

Prospective Application of Parallelization to Accelerate Biological Model Simulations



Kishore G R, Shubhamangala B R

Abstract: *Biological systems can be modeled using mathematical techniques to carry out in silico experiments and research. These models tend to have a lot of state variables and hence take a long time to simulate the model. Modern GPU architecture provides a framework for parallelizing computation-heavy processes. With the advent of GPU technology, it is increasingly used in the field of computational biology, aiming to reduce simulation times and increase the size of inputs. This paper surveys the use of GPU architecture in the field of biological modeling..*

Keywords : CUDA,GPU,CPU,GPGPUBCF,KARMA MODEL.

I. INTRODUCTION

Mathematical modeling is the process of developing a model of a system using mathematical constructs. These models describe the functioning of the system and provide insight into the elements that influence the function. Biological systems are a few of the most complex systems to be found in nature. The study of these systems using traditional experimentation can be cumbersome. By modeling the system using mathematics, we can create simulations to test hypotheses and conduct further studies. The process of modeling biological systems using mathematical equations is called Biological system modeling.

Biological modeling applies to a broad array of fields, including human organ modeling and protein synthesis modeling. These models provide a guideline for the current understanding of the topic. These models are refined to a higher degree by comparing the results of the simulation with in-vivo experimentation. The incremental refining of the system model produces an accurate representation of the system. These models can also provide insight into the functioning of cellular and sub-cellular systems and better analyze their behavior.

The biological models usually contain a set of differential equations and other mathematical systems which contain the parameters that influence the system. The inherent complexity of a biological system induces the requirement of a large number of state variables to describe the system. Simulations with a large number of variables generally take a significant

amount of time to execute. Experimentation with long time-scales is inefficient as the results of the experiment can influence the course of treatment for a patient. Due to this reason, there is a demand for faster and more accurate simulation models that can be used for rigorous experimentation.

Coarser models to describe biological systems have been developed and used to reduce simulation times. However, these compromise on the accuracy of the model to decrease simulation durations. The computer architecture in recent years has expanded to fit these demands. With the advent of multi-core and multiprocessing capabilities, computers have become much faster. There are dedicated systems called High-Performance Computers (HPCs) that provide faster computing capabilities. The increase in processing power can now be utilized to run more accurate models in real-time and produce better results.

Parallelization of tasks is one of the many methods that are used to reduce simulation durations. Specialized hardware that includes Graphics Processing Units (GPUs) is used to parallelize the simulation program. This paper provides insight into the application of parallelization in biological system modeling.

The remainder of this paper is divided into two sections: a Literature Survey and a Conclusion. The Literature Survey puts forth papers that have proposed the use of or used parallelization in biological model simulations. A comparative study is done in the form of a table at the end of the Survey Section..

II. REVIEW CRITERIA

[1] Macro-scale simulation model of the human heart (Yu et al.): Computer Simulation provides great insight into the functioning of the human heart. It empowers scientists to advance cardiac research and prevention of heart-related diseases. In this paper, Yu et al. propose a macro-scale simulation of the behavior of the human heart. The micro-scale simulation of the algorithm proposed considers the propagation of electrical potential and ignores other biochemical interactions involved in the beating of the human heart. Due to this massive demand, GPGPU (General-purpose computing on graphics processing units) computer architecture was used to parallelize the simulation and obtain the results. This paper follows a macro/minimal cellular automata model that simplifies the simulation of biochemical functioning of the heart and can be incorporated into modern large scale systems.

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The algorithm proposed assumes that the heart cells are uniformly distributed and the excitation caused in one cell is caused by the neighboring cells only. The algorithm uses a 3D model of the human heart that is reconstructed from a series of 2D parallel heart images. The distance between each point of the 3D model covers a large number of heart cells. The simulation is carried out in GPGPU devices due to its increasing popularity in research and industrial applications.

