

## Is a project for the history of Molecular Simulation timely? How to do it?

### 1. Introduction and motivation

Molecular simulation is a mature research field developed over the last sixty years. In spite of its relevance, the available literature on its historical development is extremely scarce if not at all inexistent. Time seems ripe to work toward such a goal; the field is old enough to allow the detached look required by historical investigation, but still recent enough to offer the possibility for historians to directly interact with some of the protagonists of its development. The aim of the proposed meeting is to put together professional historians of science and scientists active in the field to discuss the best way to address the issue and formulate a plan of action. In particular, and as a first step, the organization of a workshop on the history of Molecular Simulation in 2019.

### 2. State of the art

Apart from some scattered recollections by some of the “founding fathers”, and a few summary sketches in introductory chapters to textbooks and conference proceedings, no proper historical research has ever been attempted on the subject (\*). On the contrary, for other sectors of 20<sup>th</sup> century physics, and related disciplines, more or less ambitious research projects have been conducted in past times (first and foremost the project led by T. Kuhn on the Sources for the History of Quantum Physics, and then similar projects on the history of Solid State Physics, or about the development of Particle Physics), while research sectors closer to Molecular simulation have been the object of historical research (quantum chemistry, computer development, statistical mechanics...). A proposal by the organizer of this meeting for an ERC grant was submitted in 2016, but has not been accepted. In spite of that we think useful for the community of active simulators and professional historians to start an analysis of the development of the field. Contributions from historians that have done research work on similar projects and discussion with leading scientists active in the field are expected to give useful hints for planning future work on the subject. A first outcome of the present planning meeting could be the organization of a full workshop on this subject in 2019 at CECAM Headquarters in Lausanne, during or around the celebrations of the Fifty years from the foundation of CECAM.

### 3. Objectives

The primary goal of the meeting is to provide a free discussion forum where to openly debate historical perspectives and methodological issues relevant for the definition of a broad research

program on the history of molecular simulation. The objective - should the general idea appear worth being cultivated - is to set the main lines for the organization of a proper conference on the subject, to be held hopefully in 2019, and to define a convincing list of preliminary work to be achieved (interviews of founding fathers, collection of interesting material, analysis of the major events in the field, etc).

Tentative program:

1. A presentation of the problem (from the organizers)
2. Volunteering historians contribute their experience (in their own field)
3. The audience comments
4. Conclusions if any but, possibly, if considered ripe, planning of a real workshop in 2019

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