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COMPUTATIONAL SCIENCE – OVERVIEW AND SIGNIFICANCE

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ABSTRACT

The tremendous advances in computing – computer hardware, algorithm techniques, and software have been having tremendous impacts on the way studies and work are conducted in the other disciplines – engineering, physical sciences, natural sciences, health sciences, transportation, finance, business and management, social sciences, etc. A multidisciplinary area namely Computational Science has emerged and matured enough that several real–world problems which were earlier considered too complex to solve are being modeled and solved. It draws upon techniques from mathematics, computer science, numerical techniques, statistical techniques, simulation, data science, and data visualization. It is supplementing the traditional theory and experimentation in the sciences. This paper presents an overview of Computational Science, the major models used, and a sample of several complex real–world problems tackled by computational science techniques, the current state and future directions of this discipline.

Keywords- *Computational science, scientific computing, complex real-world problems, modeling, simulation*

I. INTRODUCTION

The computer, Internet, and mobile technologies have advanced and matured to a point where they have been the enabling technologies and driving forces behind the processes of several verticals and domains. However, there exist numerous real-world problems in a variety of areas which are overwhelmingly difficult to understand and develop optimal solutions. The use of traditional methods and software are not efficient or effective in developing the solutions to these problems. Some examples are: behaviors of financial markets, climate changes, development of effective vaccines, DNA based drugs, sustainable development, genetics, prediction of the effects of natural disasters, prediction of customer behavior, material science and properties of new materials, ocean modeling, etc.

The emerging discipline of Computational science has enabled modeling much more complex chemical, biological, ecological, materials, and social systems, and to understand increasingly large quantities of data, than could be done with traditional methods of science and engineering. Computational Science has been a rapidly growing multidisciplinary field which takes solving complex real–world problems to the next level by judiciously drawing upon and combining techniques from a variety of areas. It judiciously combines the techniques of computation, mathematics, data science, statistics, numerical methods, and simulation to obtain solutions to complex real–world problems. Computational Science has been having profound effects on the fundamental ways science and engineering (even business and social sciences) are beginning to be performed. It has been recognized as a promising area to harness the tremendous potential of computing power and techniques for handling and manipulating big data to achieve benefits which have immediate impacts in the real–world.

In this paper, we present an overview of Computational Science – why is it important and what it is, the different ways of understanding and predicting the behaviour of complex systems, the major steps in the modelling process which is a key component in the computational science technique to solve problems, model classifications based on the nature of models, brief description of different types of models, challenges to be addressed in the computational science discipline, samples of problems solved by computational science techniques, and the relevance and importance of courses and programs in computational science, followed by conclusions.

II. WHY COMPUTATIONAL SCIENCE?

Numerous complex real–world problems (ex. defense, security, earth sciences, space exploration, meteorology, microbiological basis of diseases, effective drug discovery, economic forecasting, epidemiology,

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weather and climate prediction, global financial markets, automobile body distortions in a crash, etc.) are far too complex to understand and solve using traditional analytical methods. Experiments in numerous scientific and other domains are highly complex, prohibitively expensive, dangerous, and risky. Computational Science is a feasible, viable method to better understand, model, and solve complex real–world problems in Physical sciences, Natural sciences, Health sciences, Social sciences, etc. Computational Science facilitates understanding of complex problems, obtain both qualitative and quantitative insights into the complex system behavior, determine the viability of solutions, and develop solutions. It enables scientists to solve in a cost– and time–efficient manner, many real-world problems which are too complex to handle experimentally. Computational Science is beginning to play an important role in the way science and engineering is being done, and is expected to play an even more dominating role in the future, impacting numerous areas in the world within us and around us.

Many of the current problems, situations, and their (adverse) effects on the environment and upon humans in contemporary society were not existent several years ago. Some examples are, greenhouse gas effects and global warming, pollution of air and water, use of chemicals in many processes, changing global weather patterns, newer diseases and their spread, public safety issues, etc. Several of the earlier problems have scaled up significantly, have changed in the basic nature, have increased number of interacting factors, etc. The conventional methods are not able to cope up the complexities nor are able to develop effective solutions using traditional methods due to various reasons, such as, huge problem sizes for which traditional solutions will not scale up, highly complex interactions of numerous factors in the newer problems, extreme difficulty in determining cause–effect relationships in many situations, etc.

