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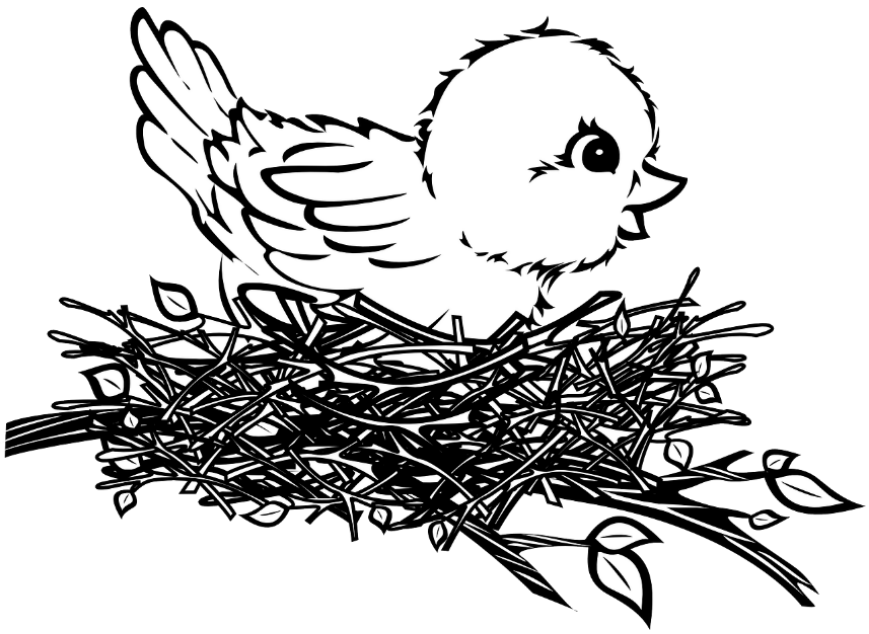
Scuola Internazionale Superiore di Studi Avanzati

UNIVERSITÀ DEGLI STUDI DI MILANO

PRESS RELEASE

In simulations, strength and quality come through communities

A group of scientists is ready to share methods and practices on a brand new platform, the PLUMED-NEST repository. The promoters say this will promote transparent and reproducible research. Nature Methods describes the initiative.



A new platform for molecular simulation and a community of scientists ready to work together to promote transparency, reproducibility and quality is now a reality. PLUMED is a 10-year-old plugin that was created by a small group of researchers. It can be used to perform the molecular dynamics simulations that underly many of the most pioneering research projects in physics, chemistry, biology and materials science. Molecular dynamics is useful as it provides a kind of computational microscope for understanding how the building blocks of matter behave. The PLUMED consortium, which is described in an article published in “Nature Methods”, expands the potential of this technique by establishing protocols that scientists can use to report their results. The consortium's mission is to maximise the impact of research by sharing data and methods. This sharing done though a tool, the PLUMED-NEST repository, which is an archive into

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which all members can enter the data, files and protocols that are necessary to replicate the simulations present in their scientific publications. This repository offers distinct advantages in terms of innovation, the ease of access to knowledge and the training of the new generations of scholars. The article published in the prestigious journal carries the signature of the PLUMED Consortium which includes Giovanni Bussi of SISSA (Scuola Internazionale Superiore di Studi Avanzati), Massimiliano Bonomi of the Pasteur Institute of Paris, Carlo Camilloni of the University of Milan and Gareth A. Tribello of Queen's University of Belfast among its leading promoters.

Computer experiments to study molecules

Molecular dynamics simulations are now an essential tool for understanding the most refined mechanisms of molecules, for predicting their behaviour and for interpreting the results obtained through experiments. Innovations in the field of simulations are emerging at an increasing pace as are novel applications to problems in medicine, industry and research and, while a great effort is being made to define best practices and to ensure maximum benefit for those who work in this sector, there is still much to be done. "Many of these challenges cannot be overcome alone" write the authors of the text in "Nature Methods" and "a concerted effort by the entire community is required".

The challenge of PLUMED

The many challenges are primarily technical. For example, "simulation methods which have a strong potential in different fields cannot be used with all the different tools that are available because each one of the tools used is optimised for specific applications and because these various tools are written in different programming languages" explain the scientists. "A strategy to resolve this problem was precisely the purpose of PLUMED" explain the scholars. "When developing PLUMED we wanted to provide technical services to overcome these limits so that so-called "enhanced molecular simulations", which are used to study the events that occur on very long time scales, could be used by all our colleagues". Over time, PLUMED has become a widely used platform. PLUMED allows newly implemented techniques to be rapidly shared and made accessible and easy for everyone to use. As PLUMED uses a unified syntax for all programs, it enables cross-validation between various molecular dynamics simulations and cross-fertilisation of ideas between areas such as chemistry, biophysics and materials science.

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From PLUMED CONSORTIUM to PLUMED-NEST

The authors of the article, which announces the foundation of the PLUMED Consortium, formed by scores of scientists and programmers active worldwide in the molecular dynamics field, say there is more to come. The goal of the initiative is, among others, to increase the reproducibility of the experiments, increase the impact of the research and promote good practices for simulation, with a community-driven approach. To do so, the scientists of the consortium have committed themselves to sharing the files and the protocols for the simulations used in their scientific work in an archive, called the PLUMED-NEST. "This initiative is also useful for training because it will allow all young scientists starting in this area to practice and repeat the experiments done by others, which is a beneficial form of training" explain the authors. They conclude: "We strongly believe that this new organisation is a good example of a community-driven project which is the heart of open-source software development. Therefore, the community welcomes all those who share our vision".

IMAGE
Crediti: neepix.com

PAPER
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