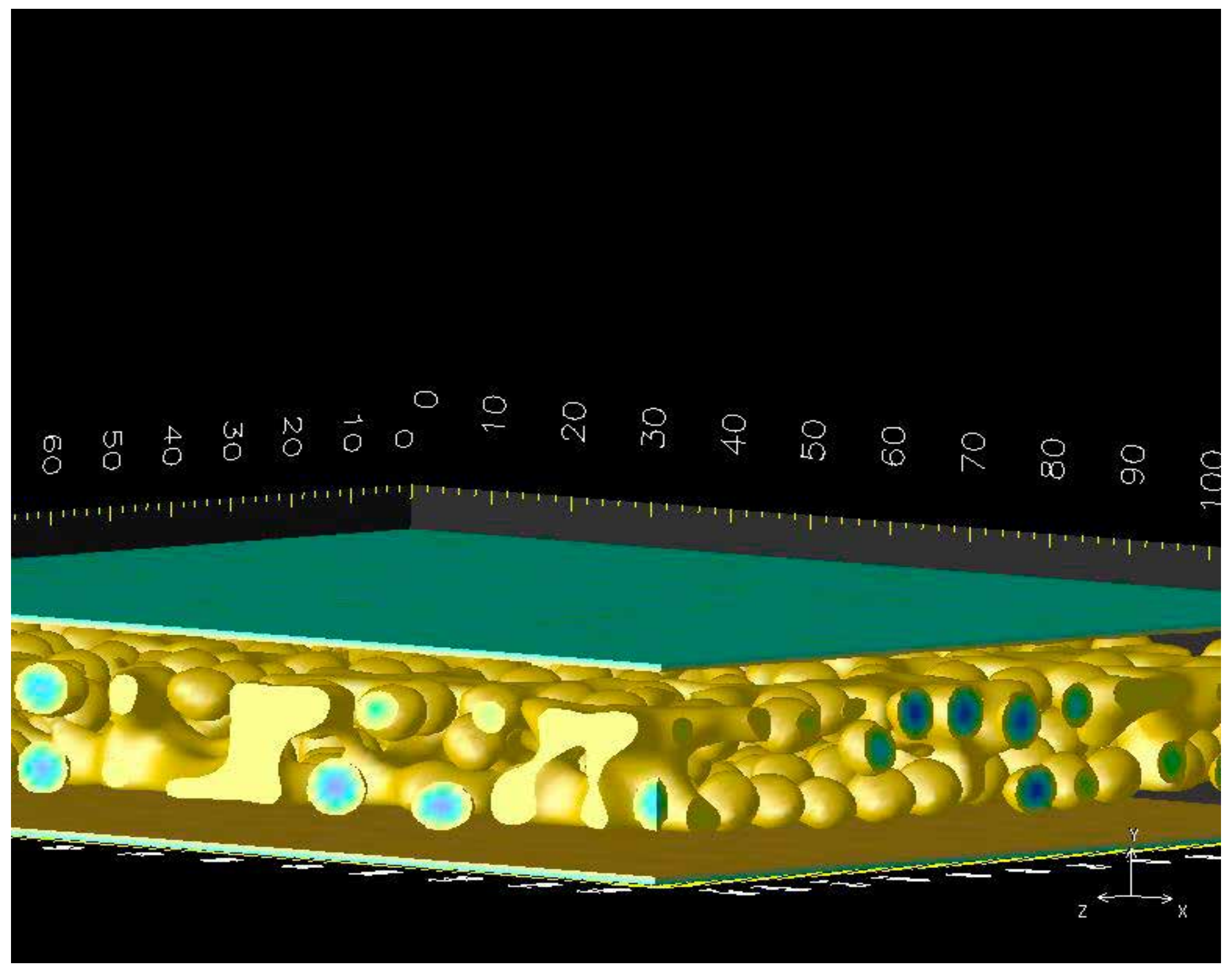
Based on the hardware limitations, in total 1014 (13,6,13) threads per block in 3 dimensions and 500 (10,5,10) blocks per grid for the system size of 128*26*128 are used.