According to [1], computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health, and economic innovation. Advances in computing and connectivity make it possible to develop computational models and capture and analyze unprecedented amounts of experimental and observational data to address problems previously deemed intractable or beyond imagination.

III. WHAT IS COMPUTATIONAL SCIENCE?

There have been numerous studies about what computational science is about. A couple of resources which present the nature, components, and practice of computational science are [3, 4, 5].

Computational Science is a multidisciplinary area which uses techniques from a variety of areas as shown in Fig. 1 to solve complex problems in physical sciences, natural sciences, health sciences, social sciences, etc. The major areas from which techniques are used in computational science are computer science, mathematics, numerical techniques, statistical techniques, modeling techniques, simulation, data science, data visualization, etc.

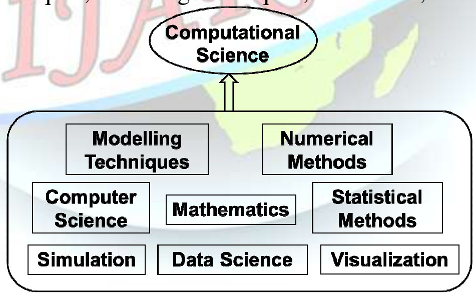

Figure 1. **Major areas contributing to Computational Science techniques**

Although Computational Science includes/draws upon elements from variety of areas such as computer science, mathematics, numerical techniques, statistical techniques, simulation, data science, data visualization, etc., it integrates the appropriate elements in the development of problem-solving methodologies and robust tools which will be the building blocks for solutions to the real-world problems of high complexity. In other words, it demonstrates that the whole is greater than the sum of the parts.

The other characteristic of Computational Science is that it requires some collaboration of expertise from different areas and the use of techniques will be domain (problem) specific. It focuses on the development and innovative use of computational tools for the solution of complex problems.

Advances in several areas have given impetus to Computational Science, for example, (a) hardware resulting in tremendous increases in computational power, (b) advanced algorithms, (c) powerful, feature–rich programming languages; (d) advanced software engineering techniques enabling development of versatile, large-scale, and highly capable software systems, (e) mathematical, algorithmic, and numerical analysis techniques to

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ensure faster and accurate computations, (f) simulation techniques to map real-world phenomena on digital computers, (g) data analytics and data visualization enabling processing, analyzing and understanding of huge amounts of data, etc. Computational Science has reached a level of maturity that it complements the traditional pillars of experimentation and theory in the sciences.

IV. UNDERSTANDING AND PREDICTING THE BEHAVIOUR OF COMPLEX SYSTEMS

The tradition ways to understand a physical phenomenon and then to be able to make predictions about the behavior of the system under various conditions are summarized in Fig. 2.

