ABSTRACTS

Paris, 30.05-01.01.2018

Giovanni Ciccotti

Title: Molecular Simulation (MS) vs Theoretical Physics

Abstract: The place of Molecular Simulations in the context of the epistemological state and evolution of Theoretical Physics will be considered to suggest that a deep change in aim and methods of Theoretical Physics is ongoing. The very scarce historical and epistemological attention that has been paid until now to the development of Molecular Simulation in the last seventy years, and the aging (when not dying) of the founding fathers of the field seem to call for an urgent concerted effort to overcome this delay. This should involve an analysis of all the disciplines/tools/institutions which have contributed to the unbelievable rate of growth of Molecular Simulation at present invading beyond condensed matter, soft and hard, materials, biology, geology and more applicative sectors. How to achieve all that is the question justifying our meeting here.

Gianni Battimelli

A project for an Archive for the History of MS

A short presentation of a project for the creation of an Archive for the History of Molecular Simulation, submitted by Giovanni Ciccotti and myself two years ago for an ERC advanced grant - and refused, will be give. Its strengths and shortcomings will be discussed, commenting the more relevant issues raised by the referees on the historiographic, methodologic and scientific ground

Oliveri Darrigol

Discrete mathematics and discrete physics in the works of Ludwig Boltzmann.

Although discreteness, in Boltzmann's time, could not be for the purpose of numerical, computer simulation, there may be

interesting similarities with some of the concerns of molecular dynamics.

Arianna Borrelli

The Monte Carlo method in early particle physics

The classical reference for the history of Monte Carlo computations is Peter Galison's (1997) study of their origin in nuclear weapon research and subsequent diffusion in scientific and engineering practices as an “artificial reality” in which experiments could be virtually performed. Casting doubts on some aspects of this picture, I will show how the view that Monte Carlo computations “simulate” reality was initially not so dominant as would be the case later on, and how the Monte Carlo method could be assimilated not only to experimental practices, but also to theoretical ones. Using examples taken mainly from early particles physics I will argue that, depending on the context, the “same” Monte Carlo computation could be seen as a simulation of physical processes, as a tool to numerically estimate analytical expressions or as a means to represent theoretical models of particle interactions. Only later on did the idea that Monte Carlo “simulates” reality became dominant.

Marie Farge

The role of supercomputers to study turbulence

The development of numerical simulation to study turbulence has been boosted by the vector and parallel architectures of supercomputers. I will explain how I have witnessed the evolution of the Cray supercomputers, how it has affected the direct numerical simulation of turbulent flows, and I will give some examples of applications in aerodynamics and geophysics.

Giovanni Paoloni

Research Institutions and Science Policy: Why and How Should One Study Them

I shall describe the work on the history of the Italian National Reserach Council: the sources that were used, the outcome, the lines of research derived from it.

Vittorio Marchis

Mechanical Fantasies, Epistemology of the Machine in the Immaterial Knowledge

Molecular mechanics, a mystery for trivial investigators.
Chance and necessity from Isaac Newton to Jacques Monod, passing through the Théorie mathématique des Effets du Jeu de Billard by G. Coriolis.
How the deterministic approach to the chaotic reality passed through the history, and how scientists and philosophers made their mistakes.
Molecular storytellers: new (ald old) ways to enter the science frontiers.

Luigi Cerruti

Folding, Unfolding, Misfolding, Non-folding …Molecular Simulation and the Proteins Folding Problem

The present communication has two purposes:

- To highlight historical-epistemological research methodologies useful for studying the development of a discipline.
- Confirming the usefulness of these methodologies with a first application to the history of molecular simulation (MS).

The historical-epistemological analysis of science in recent years finds valuable investigation tools in the bibliographic databases (Scopus, Web of Science, Scifider). The use of these databases makes possible to delineate over time the quantitative trend of a discipline, its inter-disciplinarity and finally the possible internal contradictions in the development itself (1-2). However, the qualitative analysis of the original texts remains an irreplaceable tool to understand the research methods and theoretical assumptions that have had a decisive importance in the development of a discipline (3-4). In addition to the epistemological and linguistic analysis of the texts, semiotic analysis (5) is also very reliable.

