11th Workshop on Biomedical and Bioinformatics Challenges for Computer Science: new computational models, algorithms and computer architectures*

Mario Cannataro[1][0000−0003−1502−2387], Riccardo Dondi[2][0000−0003−2868−7732], Giuseppe Agapito[1][0000−0003−2868−7732], Mauro Castelli[3][0000−0002−8793−1451], Italo Zoppis[4][0000−0001−7312−7123], and Rodrigo Weber dos Santos[5][0000−0002−0633−1391]

[1] Data Analytics Research Center, University Magna Gr æcia of Catanzaro, Italy
[2] University of Bergamo, Italy
[3] NOVA Information Management School (NOVA IMS), Universidade Nova de Lisboa, Campus de Campolide, 1070-312 Lisboa, Portugal
[4] University of Milano-Bicocca, Italy
[5] Graduate Program in Computational Modeling, Federal University of Juiz de Fora, Brazil
rodrigo.weber@ufjf.edu.br

Abstract. Emerging technologies in biomedicine and bioinformatics are generating an increasing amount of complex data. To tackle the growing complexity associated with life science challenges, bioinformatics and computational biology researchers need to explore, develop and apply novel computational concepts, methods, and tools. The 11th Workshop on Biomedical and Bioinformatics Challenges for Computer Science (BBC) aimed to present the development and use of new computational models, algorithms, and computer hardware applied to different problems of life sciences and biomedical engineering. This short paper summarizes the accepted works presented at the workshop.

Keywords: Bioinformatics · Biomedicine · Computational Modeling · High Performance Computing

1 Preface

Bioinformatics and biomedical engineering are interdisciplinary in nature. In addition to biomedicine and biology, many other disciplines are integrated, such as mathematics and systems theory, computational modeling and high-performance computing, just to name a few.

Emerging life sciences applications need to use bioinformatics tools, biological data banks, patient's molecular and clinical data as well as epidemiology data in

* Supported by CAPES, CNPq, UFJF, FAPEMIG, and Data Analytics Research Center.

a coordinated way. Therefore, new challenges to computer science arise from huge amounts of data to be integrated and the computing power necessary to analyze those big data sets or to simulate complex biological and biomedical systems. The aim of this Special Section is to discuss challenges and future directions of bioinformatics and biomedical algorithms, computational models, computer hardware and applications; and relate these to the accepted papers of the 11^{th} Workshop on Biomedical and Bioinformatics Challenges for Computer Science, held in Wuxi, China, 11-13 June, 2018. The first edition of this workshop took place in Krakow, Poland, in 2008 [1], and since then a couple of special issues with extended papers presented at the workshops were published [2–4].

2 Crossing Multiple Scales of Biomedicine

The papers presented in this Special Section deals with different scales of biology and biomedicine.

Wienbrandt *et al.* in their paper *1,000x Faster than PLINK: Genome-Wide Epistasis Detection with Logistic Regression Using Combined FPGA and GPU Accelerators* deal with challenges at the level of the genes.

Vizza *et al.* in their paper *On blood viscosity and its correlation with biological parameters* study how cells, such as Hematocrits and Erythrocytes influence human blood viscosity.

Katsushima *et al.* in their paper *Development of Octree-Based High-Quality Mesh Generation Method for Biomedical Simulation* present a simulation of the biomechanics of the tibia bone.

Reis *et al.* in their paper *Combining Data Mining Techniques to Enhance Cardiac Arrhythmia Detection* present how to use ECG signals, Electrocardiograms, taken non-invasively from patient to infer the electrical behavior of the heart.

Chillarn *et al.* in their paper *CT medical imaging reconstruction using direct algebraic methods with few projections* study how to reconstruct images of the human body from x-rays.

Finally, Varella *et al.* in their paper *A Stochastic Model to Simulate the Spread of Leprosy in Juiz de Fora* present a new model to describe the spread and dynamics of the Hansen's disease within a particular population of a Brazilian city.

Therefore, the selected papers presented in this Special Section deal with diverse spatial and time scales of life, from genes to population dynamics, passing through cells, organs and the human body.

3 Computational Models

Although the papers presented in this Special Section use computational modeling to address different challenges, the reader can find a great variety of types of models.

Empirical models are used in the works of Vizza *et al.* and Reis *et al.* in order to capture the relation between blood cells and viscosity, and the relation between ECG signals and cardiac pathologies, respectively.