The simulation of the algorithm was carried out under three different conditions, one with a CPU and two with GPUs. The results of the simulation were identical, but the GPU performance was much better than the performance of the CPU. Thus a comprehensive real-time 3D model of the heart can be developed and simulated by using modern parallelization techniques

[2] Multi-scale model to study electrical signaling in the heart (Du et al.): This paper provides a multi-scale model to study the effects of four different glycosylation conditions on electrical signaling in the human heart. The model simulates the functioning of the heart and thus is used as an alternative to studying the underlying mechanisms of the operation of the heart. It also helps overcome the practical difficulties in measuring the propagation of electrical waves through the heart tissue. The model is based on a micro/maximal model that uses numerical solver methods to improve the accuracy of the simulation.

Yang et al. have proposed mathematical models for the functioning of the human heart by considering the ion channels that are used to activate cardiac cells. The models developed include Glycosylation Modulation of hERG (human ether-a-go-go related gene product) Ion Channels, Cardiac Cell Action Potential Modeling, and Cardiac Cellular Cable and Ring Modeling. These models capture the micro-level functioning of the heart. Differential equations are used to describe these models by considering relevant external factors. The model is designed based on real-world experimental data gathered to explore the effects of human ventricular electrical signaling.

With the help of the mathematical models presented in this paper, one can predict the effects of pharmaceutical treatments on a patient's heart. The model explores the hERG channel glycosylation modulation dynamics on electrical signaling on the cardiac cells and the electrical conduction through the heart tissue. Better and accurate predictions of the condition of the human heart can be explored using this model.

[3] Comparative performance study of the simulation of cardiac tissue (Bartocci et al): Bartocci et al. have shed light on how to use GPUs for the simulation of the functioning of the human heart as opposed to the classical CPU based simulation. The models have a high computational demand as they include tens of state variables and hundreds of fitted variables. This paper shows that with careful implementation using GPUs, real-time simulations can be carried out for the complex cardiac models. This paper uses model-specific optimizations to obtain better performance. CUDA (Compute Unified Device Architecture) from NVIDIA is used for the simulation.

Cardiac tissue modeling can be done by considering the

trans-membranal potential coupled with a few differential equations. These models are then used to run the simulation using the GPU architecture. The paper simulates five different cardiac models: Karma Model, BCF Model, BR Model, TP Model, IMW model. These models have an increasing number of state variables ranging from 2 to 67. These models show promise for real-time applications and demonstrate the possibilities of the use of GPU architecture for more massive cardiac tissue model simulations.

[4] Accelerate hybrid functional Petri-Net simulations by parallelization (Chalkidis et al): Biological network simulations provide a virtual environment that can be used to accelerate personalized medicine development. The simulations also have the potential to expand the horizon of pharmaceutical research greatly. Petri nets are widely and successfully applied to biological network modeling. Extensions such as hybrid functional Petri nets (HFPNs) add additional features to capture the biological model accurately. This paper presents a method to accelerate HFPN simulations by migrating the model to a parallelized CUDA GPUs.

The HFPN implementation in this paper is done using graphs. The vertices of the graph correspond to either discrete states or continuous states. A continuous state holds a real value while a discrete state holds an integer value. The transitions (or edges) can be normal arcs, inhibitory arcs or test arcs. With these elements, the biological model is developed and is simulated under CUDA architecture. In a sequential implementation, the transitions are taken if certain conditions are met. Once taken, the values held at each node are updated. The computational throughput of the simulation is done by assigning each process to a different thread and parallelizing it. CUDA specific optimizations result in a 6.88x speedup in the simulation of HFPN.