And finally 14 kernels are developed on GPU to do the calculations and computational processing.

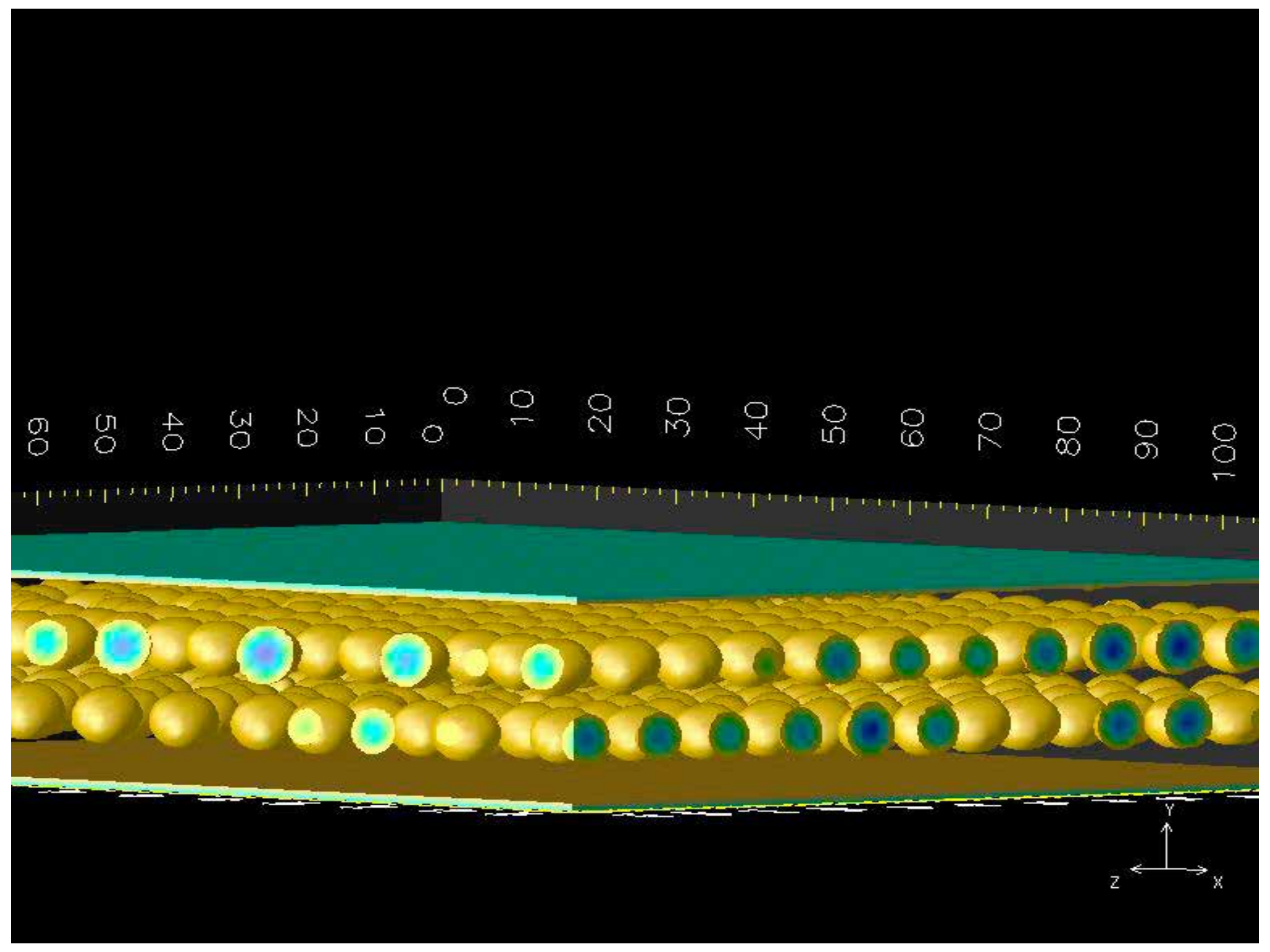
DESIGN AND RESULTS

```
Begin
Host program on CPU
 Define variables
  Read values of parameters from input files
  Allocate Host arrays
  Initialise random values for order parameters
   Allocate Device arrays
    Define time function
    Start to copy values from Host to Device
   Calculate number of threads and number of block based on the domain/system size
  Kernel programs implemented on GPU
   Kernel 1 - Define and calculate boundary condition in X axis
    Kernel 2 – Define and calculate boundary condition in Y axis
     Kernel 3 - Define and calculate boundary condition in z axis
      For all time – steps do
       Kernel 4 – 7 – Calculate Laplacian equation
       Kernel 8 – Calculate free energy
       Kernel 9 – 13 - Calculate Map function
       Kernel 14 – Calculate final value of order parameter ($\psi$)
      End For
  Copy back from Device to Host
   Write the outputs into files
   Free all Host and Device memory
   Write the elapsed time
End
```

