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Centre Européen de Calcul Atomique et Moléculaire

A European Research Centre in Orsay: Cecam 1969-1993

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Gestation and birth

Half a century after its creation, CECAM (Centre Européen de Calcul Atomique et Moléculaire) is today a solid research institution with a complex and articulated structure. Its official mission is "the promotion of fundamental research on advanced computational methods and their application to important problems in frontier areas of science and technology". With headquarters in Lausanne, where the Director, Deputy Director and the administrative staff are located, it spreads across Europe and Israel through a network of 17 operating centres ("nodes"), and is sponsored by 25 research organisations from 14 different European countries. All member organisations are represented in the Council, CECAM's supreme governing body, while the implementation of the scientific activities is controlled by a Board, chaired by CECAM's Director, whose members are the Node Directors. A Scientific Committee acts as advisor to the Board on the CECAM scientific policy.

Nothing of the sort was in sight when CECAM came into existence. Contrary to other international research institutions (of whom CERN, the European laboratory for high energy physics created in Geneva in 1954, probably represents the best and more widely known example), that were established by official agreements between the research institutions, if not the governments, of the countries involved, CECAM was at the beginning (and stayed for quite some time after) a kind of informal organisation which managed to operate successfully in spite of lacking a clearly defined institutional status. Often behind any such large cooperative enterprise are the vision and determination of a few individuals and this is particularly true in the case of CECAM, which has often been depicted as a "family affair". As a family, CECAM grew rapidly to become a large one; but it was always clear to every member of the family who the *pater familias* was. And, irony of history, the father who gave birth to the most successful European enterprise in the field of computational science was an American.

Born in Terre Haute, Indiana, in 1922, Carl Moser had received his PhD in organic chemistry at Harvard University in 1948, followed by a position as assistant professor at Johns Hopkins. In 1951 he moved to England, with a postdoctoral fellowship in theoretical chemistry, to improve his knowledge of quantum mechanics with Charles Coulson in London and Oxford. On Christmas, in 1952, he visited Paris, and got acquainted with Raymond Daudel,

the director of the Centre de Chimie Théorique de France, that Daudel had founded in 1944. It was the first and main research centre in quantum chemistry in the country, which later (1954) changed name in IMOACR (Institut de Mécanique Ondulatoire Appliquée à la Chimie et à la Radioactivité), and finally became in 1957 CMOA (Centre de Mécanique Ondulatoire Appliquée), a laboratory of the CNRS.[1] Daudel invited Moser to look forward to a career in CNRS, and to move from England to his centre for quantum chemistry. Moser accepted, and settled in Daudel's centre in the fall of 1953, thus becoming "an American in Paris". By the mid-sixties Moser had climbed the steps of the CNRS ladder, attaining the post of Directeur de Recherche and leading one of the four large research groups of CMOA, which in 1962 had moved from its previous location in rue de Sèvres to a new housing at 23 rue du Maroc, to take advantage of the facilities of the computing centre of the Institut Blaise Pascal, operating at the same place.[2]

In his first ten years or so in Paris, Moser established a dense network of relations throughout Europe with scientists and scientific managers in quantum chemistry and related fields, became quite dissatisfied with his own research, that "would never lead to a Nobel Prize"[3], and had reached the conclusion that the future advancements in his science would require large investments in computing facilities. It was, in hindsight, an easy prediction to make in the mid-sixties, given, on one side, the ongoing development of computers and, on the other, the growing need for numerical efficient techniques required in those fields, such as atomic and molecular chemistry and physics, where advances on purely analytical grounds were prevented by computing difficulties. It was still easier, for someone familiar with the state of the art in computer science and its application to fundamental research, to evaluate the extent of the gap existing at the time between the flourishing developments in the U.S. A. and the still very limited and poorly exploited availability of similar resources throughout Europe. The project of setting up some kind of cooperative effort to strengthen European activity in computational science thus started to take shape.

The idea must have been floating around for a while. From the scarce and fragmentary evidence available, it seems that it was openly debated for the first time at a meeting on molecular physics held in Blaricum (Holland) at

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[1] About CMOA, and more general developments in France, see J.L. Rivail, B. Maigret, *Computational Chemistry in France: A Historical Survey*, Reviews in Computational Chemistry 12, 1998, pp. 367-380.

