

# Multi-Scale Modeling of Nano Scale Phenomenon using CUDA based HPC Setup

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**Abstract**-The essence of High performance computing (HPC) in the field of computation Nanotechnology and problems encountered by HPC arrangement in applying HPC to Nano-enabled calculations have been presented in the paper. A proposal to optimize computations in an HPC setup has been formulated to make Nanotechnology computations more effective and realistic on a CUDA based framework. Results and findings in the expected setup and the computation complexities that will be needed in its implementation have been suggested with an algorithm to take advantage of inbuilt powerful parallelization capabilities of GPU making large scale simulation possible. Implementation of CUDA in certain complex techniques in Nanotechnology is presented with a significant improvement in performance as compared to the last work which was implemented using distributive computing toolbox in MATLAB. We have discussed about the problems that exist and how we can optimize the computations in a HPC setup and how we can make use of computational power of GPU to make Nanotechnology computations more effective and realistic. A description of the progress in this area of research, future works and a probable extension is proposed.

## I. INTRODUCTION

Nanotechnology is the realization and engineering of matter at dimensions of roughly 1 to 100 nanometers, where unique phenomena enable novel applications. Encompassing nano-scale science, engineering and technology with an involvement of nanotechnology in imaging, measuring, modeling, and manipulating matter at this length scale. Computation, modeling and simulation today play an equal role to theory and physical experimentation in discovery-driven engineering research [5]. Using the most advanced high-performance computing resources and a well worked out algorithm for innovating technology and reducing design-cycle time and reliability [7]. Compiling advanced calculations on Carbon Nanotube (CNT) [6], Micro-electromechanical systems (MEMS) and Nanofabrication and computations on characterization of CNT, calculation of various properties of CNT, integration of CNT with MEMS, nanocomposites of CNT and reliability of CNT based devices which need advanced calculations has been worked out in this paper. Introduction of a single atom or molecule in the chemical structure of CNT can change the entire configuration of the device manufactured from nano-materials. Incessant updates in existing theories in each of these areas make the study of computational Nanotechnology more arduous and

demanding as persistent revision of knowledge in the domain of nanotechnology has become mandatory.

At present the most used software solutions available are MATLAB [1] and Coventorware [4] but they do not cover all the new advancements and progressions taking place in the field of Nanotechnology as it is a rapidly evolving field. On Micro-scale software like Coventorware based on MEMS, it requires high computational power and if we add multi-scale modeling, characterization and reliability as parameters then the need for higher performance is still more eminent. Nanotechnology is a highly advanced science with many potential applications. Its impact is already being felt in materials engineering, electronics, medicine and other scientific disciplines. Current research in nanotechnology requires multi-disciplinary knowledge, not only in the sciences and engineering domain but also in the high performance computing (HPC) technology. Many nano-science explorations rely on established, efficient HPC and computational algorithms, practical and reliable numerical methods and large-scale computing systems.

In our previous operations we have been working on advanced calculations on Carbon Nanotube, MEMS, Nano fabrications [1, 2, 13, 14], and we have shown how reliability computations can benefit from HPC with MATLAB [1], MCCS [2], and various other environments, each of them having their pros and cons [3]. For example work such as characterization of CNT, calculations of various properties of CNT, integration of CNT with MEMS (Micro Electro Mechanical System), nanocomposites of CNT, reliability of CNT based devices needs advanced calculations. This is because a single atom can change the entire configuration of the device manufactured from Nanomaterials. Continuous updates and new theories in each of these areas make the application Nanotechnology more difficult.

The main thing we need to work from here is on “multiscale modeling and simulation” because from the macro to nano phenomenon everything is linked so we need high computation power to work phenomenon’s we are aware in all the intermediate scale that exists from macro to nano. The algorithm we are planning will work and breakdown the problem statement in a way so that we can distribute the computation effectively in various clusters of a HPC system.

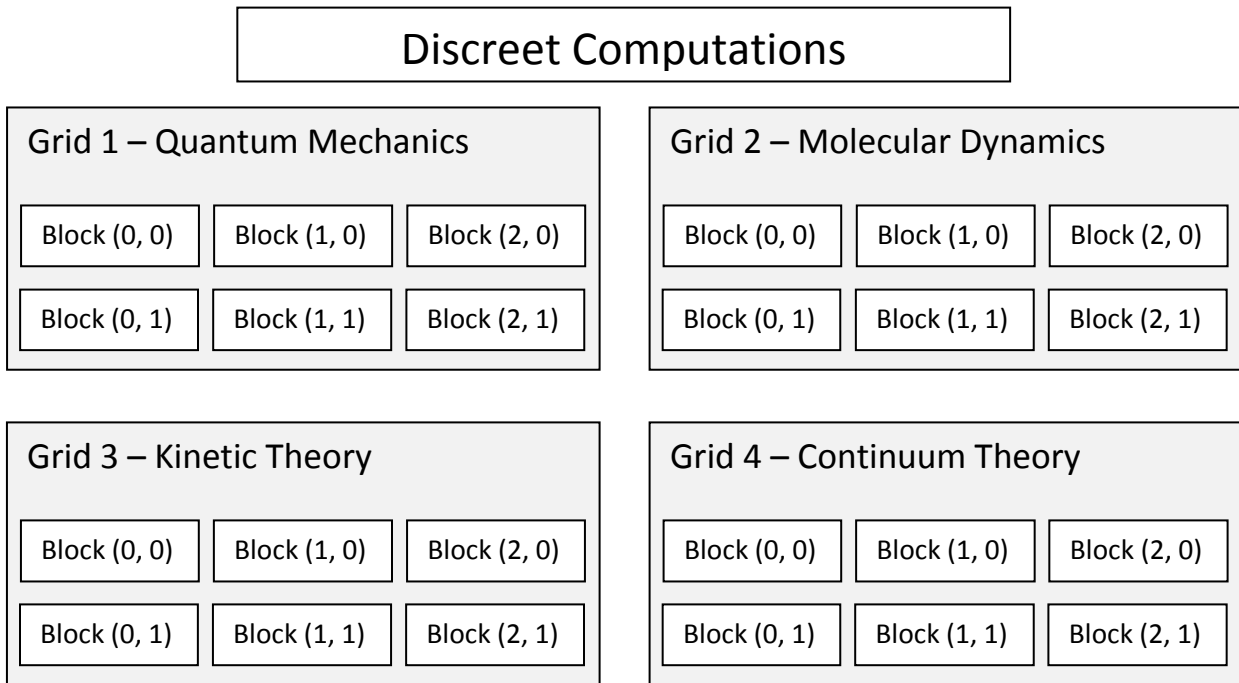


Fig. 5. Discreet Computational Grids

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