CUDA - Computational algorithm

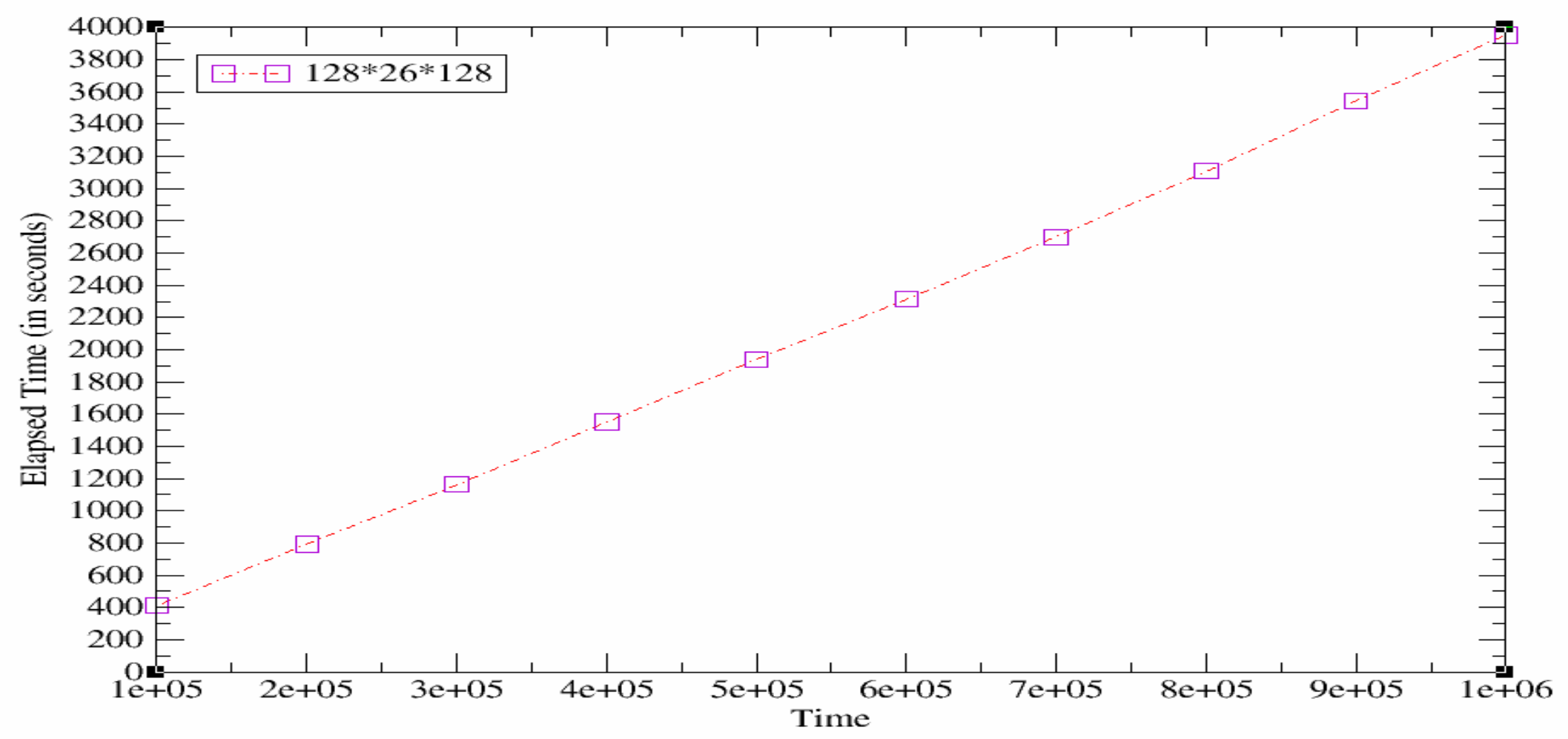


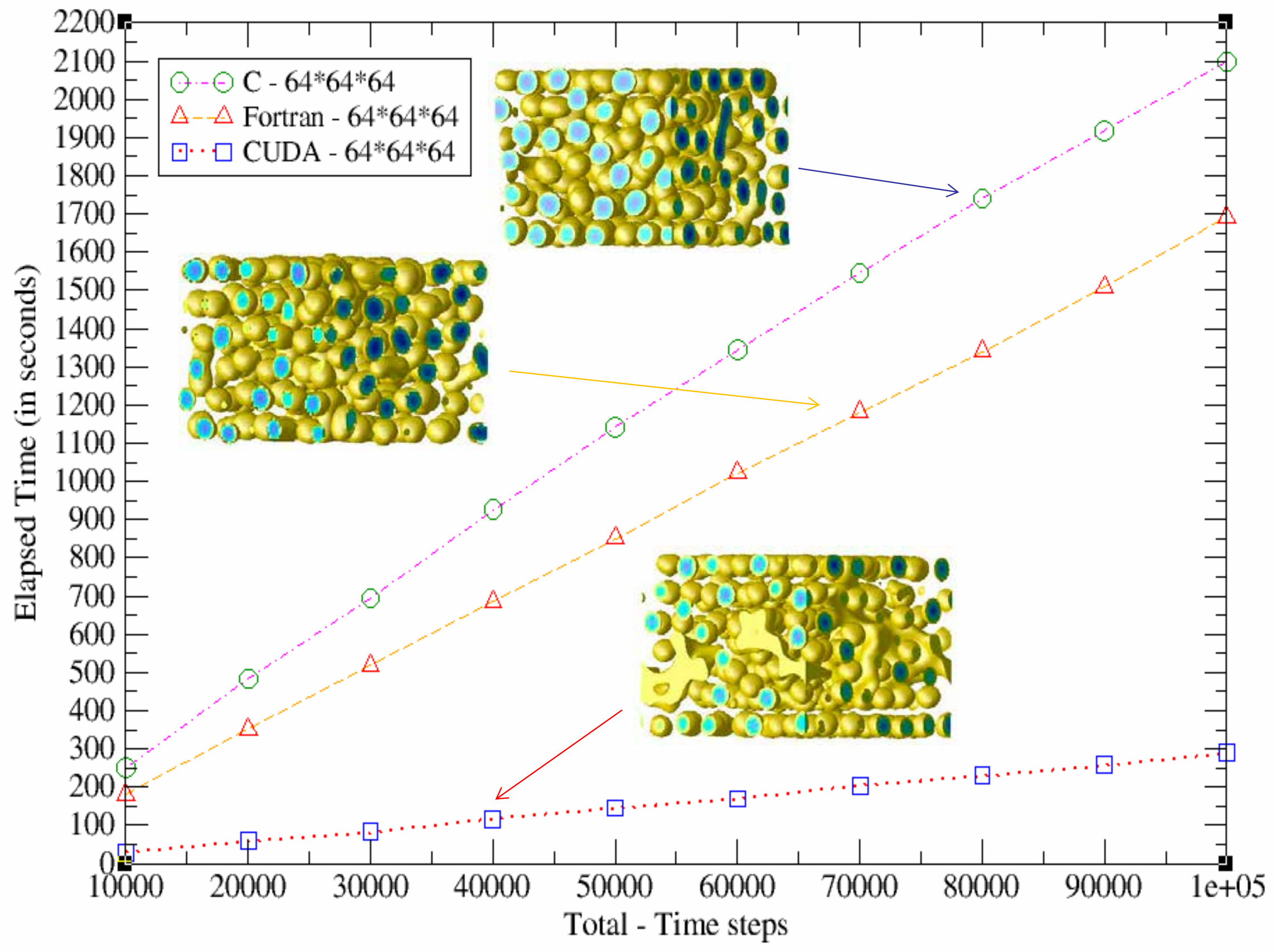
CUDA simulation result – Initial stage