[2] Created in 1946 as a centre for applied mathematics, the Institut Blaise Pascal was one of the main institutional actor in the development of computer science in France throughout the 60's. See A. Collinot, P.E. Mounier-Kuhn, *Forteresse ou Carrefour: l'Institut Blaise-Pascal et la naissance de l'informatique universitaire parisienne*, La Revue pour l'Histoire du CNRS, 27-28, Automne-Hiver 2010, pp. 79-88.

[3] M. Karplus, *Carl Mathew Moser*, Carl Moser Symposium, CECAM, Lyon 2005.

the end of March 1967, "under the leadership of C.M. Moser".[4] Blaricum was the seat of the European Education Center, founded in 1959 by IBM World Trade Corporation, a subsidiary of IBM focused on foreign operations. Nothing else is known about this meeting that is however always referred to as the moment in which the very idea of what was to be CECAM materialized. The most detailed account comes from Wim Niewpoort, professor of Theoretical Chemistry at the University of Groningen: "in 1967 Carl invited me to join his famous "Blaricum meeting", at an IBM center. There he exposed his idea about a European center for atomic and molecular calculations to a critical but knowledgeable audience including Bob Nesbet, Enrico Clementi, Paul Bagus, Gerd Diercksen, Brian Sutcliffe to mention a few. The reception was mixed. I remember my own reaction. As a true Dutchman I favoured a careful start through bilateral cooperation, rather than an all-out multilateral organization."[5] A bit more information is given by Jan Mulder, then still working at his doctoral dissertation at Leiden University: "Carl Moser came into my life at the Blaricum meeting, 29-31 March 1967. Rather early in the course of my thesis research I had started applying computational methods… and so the possible creation of a European Institute for computational physics and chemistry seemed a highly interesting development. I remember meeting Carl again in London at the Faraday Symposium "Molecular Wavefunctions", 12-13 December 1968… It had become clear that CECAM would start in the fall of 1969 and between my thesis supervisor L.J. Oosterhoff and C.M. Moser it was decided that I should go to Orsay (as it would turn out) to learn ab initio quantum-chemical calculations."[6]

Indeed, by December 1968 it was clear that something would materialize. Soon after the Blaricum meeting Moser had presented a project to the high officers of CNRS. His plan was to link his initiative with the decision taken by CNRS Director General Pierre Jacquinot to create a new large computing centre (incorporating the old centre of the Institut Blaise Pascal, which was going to be dissolved). Moser's project was first presented by Hubert Curien (which would replace Jacquinot as Director General in 1969) at a meeting of the Comité de direction of the CNRS, on September 14, 1967: the project aimed at "regrouping the researchers working on quantum computations in order to realize programs competitive with those in the United States"; it was stated that a meeting recently held in Holland had given indication that such a cooperation was desirable and feasible, that "Germany, Great Britain, Italy and maybe the USSR might give a contribution of 4 – to 500.000 Francs each", while France could participate by offering computer time

[4] The only reference I could locate in the scientific literature to the Blaricum Meeting, apart from personal recollections by some participants, is in *Proceedings of the Thirteenth General Assembly, Prague 1967*, International Astronomical Union, 1968, p. 87.

[5] W. Niewpoort, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, p. 23.

[6] J.C. Mulder, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, p. 21.

and paying researcher's salaries; the new Institut would be centred around the computer that CNRS intended to acquire.[7]

No formal decision was taken at the time. A consensus was reached one year later. In the meantime, Jacquinot's project of a new large computing facility had materialized, and work was going on at the site of Orsay to install there the new-born Centre Inter-Régional de Calcul Électronique (CIRCÉ), which was officially inaugurated on January 1969. At the meeting of the Comité de Direction held on October 7 1968, it was agreed that CNRS would support Moser's project; for the first time the acronym CECAM appeared in an official document. The minutes of the meeting relate that "since three years" contacts had been established by Moser to create a European centre on atomic computation; that the best specialists from Europe and America were expected to take part in its activities; that British, Dutch, Italians, Germans and French scientists were already showing a deep interest in the proposal (the USSR had in the meantime disappeared); that important firms such as IBM were willing to give their contribution. Moser made three requests to CNRS: computing time on the 360-75 (the IBM machine to be installed at CIRCÉ); lodging for his Centre next to CIRCÉ on the site of Orsay; an (unspecified) amount of money to cover the expenses of visiting scientists. The majority of the Committee's members "were seduced by the perspective of having an international laboratory of high scientific quality", but objected to the idea that CNRS should pay for the visits of foreign visitors. These expenses, it was agreed, should be covered by their respective countries.[8]

