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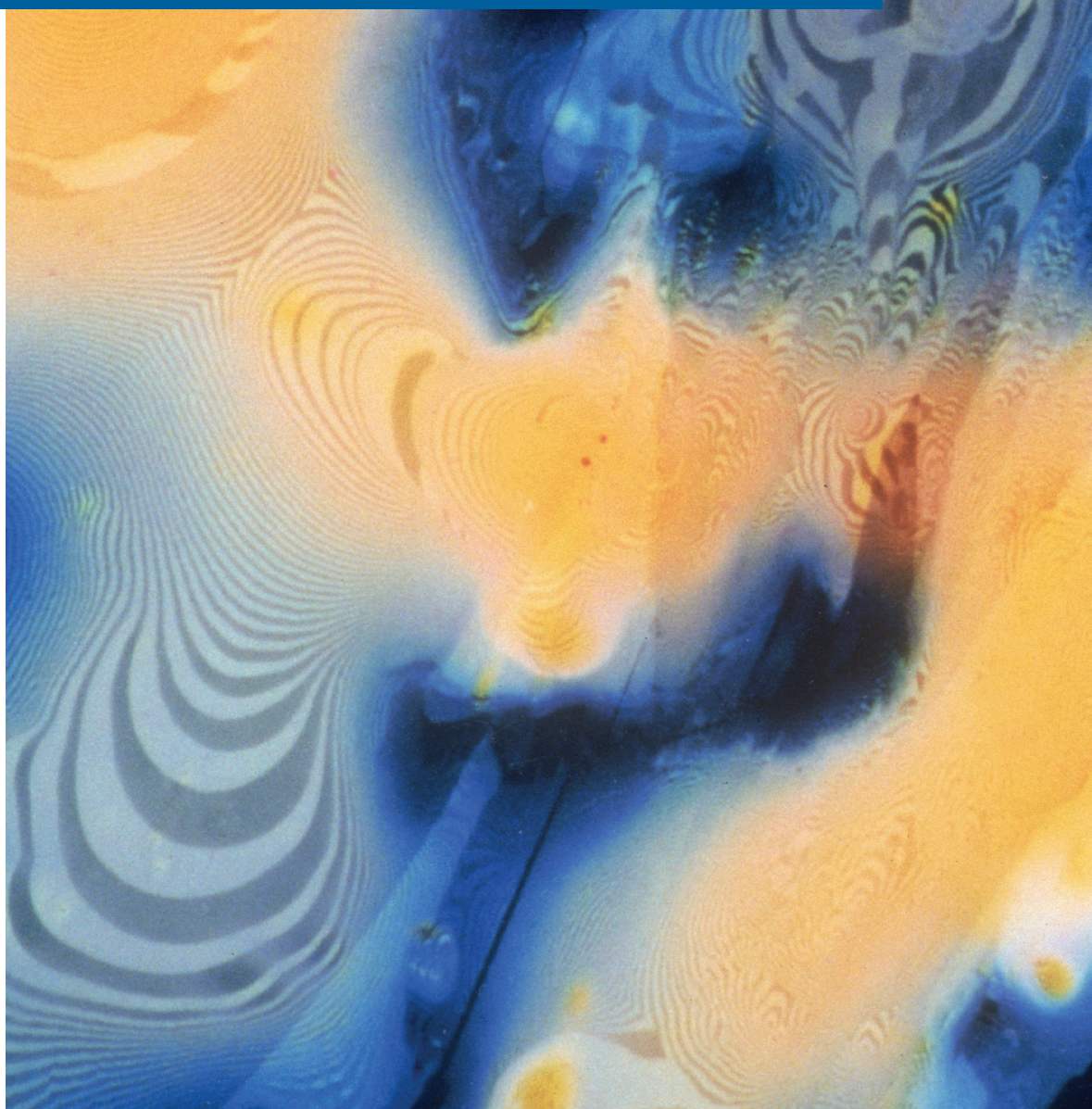
FRENCH RESEARCH NETWORKS IN CHEMISTRY