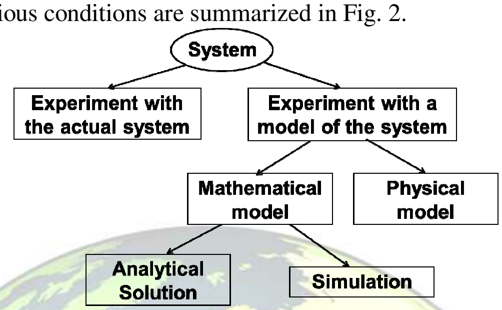

Figure 2. Different methodologies for understanding system behavior

In cases, where possible, feasible, and affordable, experiments with the actual system and gathering the results and then correlating the output with the input would enable understanding of the system behavior. However, this approach is taken if there is a strong and compelling reason, since it too limiting in most cases due to high costs of equipment. The other alternative is to develop a model of the real–world system which is an approximation with simplifying assumptions. The model could be a physical model or a mathematical model. A physical model could an actual size or scaled–down size of the real–world entity, which is tested in an actual or simulated condition. An example of a physical model is the use of physical human models in car crash tests. This is easier and more practical to study the effects on the driver/passenger in the event of a car crash under various scenarios. A mathematical model in this case would be far too complex and would be far from being accurate to be of practical use. On the other hand, there are numerous situations where a physical model is not feasible or safe (for example, modeling earthquakes and their aftereffects, predictions of predator and prey populations, etc.), and a mathematical model is the preferred way. In case of mathematical models the system is understood by solving for it analytically or by doing a computer simulation. Computational science combines several of these aspects in a judicious manner suited to the particular problem. [3] proposed a system in which FASTRA downloads and data transfers can be carried over a high speed internet network. On enhancement of the algorithm, the new algorithm holds the key for many new frontiers to be explored in case of congestion control. The congestion control algorithm is currently running on Linux platform. The Windows platform is the widely used one. By proper Simulation applications, in Windows we can implement the same congestion control algorithm for Windows platform also. The Torrents application which we are currently using can achieve speeds similar to or better than ―Rapid share (premium user) application.

V. MAJOR STEPS IN THE MODELING PROCESS

One of the key stages in the solution of problems using computational science techniques is the development of an appropriate model of the corresponding complex real–world phenomenon. The major steps in the modeling process are shown in Fig. 3.

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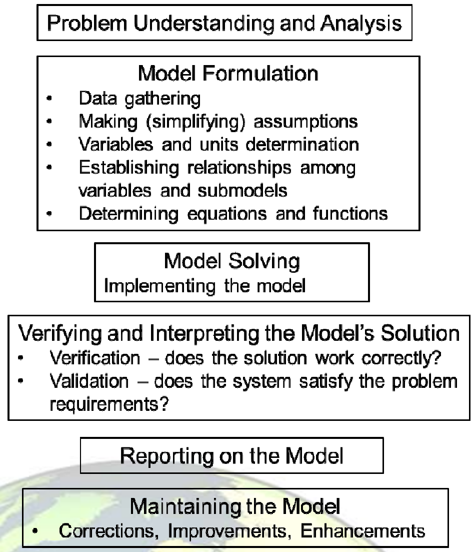

Figure 3. **Major steps in the modeling process**

Problem understanding and analysis is a very important first step in the modeling process which enable the choice of the appropriate model for the problem solution. The model formulation involves making simplifying assumptions since the original real-world problem is almost always very complex. Any submodels, relationships among variables, equations and functions governing the behavior of the system are determined. The model is then ready to be worked upon by model solvers to obtain the solution. The solution is subsequently verified (ensuring the solution works correctly) and validated (ensuring the solution satisfies the problem requirements). Then a report on the model is prepared for dissemination for colleagues and professionals. Finally the model needs to be maintained my making corrections, improvements, and enhancements, as necessary.

VI. Model Classifications Based on Nature of Models

A classification of the models based on the inherent nature of the model is shown in Fig. 4. Based on whether the input–output relationship is completely determined by a function (the output is the same for the same set of inputs) or not (there is an element of randomness in the exact value of the output), the model is classified as deterministic or stochastic (probabilistic), respectively. Depending on whether there is a time dimension involved in the model (ex. the trajectory of a rocket at different instants of time), or not (the output is independent of time, ex. gravitational force between two heavenly bodies), the model is classified as either dynamic or static, respectively. Depending upon whether the phenomenon changes continuously (ex. heat diffusion in a metal plate) or in discrete steps (ex. arrival of customers at a bank), the model is classified as continuous model or discrete model, respectively.

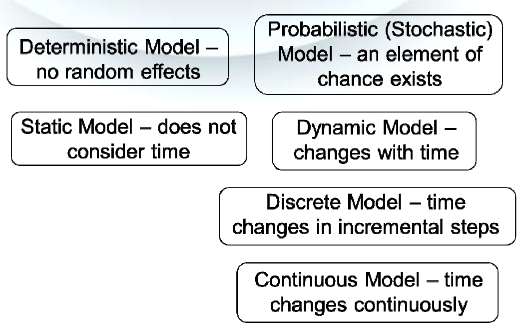

Figure 4. **Models based on different nature**

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VII. TYPES OF MODELS

There are several popular types of models which are used in the process of understanding the behavior of a system, to develop solutions to problems, and even to make predictions. These are shown in the Fig. 5, and are described below.