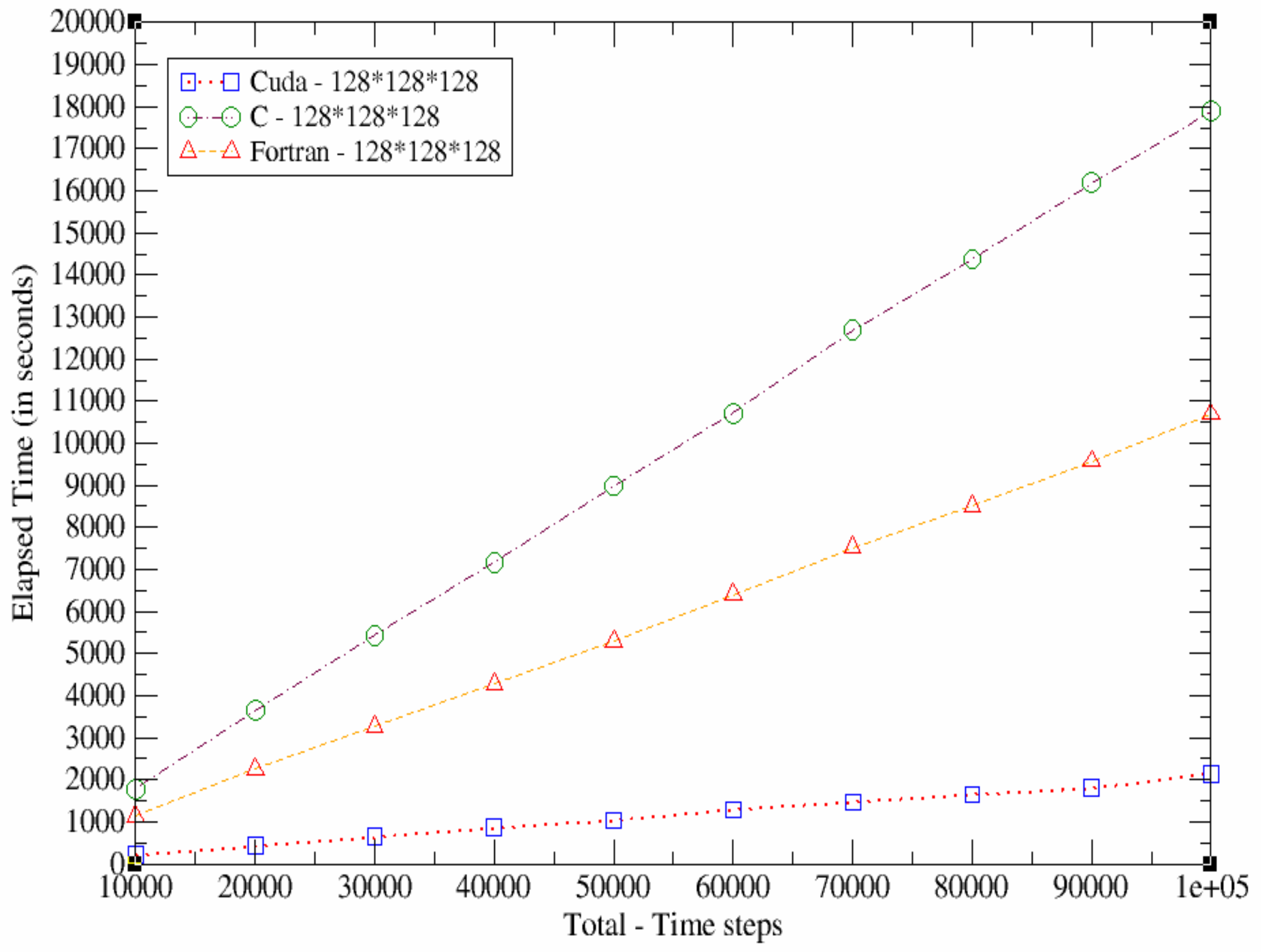
CUDA simulation result – Final stage

Total – Time for system size 128*26*128	Elapsed time (seconds)
100000	411.582886
200000	790.994629
300000	1162.659546
400000	1552.485352
500000	1939.565186
600000	2314.168071
700000	2698.750957
800000	3108.333843
900000	3544.914795
1000000	3951.440674



