Preface

Computing and science reveal today a synergic relationship, in particular when considering the nature and role of methods and techniques adopted in computer science and engineering. Is computing a science? Does computing adopt the scientific method? Can computing help science? Is science a computational processes? To what extent is science supported by computing? These are just few of the many questions we can ask when recognizing the synergic relationship between computing and science.

Computing plays an increasing role in the scientific endeavor, both in modeling and simulating entities and in practically supporting various scientific activities. Think for example of autonomous artificial systems playing an increasing role in the discovery and verification of scientific hypotheses (robot scientists); or of computer and robotic systems used to discover and test mechanistic hypotheses about intelligent and adaptive behaviors of living systems; or of computational tools applied to chemical and toxicological discovery process; or of computational models used in earth system sciences to represent, understand, predict, and manage the behavior of environmental systems. Moreover, the role of scientific method in computing is getting increasingly important, especially in providing ways to experimentally evaluate the properties of complex computing systems, such as in drawing inspiration from scientific experiments to assess and benchmark autonomous systems. Indeed, these artificial systems are so huge and intricate and can have highly unpredictable interactions with the external environment that even their designers do not know in advance their behavior in every situation.

This volume presents these issues from a conceptual and methodological perspective by addressing specific case studies at the intersection between computing and science. More precisely, we intend computing both as an infra-science and as a science, and we organize the contributions accordingly. In the first role, computing is a tool for scientific disciplines (chemistry, biology, environmental sciences, animal behavior, ...) and the privileged direction of the knowledge flow is from computing to science. In the second role, computing is a science, even with some important peculiarities, and the privileged direction of the knowledge flow is from science (in particular the experimental scientific method) to computing. The volume attempts to offer an insight on how computing and science can influence each other both at a practical level and at a theoretical one. Since we cannot cover all the issues related to the common ground between computing and science, we go in depth for some significant questions, on the basis of the specific case studies presented.

This volume stems from the experience of the course "Computing and Science: What Can They Do for each Other?" for graduate students in the PhD program in Information Engineering held at Politecnico di Milano during the Spring of 2012. As for the course, our aim here is to present an integrated overview over the relationships between computing and science that goes beyond their specific field of study.

Part I of the volume investigates the impact of computing on different scientific fields. Chapter 1 ("Computational Models for Environmental Systems" by Francesca Pianosi) illustrates, by means of examples taken from various environmental contexts, how numerical computing has unlocked new uses for existing environmental models with terrific impacts from both the scientific and the engineering perspectives. Indeed ever growing computing power and its increasing availability are revolutionizing the way environmental models are constructed and used. Besides model use, this chapter considers how numerical computing has also significantly impacted model construction, especially in the context of the so-called empirical models, which simply could not exist without the computer programs used for their construction. Chapter 2 ("How Far Chemistry and Toxicology Are Computational Sciences?" by Giuseppina Gini) describes the basis of computational chemistry and how computational methods have been applied to biology, and to toxicology in particular. It discusses how and why the experimental practice in biological science is moving toward computational modeling and simulation to confirm hypotheses, to provide data for regulation, and to help designing new chemicals.

Part II of the volume analyzes the possible role of scientific concepts, like the experimental scientific method, on some fields of computing, in particular on autonomous robotics, which shows challenging issues related to the interaction between computational entities, the autonomous robots, and the real world. In this part, by investigating to what extent traditional experimental principles can be applied to some fields of computer science and engineering, we argue in favor of the importance of a methodological characterization of computing, and of computer engineering in particular, considering the role played by experiments. This is also a way to reflect on the status of the discipline not from the perspective of its object, but from the perspective of its method, whereas the debate on the disciplinary status of computer science has been mostly revolved around the issues on what computer science is (science, engineering, or else) and whether computing is a scientific discipline. Chapter 3 ("Good Experimental Methodologies for Autonomous Robotics: From Theory to Practice" by Francesco Amigoni, Viola Schiaffonati, and Mario Verdicchio) presents an analysis of experimental trends in autonomous robotics by surveying the autonomous robotic articles presented over the last dozen of years at the International Conference on Autonomous Agents and Multiagent Systems (AAMAS). By starting from some experimental methodologies proposed for autonomous robotics, this chapter reflects on the way they are implemented in the current robotic research practice. Chapter 4 ("RAWSEEDS: Building a Benchmarking Toolkit for Autonomous Robotics" by Giulio Fontana, Matteo Matteucci, and Domenico G. Sorrenti) takes a further step in this direction by illustrating the RAWSEEDS toolkit for benchmarking robots that perform simultaneous localization and mapping activities. The chapter shows both the benefits and the difficulties of building tools for the rigorous experimental evaluation of robotic performance.

Part III of the volume presents an attempt to investigate on the relationship between computing and science while considering, at the same time, computational tools as support to experimentation and some experimental principles as inspiration for the development of good experimental methodologies in computing. Chapter 5 ("Biorobotics: A Methodological Primer" by Edoardo Datteri) presents some interesting roles played by biorobotics in the study of intelligent and adaptive behavior, where biorobotic experiments can give rise to different theoretical outcomes, such as the evaluation of the plausibility of an hypothesis or the formulation of new scientific questions. Moreover, this chapter illustrates some methodological and epistemological problems raised by biorobotics, arguing that dealing with these problems is crucial to justify the idea according to which robotic implementation and experimentation can offer interesting theoretical contributions to the study of intelligence and cognition.

Finally, some concluding remarks recall that one of the goals of this volume is to leave the reader with the recognition that many of the issues at the intersection between computing and science are still open and represent excellent topics for future investigations.

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