Therefore, by the end of 1968 the CNRS agreed to start the project, but it was not clear what formal status the new Centre would be given.[9]

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[7] "M. CURIEN expose le projet de M. MOSER tendant à regrouper les chercheurs spécialisés dans les calculs quantiques, afin de mettre au point des programmes susceptibles de rivaliser avec ceux qui sont montés aux Etats-Unis. Une première réunion de ces chercheurs, qui a eu lieu récemment en Hollande, a montré que les possibilités de cette coopération sont réelles. M. MOSER propose de regrouper cet institut autour de l'ordinateur que le C.N.R.S. a l'intention d'acheter. Il estime que le budget de fonctionnement s'élèverait aux environs de 6 (?) millions de francs pour une vingtaine de personnes. L'Allemagne, la Grande-Bretagne, l'Italie et peut-être l'U.R.S.S. pourraient y contribuer à raison de 4 à 500.000 F pour chaque pays. La France pour sa part, y participerait par la fourniture d'heures-machine et le paiement des chercheurs." Extrait du compte-rendu du Comité de direction n° 56 - Séance du jeudi 14 septembre 1967 - Point n° 6 – Projet d'institut européen de recherches moléculaires, CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[8] Extrait du compte-rendu du Comité de direction n° 157 - Séance du lundi 7 octobre 1968 - Point n° 4 – Centre de recherche européen de calcul atomique et moléculaire (C.E.C.A.M.), CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[9] Several holes in the documentation preserved both in Lausanne and at the CNRS archives regarding the early stages of CECAM make it difficult a detailed reconstruction of events, and offer sometimes puzzling evidence. Such is the case of a "CECAM brochure", found among other scattered documents in the CNRS archives. Only pages 7, 11 and 13 have been photocopied and preserved. Since the first pages are missing, the exact date of the document

Disregarding such bureaucratic subtleties, Moser went ahead, and by October 1969 CECAM was installed at its new premises on the hill in Orsay; that is, Moser moved himself, his office, his secretary and his beloved dogs from rue du Maroc to a room in the Laboratoire Aimé Cotton (the CNRS laboratory for atomic spectroscopy), located at Batiment 505, next to the building where CIRCÉ was installed. Not much later (when exactly we cannot say) CECAM crossed the street and settled finally in Batiment 506, where enough space for its activities was afforded by the CIRCÉ director, Janine Connes. Connes, an astrophysicist who had acquired a solid competence in computational science working in 1963 at the Jet Propulsion Laboratory in Pasadena, had been entrusted by Jacquinot to be responsible of the management of the new large computing centre at Orsay; although completely foreign to the field of quantum chemistry, she shared with Moser the feeling that a strong effort was needed from Europe to become competitive with the U.S. in computational science, and was sympathetic with his plans for such a cooperation. She therefore proposed to Jacquinot to host Moser's new centre in the CIRCÉ's building where (at least for the moment) space was available and not yet fully utilized.[10]

A European network

"How he did it I do not know, but in 1968 [must be 1969] I got word that an organization called CECAM was brought into existence under his

