International Journal of Trend in Research and Development, Volume 6(4), ISSN: 2394-9333
www.ijtrd.com

Computational Science

[1]Matthew N. O. Sadiku, [2]Kelechi G. Eze and [3]Sarhan M. Musa,
[1,2,3]Roy G. Perry College of Engineering, Prairie View A&M University, Prairie View, TX, United States

Abstract: Computational science refers to the use of computer hardware and software to solve scientific problems in diverse areas such as sciences, engineering, finance, and humanities. It is at the intersection of mathematics, computer science, and the core disciplines of science and engineering. It has become an indispensable partner along with theory and experiment. It is crucial to the security and welfare of any nation. It is becoming indispensable in many scientific investigations ranging from chemistry, physics, mathematics, engineering, economics, and finance. This paper provides a brief introduction to computational science.

Keywords: *Computational Science, Computational Science and Engineering, Computational Methods, Scientific Computing*

I. INTRODUCTION

Since the invention of digital computer, its potential to aid scientific investigation has been well recognized. Computer is an indispensable tool in solving complex problems in every sector, from traditional science and engineering domains to such key areas as finance, national security, medicine, and public health. Computers have come a long way within a few decades.

Computational science (CS) refers to the application of computer simulation to solve problems in various scientific disciplines. It is commonly regarded as the third pillar of scientific investigation, complementing theoretical analysis and laboratory experiment. The triad of theory, experiment, and computation is shown in Figure 1 [1]. CS provides the means of solving problems that are either mathematically intractable or inaccessible to traditional experimentation. Sometimes the computation involves massive amounts of calculations and is often implemented on high performance computers or supercomputers [2]. Some areas of computational science utilize large databases and require terabytes of storage, while other areas may require networks of computers. Software and programming are also important in computational science: FORTRAN, C++, Java, CORBA, MATLAB, Linux, Python, etc.

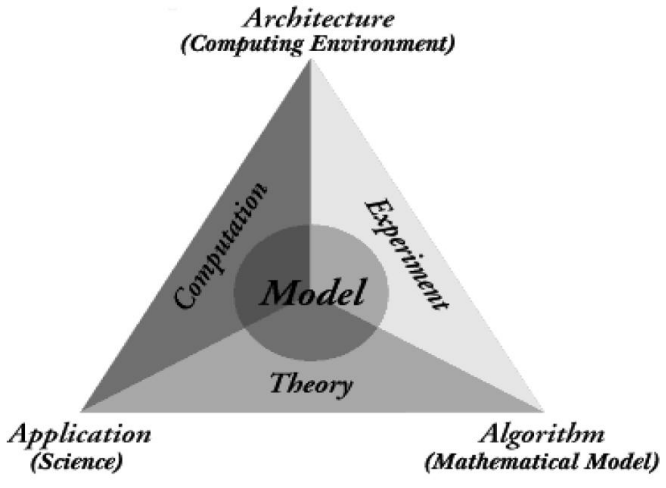

Figure 1: Triad of theory, computation, and experiment [1].

A computational scientist is usually a scientist, an engineer or an applied mathematician who is skilled in scientific computing, programming languages, operating systems visualization software, and parallel computing. Common numerical techniques used by computational scientists include finite elements, moment methods, finite difference method, Monte Carlo methods, methods of integration, and methods of line.

II. APPLICATIONS

Many disciplines have undergone a computational turn in the past decades. The recent computational turn has produced sub-disciplines such as computational biology, computational chemistry, computational physics, and computational finance.

- *Computational Biology*: This is the science of modeling biological systems. Computational techniques are revolutionizing biology. A major challenge here is to understand how gene regulation controls fundamental biological processes. Computational anatomy and medicine have greatly helped in the analysis of biological information. Computational tools are now in the hands of doctors who treat patients with all kinds of illnesses.
- *Computational Chemistry*: Computational chemistry is a rapidly developing branch of chemistry that applies computational methods to solve chemical problems. It is basically the application of chemical, mathematical, and computing skills to the solution of problems. It uses computers to generate information such as properties of molecules and materials. Computational chemistry has become a vital collaborator with experimental chemistry, whether it be physical chemistry, organic chemistry, biochemistry, medicinal chemistry or chromatograhy. It is a multidisciplinary field with applications in chemistry, biology, and material science. The use of computational chemistry in drug design has become a standard practice [3].
- *Computational Physics:* Computers are playing an increasingly important role in the lives and education of physicists. Several areas in physics have problems which cannot be treated exactly or analytically and must be solved numerically. Computational physics allows developing models of physical phenomena and understanding things at depths greater than possible otherwise. It deals with applying numerical methods in solving physical problems. It enables learning physics with computers. Depending on whether the researcher is a born digital or digital immigrant, programming languages used in computational physics include FORTRAN, C, C++, and Python [4].
- *Computational Finance:* Computational finance is an important aspect of modern commerce. It combines the power of computing and statistical analysis with the principles of finance and investment management. While traditional finance deals with actually making transactions that range from stock trades to corporate acquisitions, computational finance is more concerned with algorithms, modeling, and the computer software

that powers most of the modern financial world. Modeling is an important activity in computational finance. With models built, researchers in computational finance sometimes experiment with human participants [5].