In the present communication the different historical-epistemological research methodologies are not treated separately, but directly applied to the history of MS. The history of MS is understood as the development of a particular

theoretical approach to the atomic-molecular world, with an evident interdisciplinary interaction / attraction between MS and chemistry and biology. This interaction / attraction is easily demonstrable with bibliometric methods, when choosing an intrinsically trans-disciplinary chemical-biological theme of great importance such as proteins folding. The communication will therefore deal with three points:

- To clarify the relevance of the proteins folding problem, the main steps of the history of knowledge on this phenomenon will be synthetically illustrated, from the discovery of the reversibility of folding to that of the importance of misfolding in neurovegetative diseases, and the questions posed within genomics (6).
- Quantitative methods will be applied to evaluate, from an interdisciplinary point of view, the trend over time of the scientific production of MS, in the two fundamental components of molecular dynamics and Monte Carlo methods.
- Qualitative methods will be applied to highlight the explicit and implicit dialogue among scientists on the effectiveness of MS in solving the multifaceted issue of proteins folding.

Bibliography

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Sara Bonella
Ignacio Pagonabarraga

CECAM Historical Archives: First steps and a Few Questions

The Centre Europeéen du Calcul Atomique et Moléculaire (CECAM, www.cecam.org) is the oldest European Institute for the promotion of fundamental research on advanced computational methods and their application to problems in frontier areas of science and technology. For almost 50 years, it has contributed to the development of new ideas in the field via a rich activity of workshops, schools, and scientific .
The documentation of these activities - consisting of scientific reports, publications, photographs, management and administrative papers of the center, and the Center's website - is conserved at CECAM Headquarters, Ecole Polytecnique Fédérale de Lausanne. This documentation is not complete, due to losses that occurred mainly in the two transfers of CECAM's home venue (first from Paris to Lyon, then from Lyon to Lausanne). The material is, however, of potential great value to document the history of the Center and, more generally, as a source for studying the historical development of simulation in modern science.
CECAM has recently started, in collaboration with the Haute Ecole de Gestion de Geneve, cataloguing the material (via an inventory and a preliminary upload of some data on the website) with the long term plan to create an accessible Historical Archive and to foster projects on the history of modeling and simulation. Plans for a first paper on the history of the institution have also been initiated in collaboration with Prof. Giovanni Battimelli, University of Rome La Sapienza.
In this talk, we shall present the state of our activities in this area, and outline the current strategy and outlook for preservation and acquisition of further material. Our goal is to receive feedback and comments from the participants to the workshop to improve and further develop the construction of the archive, also in view of the upcoming celebrations for CECAM's 50th anniversary.

Gianni Battimelli (speaker)
Giovanni Ciccotti

A Case Study on the History of Molecular Simulation: B.Alder and the Inception of Molecular Dynamics

On the basis of a paper (just submitted to EPJH) on the early scientific activity of Berni Alder, covering about thirty years from the early 50's to the early 80's, I will sketch the main results of our research, focusing on several sidelines that our findings suggest for a wider work attempting to place Alder's own contributions in a wider context.

Michel Mareschal

The Early Years of Computational Statistical Mechanics

In 1957 evidence was provided by two new numerical methods of the existence of a first-order fluid-solid transition for the hard-sphere model. The two papers, jointly published in the Journal of Chemical Physics, were the result of a collaboration between Wood in Los Alamos, developing Monte Carlo, and Alder, inventing molecular dynamics in Livermore. We will reconstruct the story of this collaboration and put it in perspective with respect to equilibrium and non-equilibrium statistical mechanics.

Martyn Guest

The Story of two Community Codes, DL_POLY and GAMESS-UK, with an Overview of their Performance Evolution: Analysing, Understanding and Exploiting HPC Technology

This talk considers the evolution of the performance of two of the computational chemistry codes developed under the auspices of the UK's Collaborative Computational Projects (CCPs), as measured and analysed over the past two decades. We focus on DL_POLY, the molecular simulation code developed by CCP5 and GAMESS-UK, the molecular electronic structure code from CCP1.
Following a brief overview of the evolution of HPC technology over the period in question, we define the benchmark cases used in assessing the performance of the codes across well over 100 HPC systems – from the Cray T3E/1200E to today's Intel Skylake clusters. Consideration is given to the tools that have proved helpful in analysing this performance.

Paul Durham

Origins and Development of the Collaborative Computational Projects at Daresbury Laboratory

One of the notable aspects of the development of molecular simulation, and of computational science more widely, is the role of various institutions or associations in providing a framework within which collaboration and sharing could take place. CECAM played such a role with regard to molecular dynamics. In the UK, the establishment of the so-called Collaborative Computational Projects (CCPs) was a particularly striking embodiment of this idea. I will give a very brief account of the origins and development of the CCPs, their structure and funding (mostly at Daresbury Laboratory), and their current status.