is unknown (although from its content it could be located around the beginning of 1969), nor is it possible to ascertain its author (which may well be Moser himself). It is announced that CECAM will be opened at the CNRS Computing Centre in Orsay in October 1969. About twenty scientists are expected to visit the Centre for a long period of time (hopefully "a year at least"), mostly but not exclusively from Europe. Mention is made of a "Comité de Direction Européen" that should determine the amount of the financial contribution from each foreign institution taking part in the Centre's activities. Most interesting is a list of scientists (all of them active in quantum chemistry) to whom aspiring visitors to CECAM are addressed to establish contacts: besides Moser, we find for France also R. Chabbal from the Aimé Cotton CNRS laboratory at Orsay, W.A. Bingel and W. Kutzelnigg (both from Göttingen) for Germany, for Britain D.W. Cruikshank from Manchester and J.W. Linett from Cambridge, and Italians M. Simonetta from Milan and A. Vaciago from Rome. The closing lines of the booklet stress the provisional form of the Centre, that will be "certainly closed five years from now, should it prove to be a failure"; while "if, as we strongly believe, it will be a success, it will be necessary to set up an European Organisation for its administration". CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[10] The information that hosting CECAM in Batiment 506 was a suggestion by Janine Connes was given to me by Mme Connes herself, in a short conversation we had on June 13, 2019 in the office of IDRIS Director Denis Giroud, in that very Building 506 at Orsay (IDRIS is the new computing centre that took the place of CIRCÉ in 1994). That the first space occupied by CECAM in Orsay was at the Laboratoire Aimé Cotton is confirmed by Carl Moser in his introduction to the 1978 CECAM Scientific Report (written in 1979): "I would not wish to finish this introduction without a reminder that on October 1 of this year ten years will have passed since we started operation in the Laboratory Aimé Cotton here in Orsay".

directorship and located at Batiment 506, Campus d'Orsay. Interested scientists were invited for research stays during which they could use computational facilities of CIRCÉ with generous limits."[11] No doubt, "how he did it" was largely due to Moser's determination, and disregard of bureaucratic matters. In dealing with scientific administrators, Moser displayed a pragmatic attitude coupled with a distinctive tendency to "think big" (and ask consequently). "Above all, Carl had the streak of outrageousness, which was essential in setting up a major facility and convincing governmental bodies. His first tool in these enterprises was making shameless demands. At CMOA he asked for an annual budget of computer times of 1000 hours, while the rest of the department asked for 20! He got 800."[12]

While CECAM started operating on scientific grounds, its existence at the formal level was still a matter of embarrassment for high CNRS officials. It was difficult indeed to find an adequate way to give official life to an institution that consisted only of a Director and a secretary, with no permanent personnel. Already at the 1967 meeting where Moser's project was first discussed it had been decided to avoid the creation of "an independent moral figure" to define the legal status of the proposed centre, and it was rather suggested to have it in some way directly supported on formal aspects by CNRS.[13] Exactly which way, however, was left undefined, and such was the situation when CECAM moved to Orsay. A first suggestion to establish the centre under the form of a Recherche Coopérative sur Programme (RCP) was abandoned, just as the idea of creating it as an association following the lines of the 1901 Loi des

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[11] W. Niewpoort, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, p. 23.

[12] G. Richards, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1989, p. 25. Richards also mentions a second strategic move used by Moser to have his requests promptly accepted, which though anecdotic deserves to be reported: "The second line of attack on ministers and hautes fonctionaires was Gunther. Gunther was Carl's child – a dachshund who had a spinal injury and was in consequence paraplegic. Carl very much judged people by their reactions to Gunther, whom he loved and cared for indefatigably. Being a spastic, however, Gunther had no control over his bladder. Thus when Carl went to see the minister to demand resources for CECAM he took Gunther into the carpeted offices, and many of us felt that funds were often forthcoming because officials were worried about their carpets and gave in to Carl to get him out of their suites."

[13] "Quant à la forme juridique de cet institut, M. DAURY (?) souhaiterait éviter la création d'une personne morale indépendante. Aussi est-il décidé par le comité de proposer à M. MOSER une formule qui ferait du C.N.R.S. le support juridique de cet organisme sous la forme d'une R.C.P. européenne assortie d'apports étrangers régis comme les ressources affectées. Le comité propose aussi de modifier la dénomination de cet institut, le terme de « recherches moléculaires » lui paraissant un peu large pour un objet qui est en réalité assez spécialisé." Extrait du compte-rendu du Comité de direction n° 56 - Séance du jeudi 14 septembre 1967 - Point n° 6 – Projet d'institut européen de recherches moléculaires, CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