- *Computational social science* (CSS): This is an academic discipline that combines the traditional social sciences with computer science. CSS can span all the five traditional social science disciplines: psychology, anthropology, economics, political science, and sociology. It is team work of computer scientists and social scientists. While social scientists provide research questions, data sources, and acquisition methods, computer scientists contribute mathematical models and computational tools. CSS uses computationally methods and statistical tools to analyze and model social phenomena, social structures, and human social behavior [6].

Other areas of application include computational sociology, computational economics, computational mechanics, computational fluid dynamics, computational electromagnetics, computational medicine, computational archaeology, computational materials science, computational engineering, computational fluid dynamics, computational forensics, computational geophysics, computational history, computational informatics, computational intelligence, computational law, computational linguistics, computational mathematics, computational mechanics, computational neuroscience, computational pharmacology, computational anatomy, computational imaging, and computational statistics. The list keeps growing.

III. CHALLENGES

While computational science offers great value to society, it faces some challenges. Some software used in CS are large and expensive to maintain. Such limitation has caused some industries to develop internally written and maintained codes [7].

There are some "unsolved problems in computational science. These tough problems are related to number theory, geometry theory, combinatorics, graph theory, linear Algebra, and group theory [8].

Since CS is multidisciplinary field, there are challenges in working across disciplines. Communication can present a challenge among interdisciplinary teams since each discipline has its own unique vocabulary [9].

CONCLUSION

Computational science complements theory and experiments. It is a fast growing interdisciplinary and exciting field that uses advanced computing and data analysis to solve complex problems. The dramatic advances in software and hardware development during the past half-century suggest that our computational efforts in the next half-century will supersede all imagination. By applying digital tools, researchers have begun to build models that can unravel complex physical mysteries. The field of computational science is exciting and growing.

Computational Science and Engineering (CSE) is a multidisciplinary area of study that is offered in some universities today at undergraduate and graduate levels [9,10]. It is a rapidly evolving field that is distinct from pure computer science and computer engineering. The next generation of computational scientists should obtain competences in several disciplines. More information about computational science can be obtained from books on CS available on Amazon.com and two major journal exclusively devoted to it: *Journal of Computational Science* and *The international Journal of Computational Science*.

References

[1] M. Kafatos, P. Becker, and Z. Boybeyi, "Computational sciences: at the intersection of science and engineering - Case study for academic and research programs," Turkish Journal of Electrical Engineering and Computer Sciences, vol. 14, no. 1, 2006, pp. 77-90.

[2] "Computational science," Wikipedia, the free encyclopedia https://en.wikipedia.org/wiki/Computational_science

[3] M. N.O. Sadiku, S.M. Musa, and O. M. Musa, "Computational Chemistry," Computational Chemistry, vol. 110, 2017, pp. 48184-48185.

[4] M. N. O. Sadiku, A. E. Shadare, and S.M. Musa, "Computational physics: an introduction," International Journal of Engineering Research, vol. 6, no. 9, Sept. 2017, pp. 427-428.

[5] M. N. O. Sadiku, S. M. Musa, and O. S. Musa, "Computational Finance," International Journal of Trend in Research and Development, vol. 4, no. 5, Sept./Oct. 2017, pp. 375-376.

[6] M. N. O. Sadiku, S. M. Musa, and O. S. Musa, "Computational Social Science," Invention Journal of Research Technology in Engineering and Management, vol. 1, no. 12, Sept. 2017, pp. 25-26.

[7] A. M. Heroux and G. Allen, Computational Science and Engineering Software Sustainability and Productivity (CSESSP) Challenges Workshop Report. Arlington, VA: Networking and Information Technology Research and Development (NITRD). September 2016, https://www.nitrd.gov/PUBS/CSESSPWorkshopReport.pdf

[8] S. Gao and K. H. Chen, "Unsolved problems in computational science: III A special self-avoiding walk," Proceedings of International Conference on Computational Science and Computational Intelligence, 2016, pp. 1371-1374.

[9] L. Carter, R. Botts, and C. Crockett, "Computational science programs: the background research," Proceedings of Frontiers in Education Conference (FIE), 2012.

[10] O. Yasar and R. H. Landau, "Elements of computational science and engineering education," SIAM Review, vol. 45, no. 4, 2003, pp. 787-805.

AUTHORS

Matthew N.O. Sadiku is a professor in the Department of Electrical and Computer Engineering at Prairie View A&M University, Prairie View, Texas. He is the author of several books and papers. His areas of research interest include computational electromagnetics and computer networks. He is a fellow of IEEE.

Kelechi G. Eze is a doctoral student at Prairie View A&M University, Texas. He is a student member of IEEE. His research interests include Internet of things security, data security and privacy, blockchain technology, wireless sensor networks, and machine learning.

Sarhan M. Musa is a professor in the Department of Engineering Technology at Prairie View A&M University, Texas. He has been the director of Prairie View Networking Academy, Texas, since 2004. He is an LTD Sprint and Boeing Welliver Fellow.