Data Driven Models	Cellular Automaton	Agent–Based Models
Matrix Models	Markov Chains	Graph Models

Figure 5. **Different types of models**

Data Driven Models

In a data driven model, measurements data is available. An attempt is made to "understand" the pattern of data by trying to obtain a function to fit the data (with least error). The function could typically be linear, quadratic, exponential, logarithmic, logistic, trigonometric, or non–linear (with multiple terms–piecewise linear approximation). Subsequently the function is used to find estimates (where no data is present). This is also called empirical model.

Cellular Automaton

This model (usually) consists of a 2–dimensional array of cells. Each cell is associated with a function which determines the value of a cell based on its neighboring cells (Von Neumann neighborhood of 4 neighbors or Moore neighborhood 8 neighbors). The boundary cells are handled suitably. Initial conditions need to be appropriately determined and set. Then, the model is subjected to a set of iterations until some convergence / equilibrium is achieved.

Agent–Based Models

In this model, each entity of the system being modeled is an autonomous, decision–making agent. Each agent has a state (a set of state variables) and behavior(s). There is a method (or procedure) associated with a class / group of agents. Agents operate in an environment. The next state of an agent is a function of the environment, neighboring agents, current state of agent, and behavior of agent. The state of each agent is updated at each step of the iteration.

Matrix Models

In this model, entities and attributes are represented as matrices and vectors. The matrices and vectors represent systems of equations. The equations are solved using several well–known approaches to obtain solutions. Special matrices and their characteristics have been studied which aids the solution process.

Markov Chains

In this model, the system is represented as a set of states and transitions. The next state is a function of current state and input. There are probabilities associated with transition(s) to next state(s). The matrix employed is called a Markov matrix which is a matrix of probabilities where column values add up to 1. The values in the matrix are based on observed / experimental data. Markov chain is a sequence of variables. In a first order Markov chain, the value of a variable depends on value of the immediate predecessor, while in an Nth order Markov chain, the value of a variable depends on values of the previous N predecessors.

Graph Models

In a graph model, the problem is represented as a graph. The solution sought usually involves finding a special property in that graph for which there are well–known graph algorithms. A Graph G is a tuple (V, E), where V is a set of vertices (points), and G is a set of edges (an edge being an arc connecting two vertices). Edge could be undirected, directed, weighted, etc. There are numerous kinds of graphs such as undirected, directed, planar, bipartite, etc. etc. There are numerous properties of graphs that solutions look for such as connectedness, colorability, minimum spanning tree, least cost paths, cliques, etc. etc., for which numerous, well–studied graph algorithms are usually available.

VIII. CHALLENGES IN COMPUTATIONAL SCIENCE

Almost all real–world phenomena are dynamic and continuous systems. However, the computational solutions to the real–world problems must be developed to cater to the discrete nature of digital computers. In addition, computers can only handle numbers and data of limited precision. Therefore the continuous phenomena/signals need to be appropriately discretized without loss their essential characteristics. Sophisticated

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mathematical, numerical analysis, and simulation techniques have been developed to handle the above requirements, which form part of the basis of computational science.

The other challenges in computational science are, (a) choice of appropriate model for the underlying physical, real-world problem; (b) the right set of assumptions and simplifications of the model; (c) the conversion of physical events and principles into mathematical representations; (d) the development of correct and efficient algorithm; (e) the correct and efficient implementation using a program or an already existing software and/or computational tool suited for the solution; (f) taking care of round-off and other errors in numerical computations; (g) verifying the results of computation to ensure it is correct; (h) validating the results of computation/simulation to make sure it is solving the right problem; (i) refining the model as necessary to improve the solution; etc.