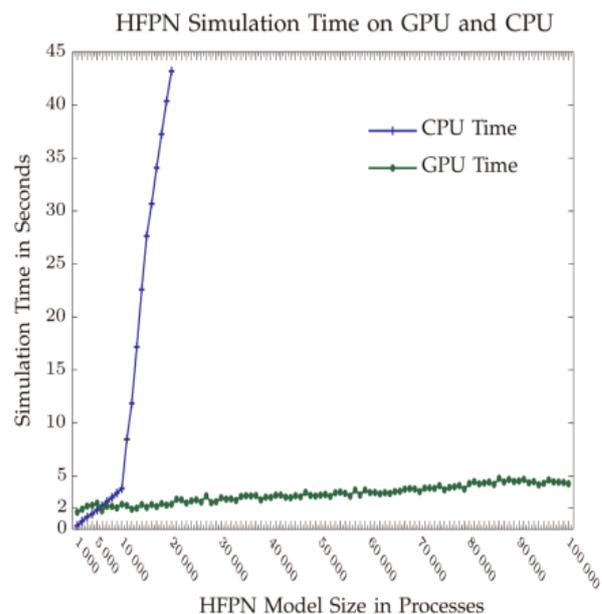


Fig 1: A comparison of CPU and GPU simulation times in HFPN simulation

If you are using *Word*, use either the Microsoft Equation Due to the heavy computation demands of biological model simulations, it is imperative to shift to parallel processing on GPUs.

Chalkidis et al. have provided a CUDA based GPU implementation of the HFPN models. The results of the paper are promising and reinforce the need to shift the biological model simulation to GPUs.

[5] Protein threading problem in parallel (Yanev and Andonov): The Protein Threading Problem is considered as the “holy grail” in computational biology. The problem states that given a particular target sequence query whether or not it folds into a 3D template core with an alignment that minimizes a suitable score function. The protein threading problem is proven to be NP-Complete and non-approximable. This paper formulates the Protein Threading problem as a network flow model, which is proven to be similar to the Shortest Path Problem with a specific structure. The paper also provides a mechanism to parallelize the solution and improve the efficiency of the algorithm.

Yanev and Andonov initially provide a mechanism to convert the Protein Threading Problem to a Network Flow. The conversion gives the optimization expression, which must be minimized. Specific instances such as the self-threading (of the protein) cases are also considered in this conversion. The algorithm is then parallelized by using a centralized load balancing strategy by using atomic processor threads. This strategy was found to result in one processor getting a “hard” subproblem, thereby slowing down the global processing time. The CPLEX callback function technique is used with non-atomic tasks assigned to the processor threads to ensure that the “hard” subproblem doesn’t slow down the execution of the program.

This paper demonstrates the power of mathematical programming with parallel programming and algorithm design. These methods can be used to tackle various problems that arise in computational biology. The paper successfully models a non-linear combinatorial problem linearly and solves huge instances of the Protein Threading Problem in a reasonable time.

[6] A Lattice-Based, Reaction-Diffusion model to simulate in vivo diffusion (Roberts et al): Roberts et al. in their paper have developed a lattice-based, reaction-diffusion model that uses GPUs to speed up the long time-scale simulations of biomechanical pathways under in vivo cell conditions. Multi-particle cellular automata model with adaptations specific to the problem is used in this paper to perform the simulation. Cellular automata are theoretically well suited for parallelized implementations and thus forms the motivation of this paper.

The paper introduces the cellular automata used for the simulation as a derivative of the multi-particle model. The model consists of a cubic lattice with three spatial coordinates for each particle. The Brownian Motion of particles in a system is simulated as a random choice of the walk of the particle in the three spatial dimensions. The random walks of each particle govern the time evolution of the model. The parallelized implementation of the simulation adopts a specified processing strategy. Random number generation is one of the key steps in this simulation. The paper uses a linear congruential generator, followed by a 64-bit xor shift and finally a pass through a multiplicative linear congruential generator to produce the three random numbers. Overall the cellular automaton captures the intrinsic behavior of in vivo

diffusion, and the simulation duration is well within the second's range. The paper presents a unique method of using cellular automata to simulate in vivo diffusion in real-time. The cellular automata described in this paper is explicitly designed to run on GPUs and take advantage of its unique characteristics. The paper introduces the use of GPUs to provide real-time simulations for previously long time-scale simulations of in vivo diffusion.

[7] Protein-Protein Docking Pipeline using HPCs (Hu et al.): Protein-Protein Interactions (PPIs) underlie most biological interactions. The 3D structure of a protein determines its interaction with other proteins, which is fundamental for antimicrobial drug and vaccine design. Recent advancements in the field of computational biology have made in silico protein-protein docking a promising methodology to determine PPIs. This paper outlines a Protein-Protein docking pipeline developed by integrating well-defined docking algorithms such as ZDOCK and RosettaDock in a state-of-the-art High-Performance Computing (HPC) system.