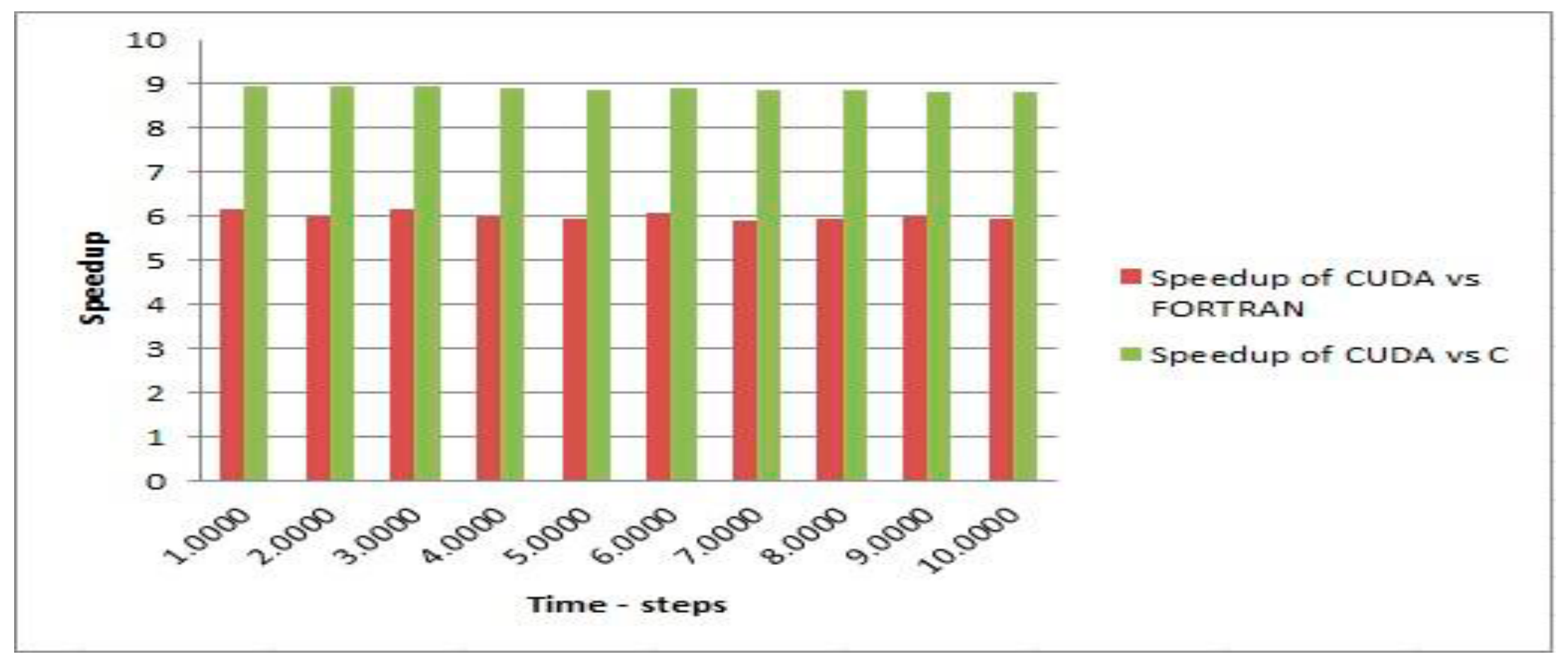


Speed comparison of CUDA vs C vs FORTRAN in 64*64*64 system size

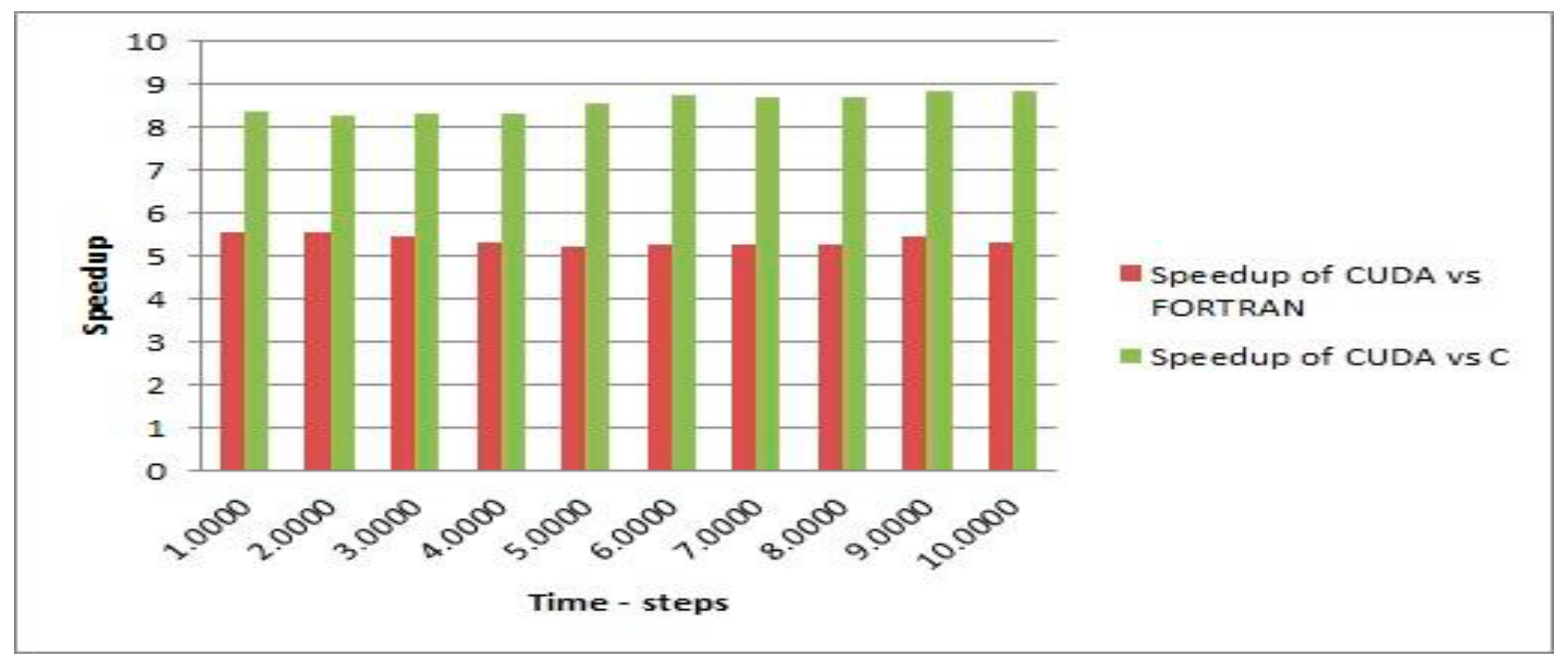


Speed comparison of CUDA vs C vs FORTRAN in 128*128*128 system size

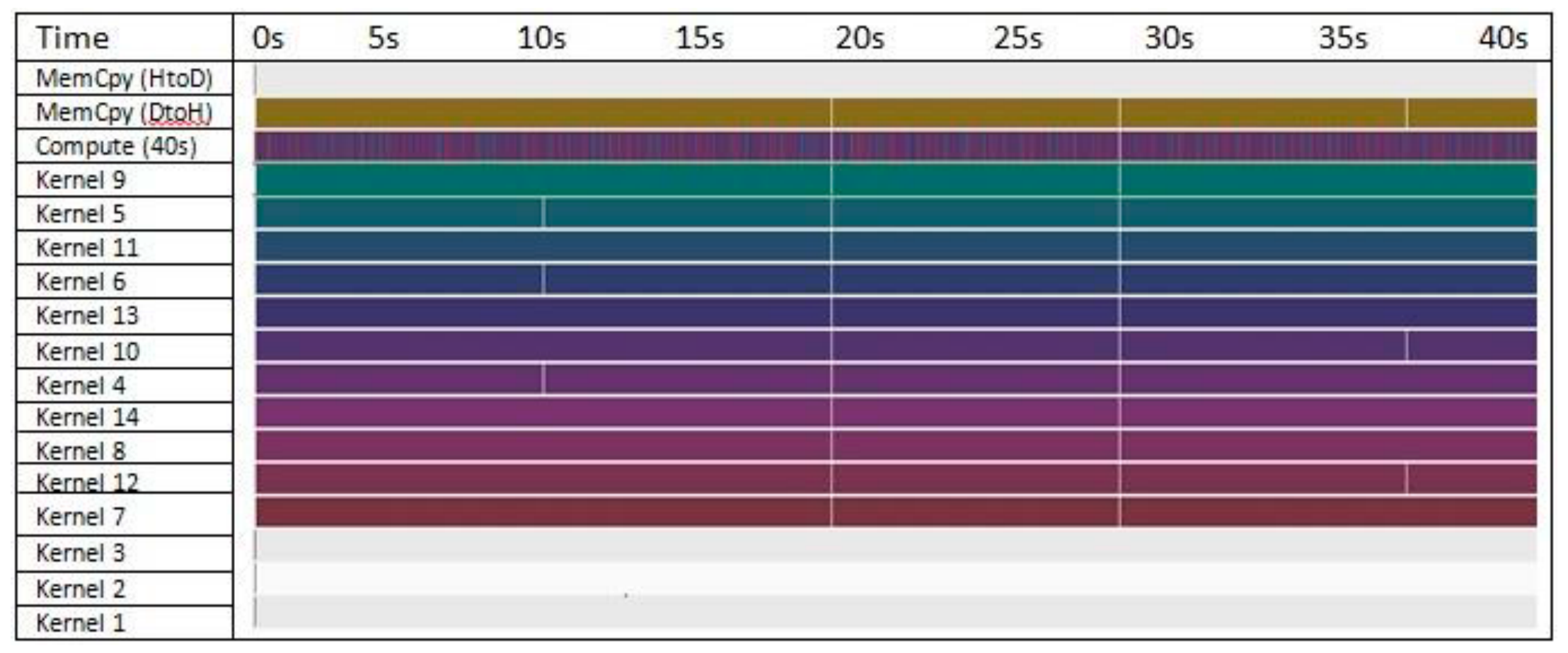
RESULTS



Benchmark result of performance enhancement (speedup) for the system size 64*64*64



Benchmark result of performance enhancement (speedup) for the system size 128*128*128



CUDA Compute Visual Profiler of all kernel executions and memory copies for the system size 128*26*128 in first 40 seconds

CONCLUSIONS AND FUTURE WORK

In this poster, we present a CUDA based simulation algorithm and results with the technique of cell dynamic simulation. We illustrate a GPU enhanced and accelerated high speed results compare with CPU. Therefore, future work must improve the performance of current program with using other optimization techniques for reducing memory access time, and finally examine and compare the CUDA accelerated results with cluster results.

REFERENCES

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