IX. SAMPLES OF PROBLEMS MODELED AND SOLVED USING COMPUTATIONAL SCIENCE

In this section, we present a few representative samples of problems (in no particular order) from a variety of disciplines which are very complex but are very important and useful, and are modeled and solved using computational science techniques. By no means are these exhaustive.

- Simulation of earthquakes including quantitative predictions of infrastructural damages, response and recovery to minimize damage, death, and injury
- Models to develop DSS (Decision Support Systems) for drones (UAV – Unmanned Aerial Vehicle) for monitoring air quality, aerial reconnaissance, etc.
- Better understanding of Arboviruses (arthropod–borne) viruses causing West Nile encephalitis, dengue fever, and yellow fever, and to improve outbreak predictions, interventions, responses
- Determination of prescribed usage for a drug, considering a number of factors such as absorption, distribution, metabolism, and elimination. (Pharmacokinetics)
- Modeling the changes in the populations of predators and preys
- Mapping all of the human genome / genetic code which consists of 20,000-25,000 genes, composed of about 3 billion nucleotides
- Cataloguing the complete human proteome – the set of proteins that are produced and expressed in the cells of our bodies (which is of vastly greater size and complexity than the sequences of the human genome)
- Development of quantitative approaches for understanding the mechanisms, diagnosis and treatment of human disease (computational medicine)
- Predictions of Greenhouse effects, global warming, and long–term climatic changes
- Gene editing on human embryo to correct a disease–causing mutation
- Detection of gravitational waves (ripples in the fabric of space-time, hypothesized by Albert Einstein a century ago)
- Understanding how the HIV virus interacts with the cells it infects and to discover/design new drugs that can attack the virus at its weak spots
- Study and modeling of decompression sickness in deep-sea divers
- Modeling and design of Bathysphere – pressurized metal vessel which allows exploration of the oceans to much greater depths than possible by skydiving

X. RELEVANCE AND IMPORTANCE OF COURSES AND PROGRAMS IN COMPUTATIONAL SCIENCE

In today’s world there are far too many problems which are complex which cannot be solved by traditional computing methods. Several of these problems and the scale of the problems were not existent a few years ago. A few examples are, public transportation management in mega cities, alleviation of congestion in roads and highways, public safety issues, public health issues with growing population and movement of people across wide distances, pollution of various kinds due to industrialization and personal vehicles, etc. In order to understand the problem and develop an effective solution requires Computational Science methods. In this regard, it is important develop a workforce which is adept in Computational Science methods and techniques. According to [2] there is a need for approximately one million people in information and computational technology, a need that cannot be met solely by all computer science departments working at full capacity. The key to filling the need starts in institutes of higher education by developing courses and programs in Computational Science.

One of the earliest studies to come up with the components and elements of computational science and engineering education is [6]. A few challenges and opportunities in computational science and engineering study are presented in [7]. A survey of computational science education is provided in [8]. A popular and widely used resource for undergraduate and first year graduate course in computational science has been [9].

In our analysis, some of the main challenges to teaching in Computational Science are:

- Development of a systematic 'first principles' approach to modeling, simulation, analysis and control of complex, nonlinear, dynamic behavior of systems.
- To make seamless connections of principles and techniques from diverse disciplines/areas.
- Complexity of the real–world problems.
- Development of capabilities in the use of high-performance computing and highly accurate numerical methods.
- Application of computational modeling methods to complex problems from diverse areas

XI. CONCLUSIONS

Computational science is an emerging multidisciplinary discipline which has demonstrated high potential in modeling and solving numerous complex, real–world problems from across several diverse disciplines. It draws upon and integrates techniques from a variety of areas such as computer science, mathematics, numerical methods, modeling, statistical methods, data science, data visualization, etc. Advances in computer hardware, algorithms and programming languages, numerical methods, data analytics and data visualization, have given impetus to computational science. It is crucial to develop workforce adept in understanding and solving complex real–world problems from across diverse disciplines. In this regard, it is important for the students of science and engineering to be exposed to computational science. It is also important for institutes of higher education to develop courses and programs in Computational Science.

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