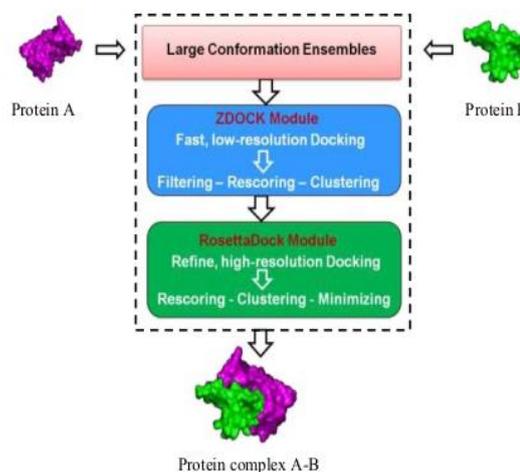


Fig 2: A visual representation of the Protein-Protein Docking Pipeline

Hu et al. have developed a Web-based tool for the simulation of their Protein-Protein Docking Pipeline (PPDP). The pipeline is an amalgamation of ZDOCK and RosettaDock algorithms with HPC specific optimizations. The PPDP provides a systematic platform to design and optimize different docking protocols for PPI study. The HPC specific implementation of PPDP allows for the parallelization of large data sets and the study of large-scale PPI networks. The pipeline developed in this paper can be used to study bacterial virulence effector/chaperone interactions and other related areas effectively. [8] A particle model to simulate intracellular functions (Falk et al.): Biological system interaction and functions are highly complex, even in the case of a single cell. Mathematical models for intracellular interactions provide an insight into the functioning of a cell and also give a framework for in silico simulations of the same. This paper focuses on a parallelized simulation method that accounts for the important intra-cellular architecture of the cell.

The article also highlights the benefits of migrating particle-based simulations to the parallel architecture of GPUs. A comparison of CPU and GPU implementation presented in the paper reinforces the point above.

A particle-based simulation tracks all the molecules of biochemical reaction and their positions in the cell. The initial conditions such as relative abundance, distribution of the cell are the input to the simulator provided by the user. The time-evolution of the system is studied by following a series of well-defined steps. Random numbers are generated at each step of the simulation to provide a virtual random motion of particles inside the cell. The cytoskeleton is fixed during the initialization phase of the simulation and the collision of particles with the cytoskeleton is detected by referring to the position of the particle. The reactions between the molecules are carried out *in silico*, and a delayed update to the state values is done. This encapsulates the functioning of a cell. The overall results of the experiments show that the simulation benefits from GPU performance.

Falk et al. in their paper have presented a parallelized strategy to run a particle-based simulation to model the functioning of a cell. The model allows the use of large datasets and a high number of particles with as many molecular reactions. The simulation accurately captures the structure of the cell. The results of the work show an approximate 2000x speed-up as compared to the CPU implementation and thus has a lot of scope for real-time application.

[9] A survey on the Clinical Bioinformatics (Akanksha et al.): Bioinformatics is an interdisciplinary field that combines biology, computer science, information science, mathematics, and statistics to analyze biological data. Bioinformatics is proving to be extremely useful for clinical research. Clinical bioinformatics is the application of bioinformatics methods to clinical research and potential therapies for human diseases. This paper surveys the various databases, the prospective applications, challenges and opportunities of clinical bioinformatics in the future.

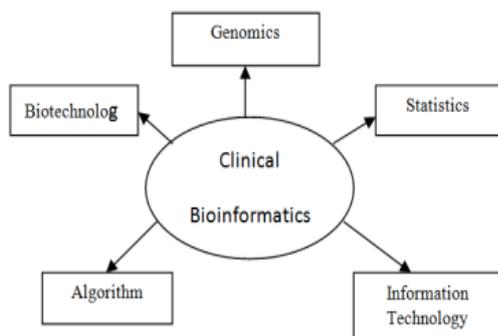


Fig 3: Constituents of Clinical Bioinformatics

The collection and storage of data form the basis of Bioinformatics. A secure database is necessary to exploit the techniques of clinical bioinformatics. Suman et al. in their paper have outlined various databases that are currently in use. These include databases on heart tissues, genetic information, malaria patients, tooth tissue, etc. These databases act as a readymade tool to access and make experimental conclusions. The article also outlines the applications, challenges, and opportunities of clinical