On the other hand, mechanistic models are used by Katsushima *et al.*, Chillarn *et al.*, and Varella *et al.*. Katsushima *et al.* present simulations of the structural biomechanics of the tibia bone using partial differential equations. These simulations can be used to help the planning of High Tibial Osteotomy (HTO), a surgical procedure that aims to disperse excessive load on the bone due to bow leg deformation. Chillarn *et al.* also use deterministic models, in the form of algebraic equations, in order to reconstruct CT-images from X-rays.

Finally, mechanistic but stochastic models are proposed by Varella *et al.* to describe the evolution of the Hansen's disease within a particular city. Stochastic models were needed to capture the limited number of infected persons, as described by the public health database of the aforementioned city.

Therefore, the selected papers presented in this Special Section use different types of models, from empirical to mechanistic, from deterministic to stochastic ones.

4 New Algorithms

All the papers presented in this Special Section propose new algorithms or new implementations to address different challenges of biomedicine and bioinformatics.

Wienbrandt *et al.* developed a new parallel algorithm to compute a logistic regression. The algorithm is based on a modified version of the classical Newton's method specially tailored to FPGAs and GPUs.

Katsushima *et al.* developed an octree-based high-quality mesh generator to support biomedical simulations, such as those based on the Finite Element Method.

Reis *et al.* combine different data mining techniques, such as clustering, feature selection, oversampling strategies and automatic classification algorithms to create efficient classification models to identify cardiac diseases based on ECG signals.

Chillarn *et al.* present two new direct algebraic algorithms for CT-imaging reconstruction, one based on Sparse QR (SPQR), and another based on singular values decomposition (SVD).

Finally, Varella *et al.* implement the Gillespie algorithm to solve the new proposed stochastic and compartmental model of epidemiology.

5 High Performance Computing

Modern challenges of life sciences involve a large amount of data and complex models, posing considerable requirements for computing power and storage resources. Not surprisingly, high performance computing is often used to deal with these complexities.

The numerical methods developed and presented by Chillarn *et al.* for CT-imaging reconstruction were run on a cluster composed of 128 cores.

The simulations of the structural biomechanics of the tibia bone performed by Chillarn *et al.* were executed on a shared-memory system composed of a total of 512 cores.

Finally, the new parallel algorithms to assess gene-gene interactions developed by Wienbrandt *et al.* were executed on a modern and heterogeneous high-performance platform that combines CPUs, FPGAs, and GPUs. The combinations of FPGAs and GPUs resulted in a speedup of more than one thousand when compared to a classical parallel algorithm that was executed on 32 cores. These new computer architectures enabled the reduction of execution times from months to a couple of hours.

6 Conclusion

Modern biology and medicine are on a regular basis challenging computer science in many aspects: (i) by demanding new concepts and models or the integration of them; (ii) by promoting the development of new algorithms, methods and techniques to solve problems that arise from life sciences or biomedical engineering; (iii) and even by requesting novel computer architectures that can cope with the ever-increasing tasks of processing large amount of data and simulation of complex computational models. The selection of papers of the 11^{th} Workshop on Biomedical and Bioinformatics Challenges for Computer Science discusses all these issues and suggest novel directions and approaches to tackle them.

References

1. Cannataro M., Romberg M., Sundnes J., Weber dos Santos R. (2008) Bioinformatics Challenges to Computer Science. In: Bubak M., van Albada G.D., Dongarra J., Sloot P.M.A. (eds) Computational Science ICCS 2008. ICCS 2008. Lecture Notes in Computer Science, vol 5103. Springer, Berlin, Heidelberg
2. Cannataro M., Romberg M., Sundnes J., Weber dos Santos R.: Special section: Biomedical and bioinformatics challenges to computer science. Future Generation Computer Systems **26**(3), 421–423 (2010). https://doi.org/10.1016/j.future.2009.10.00
3. Cannataro M., Weber dos Santos R., Sundnes J., Veltri P.: Advanced computing solutions for health care and medicine. Journal of Computational Science **3**(5), 250–253 (2012). https://doi.org/10.1016/j.jocs.2012.07.002
4. Agapito G., Cannataro M., Castelli M., Dondi, R., Zoppis I.: Editorial of the Special Issue of the 10th Workshop on Biomedical and Bioinformatics Challenges for Computer ScienceBBC 2017. Computers **7**(1), (2018). https://doi.org/10.3390/computers7010017