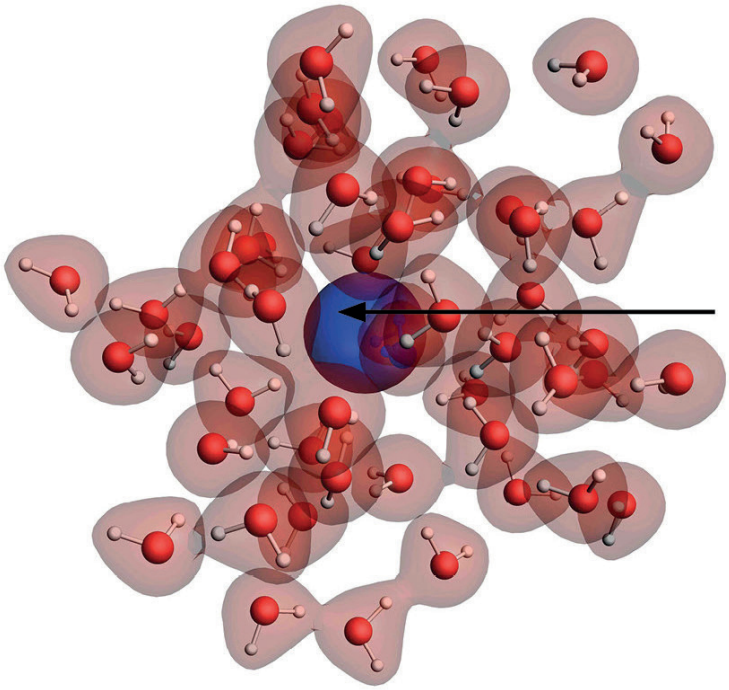


GDR NBODY

Quantum n-body problem in chemistry and physics

OBJECTIVES

The research network aims to bring together the community working on the quantum N-body problem, mostly from the viewpoint of quantum chemistry, but also including the viewpoints of condensed-matter physics, nuclear physics, and mathematics. The idea is to foster the development of new computational methods in quantum mechanics, the transfer of these methods from one discipline to another, and their efficient computer implementations. To reach this goal, the research network organizes interdisciplinary conferences and workshops. It is also particularly involved in training students and researchers via the organization of several interdisciplinary international schools.



Quantum calculation for the system I-$(H_2O)_{50}$

THEMATICS

- Quantum chemistry
- Condensed-matter physics
- Nuclear physics
- Mathematics

$$E^{\mathrm{w}}_{\mathrm{c},J}[n^{\mathrm{w}}] = \mathscr{E}^{\mathrm{w}}_{\mathrm{c},J}[n^{\mathrm{w}}] + \sum_{K\geq 0} \mathtt{w}_K \sum_{I>0} (\delta_{IJ} - \mathtt{w}_I) \frac{\partial \left(\mathscr{E}^{\mathrm{w}}_{\mathrm{c},K}[n^{\mathrm{w}}] \right)}{\partial \mathtt{w}_I} + \sum_{K\geq 0} \mathtt{w}_K \int d\mathbf{r} \frac{\delta \mathscr{E}^{\mathrm{w}}_{\mathrm{c},K}[n^{\mathrm{w}}]}{\delta n(\mathbf{r})} \left(n_{\Phi^{\mathrm{KS,w}}_J}(\mathbf{r}) - n_{\Psi_J}(\mathbf{r}) \right)$$

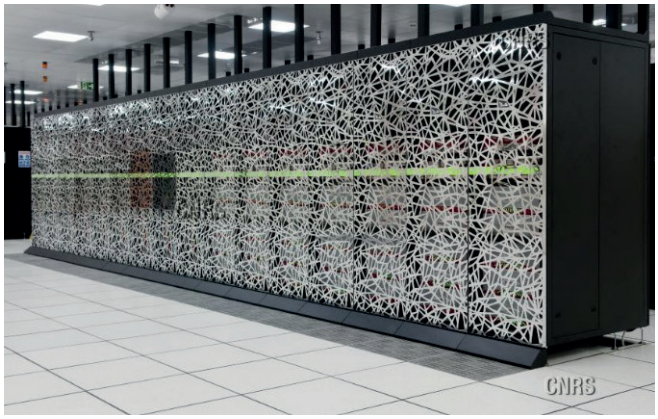
Development of a density-functional theory for excited states.

100 RESEARCHERS
INVOLVED IN
37 LABORATORIES

PROSPECTS

We are witnessing a remarkable evolution of quantum chemistry at the international level. New approaches based on methods coming from different fields are proposed. This is so for example for wave-function approaches in which new methods overcoming the limits of the current methods are developed. For example, CASSCF calculations with active spaces corresponding to about 50 electrons in 50 orbitals can now be performed. New wave-function representations coming from Physics *(Tensor Network)* are used and provide a much deeper picture of the physical contents of the wave function. The development of stochastic approaches is also very active. For example, the FCI-QMC method introduced a few years ago allows one to sample active spaces that were previously beyond reach. The development of deterministic variants of the FCI-QMC method, such as the selected configuration interaction, is also a very active research field. For all these methods, high-performance computing implementations are crucial. Very efficient implementations adapted to the architecture of current supercomputers, involving in particular massive parallelism, have to be developed. Regarding systematic calculations of numerous molecular systems, we are witnessing a spectacular development of *machine learning* techniques. At a more fundamental level, it is now proposed to use *machine learning* for selecting the most important configurations in configuration-interaction calculations.

Beyond wave-function methods, one can mention the evolution of green-function techniques, a central tool of physicists, and their application to quantum chemistry which progresses. In the same spirit, one can also point out *embedding* methods including environment effects similarly to DMFT methods. Regarding DFT, one can mention the combination of wave-function methods with short-range density functionals in order to correct for the incompleteness of basis sets and include dynamical correlation at low computational cost.



Super computer CURIE.

This booming activity around *ab initio* computational methods requires mobilizing various methodologies which are not well known yet by all. The NBODY research network has the mission to structure these developments with strengthened interactions between chemists, physicists, and mathematicians.

CONTACT

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NBODY Quantum n-body problem in chemistry and physics