bioinformatics. Bioinformatics can play a vital role in the detection and cure of diseases such as cancer, diabetes, and so on. One of the significant challenges that clinical bioinformatics face is economic sustenance. Moreover, there is an argument on the ethics of holding such information which may be personal to certain people. Thus, even with its vast application and opportunities, clinical bioinformatics remains in its infancy and needs careful attention to realize its full and true potential.

[10] A mass univariate framework to image a 3D phenotype of the heart (Biffi et al.): Many factors affect the structure of the human heart. Genetics and the environment form the most prominent ones. The degree of expression of these genes and the effect of the environment on the genes affect the 3D structure of the heart. In this paper, Biffi et al., extend the techniques of neuroimaging to cardiovascular imaging by developing a framework to map genetic variations and their expression in the 3D model of the heart. The mapping of the genotype and phenotype is based on the statistical expression of each gene at every point in the 3D image of the heart.

In this paper, a mass univariate framework images the 3D heart and maps the relationship between genotype and phenotypic expression of the genotype. Data collected from collegewide studies form the dataset of this experiment. Every point in the 3D model contains a linear model to extract the regression coefficient connected to a gene. Threshold-free cluster enhancement (TFCE) enhances the map derived in the previous step. Multiple tests refine the obtained model and its many permutations to produce a final 3D model of the heart.

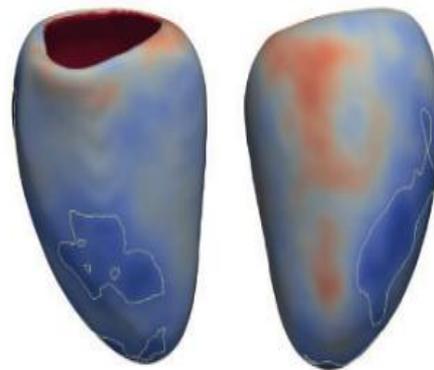


Fig 4: A 3D model of the human heart developed using the univariate model

Overall, this paper presents a robust framework to study the effects of genes and environment on the structure of the human heart. The 3D model encompasses many phenotypic traits that are aligned to the clinical datasets available. The model offers immense power to study and experiment on the expression of genes in the human heart.

[11] Survey on different methods to prevent human heart-related diseases (Liew et al.): Determining and possibly preventing heart failures is a difficult task — factors such as genetics, lifestyle, diet, and previous medication effect the analysis.

This paper calls for a unification of many different techniques to determine the reasons for heart failure. Liew et al. also realize the need for bioinformatics to manage the vast data required for each method. The unification of the techniques minimizes the various drawbacks of each method and can predict heart failures more accurately.

This paper discusses the various techniques involved in detecting human heart failure. The Gene array method forms one of such methods. The method currently is reasonably advanced concerning to human heart failure. The authors

suggest that by sampling data of normal-functioning hearts and cases of heart failure can increase the accuracy of the gene array method. Methods like electrophoresis (e.g., two-dimensional polyacrylamide gel electrophoresis (2DGE)), protein arrays have their drawbacks. The authors aim to reduce these drawbacks by intertwining all the methods with a larger dataset and bioinformatics. The additional data facilitates better prediction and detection of heart failure.

III. GAP IDENTIFICATION

TABLE I. Comparative Study

Sl No.	Author(s)	Year	Approach	Description	Gap Identification
1	Di Yu, Dongping Du, Hui Yang, Yicheng Tu	2014	Macro-scale simulation model of the human heart	A 3D model of the heart is generated from a number of 2D images and the simulation durations on CPU and GPU are compared.	There is a compromise on the accuracy of the model by considering a minimal approach. It can lead to inaccurate analysis.
2	D. Du, H. Yang, S.A. Norring, E.S. Bennett	2011	Multi-scale model to study the effects of glycosylation on electrical signaling in heart	Developed various models to capture the micro-level functioning of the heart. Proposes the use of GPU architecture for simulation.	Micro-level models require a complex parallelization system to run real-time simulations. There is a trade-off between accuracy and speed
3	E. Bartocci, E. M. Cherry, J. Glimm, R. Grosu, S. A. Smolka, S. A. Smolka, and F. H. Fenton	2011	Comparative performance study of the simulation of cardiac tissue	Different models with different number of state variables are simulated on CPU and GPUs to compare the performance	Analysis of larger models would provide more conclusive evidence for migrating to GPUs.
4	Georgios Chalkidis, Masao Nagasaki, and Satoru Miyano	2011	Accelerate hybrid functional Petri-Net simulations by parallelization	A graphical model is simulated by using the CUDA architecture to propose the migration of simulations to GPU architecture.	Analysis of graphical model of HFP using CUDA architecture in the migration of GPU simulation architecture.
5	Nicola Yanev, Rumen Andonov	2003	Use Algorithm design and parallelization to provide a possible solution to the Protein-Threading Problem	Convert the problem to a Network flow and use load balancing parallelization technique by ensuring no processor gets a "hard" sub problem	Can incorporate amino acid interactions to the model to improve the accuracy of prediction of the folded protein structure

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6	Elijah Roberts, John E. Stone, Leonardo Sepúlveda, Wen-Mei W. Hwu and Zaida Luthey-Schulten	2009	A Lattice-Based, Reaction-Diffusion model to simulate <i>in vivo</i> diffusion.	Uses a cellular automaton to model the system and use an architecture-specific parallelization technique to reduce simulation time into the seconds range.	It can be analyzing different cellular automation of the model and how you can involve in the parallelization technique to reduce simulation
7	Xin Hu, Michael Lee, Kamal Kumar, and Anders Wallqvist	2010	Protein-Protein Docking Pipeline using state-of-the-art High-Performance Computing systems.	A generalized docking pipeline based on well-defined pipelines to simulate protein-protein docking.	Adopts a clustered approach to produce real-time results. Fails to highlight the use of GPUs in the simulation.
8	Martin Falk, Michael Ott, Thomas Ertl, Michael Klann, Heinz Koeppl	2011	A particle model to simulate intracellular functions.	The paper provides a parallelization strategy to run a particle-based simulation model with a large number of initial particles.	The results of the work show an approximate 2000x speed-up as compared to the CPU implementation and thus has a lot of scope for real-time application.
9	Suman Akanksha, Chaudhary Nidhee and Neetu Jabalia.	2015	A survey on the Clinical Bioinformatics	Describes the application, need, opportunities, and drawbacks of Clinical Bioinformatics.	Fails to recognize the importance of Parallelization for the development of Clinical Bioinformatics
10	Biffi, Carlo, Antonio de Marvao, Mark I. Attard, Timothy JW Dawes, Nicola Whiffin, Wenjia Bai, Wenzhe Shi	2017	A mass univariate framework to image a 3D phenotype of the heart to study the effects of genes.	Uses a regression model to statistically determine the structure of a human heart based on the genetic information available to study the relationship between genotype and phenotype.	Effective parallelization schemes can be adopted to explore larger and more sophisticated models.
11	Dos Remedios, C. G., C. C. Liew, P. D. Allen, R. L. Winslow, J. E. Van Eyk, and M. J. Dunn.	2003	Surveys different mechanisms to study, detect and prevent human heart-related diseases	Describes methods that are in general use today, and calls for a unified effort with a large dataset to detect human heart diseases	Performing large dataset simulations in real-time require parallelization strategies. The author fails to touch upon this regard.

IV. CONCLUSION

Conclusion: Recent advances in systems biology research have resulted in larger model sizes, and hence computationally heavy simulations. Thus the demand for faster simulations has increased. Parallelization with GPUs offers a prospective solution to reduce execution times. This paper outlines the use of GPU architecture and parallelization in biological system modeling. The speed-ups achieved by the papers described in this article show a promising future for the use of GPUs for faster *in silico* experiments.

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