Associations.[14] On December 12 1969, CNRS Director General Hubert Curien wrote to the Director of cultural, scientific and technical relations at the Department of Foreign Affairs, on the general subject of European cooperation, raising the issue of how to deal with the legal status of CECAM. Curien underlined the specific difficulty of the problem: it was neither the case of a cooperation between two (or more) laboratories from different countries, that could have been easily defined through bilateral conventions or the application of the existing formula of the RCPs, nor of a large European or international project requiring for its implementation the official ratification of complex intergovernmental agreements. The case at hand ("the creation of a European centre for atomic and molecular computations, that could be installed next to the CNRS computing centre at Orsay") was of an intermediate size, making a formal intergovernmental agreement unnecessary, but still requiring "a formal structure to guarantee coordination of research and proper operation handling". For the time being, Curien concluded, CNRS would find a provisional way of handling the matter, but, should the initiative be successful, a "more definitive solution should be found in the forthcoming years".[15]

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[14] The CNRS files keep a copy of the (undated, but clearly end of 1969) draft of a document "Statuts du Centre Européen de Calculs Atomiques et Moléculaires". CECAM was there conceived as a private association among individuals, having as founding members R. Chabbal, H. Curien and C. Moser for France, and V. Caglioti, M. Simonetta and A. Vaciago for Italy. The document had been prepared for approval from the competent CNRS offices, and rejected on administrative grounds, as stated by H. Curien in his letter on the matter cited in note 14. Most likely the rebuttal of the proposal had to do with the fact that in the Statute of the proposed association no mention at all was made of any role of CNRS, and the question of how the financial aspects would be handled was left totally undefined.

[15] In view of its interest, we reproduce the full text of the letter: "Décembre 12, 1969 - Le Directeur General du CNRS à Monsieur le Directeur General des relations culturelles, scientifiques et techniques, Ministère des Affaires étrangères - Objet: Coopération européenne.

Au cours d'une récente conversation, nous avons évoqué le développement nécessaire d'actions européennes en matière de recherche scientifique et l'insuffisance actuelle des moyens juridiques permettant de promouvoir de telles actions.

Lorsqu'il s'agit d'une collaboration directe entre deux laboratoires, l'un français, l'autre étranger, chacun apportant ses moyens à l'exécution du programme, aucune difficulté ne se présente. Cette collaboration peut s'inscrire soit dans le cadre des protocoles d'application des conventions de coopération scientifique et technique relevant de votre Département, soit dans celui des conventions passées entre le C.N.R.S. et certains organismes nationaux de recherche étrangers.

Dans le même esprit, quelques laboratoires étrangers participent avec des laboratoires français à l'exécution de "recherches coopératives sur programme". Il s'agit, ici encore, de rapports directs entre laboratoires sur des sujets de recherche fondamentale. Cela ne soulève pas de problème particulier et cette formule pourrait sans doute être développée à l'avenir.

Par ailleurs, s'il s'agit de projets européens ou internationaux de grande envergure, il est normal que ces projets fassent l'objet d'accords entre gouvernements, mais la procédure est généralement assez lourde et demande des délais assez longs.

From the available documentation it seems that CNRS took a decision about the "provisional way of handling the matter" on January 14 1970, creating "a specific action for the opening of the Centre européen de Calcul atomique et moléculaire".[16] The final arrangement left to the CECAM director full autonomy for the scientific management of the centre, while the financial issues connected with the sponsoring of CECAM activities by foreign partners would be regulated by specific conventions between those partners and CNRS, which would operate as administrator of CECAM related funds. In particular, Moser insisted (and this line of action was strictly enforced, despite episodic objections from some of the member institutions) that funds allocated by the different partners should go into the general budget for CECAM activities, and not exclusively used to cover the expenses of the scientists from that specific country. By so doing, Moser intended to leave open the possibility to use CECAM money for all sort of general scientific activity and eventually allow participation to those activities also for researchers coming from countries whose institutions were not official CECAM partners. Benefit for the financing countries would come mostly from having their scientists taking advantage of the computing facilities of CIRCÉ and interacting with a broadly international network of colleagues.

Contacts with various national agencies were soon established through the thick network of Moser's personal relations. Wim Niewpoort acted as the "CECAM connection man" with Holland: "Carl and I did our best to gain support for a formal agreement with CECAM in Holland. In 1970 I went to Orsay for three months with the specific aim to prepare a fact-finding report and advice ZWO, the Dutch science foundation. Shortly after negotiations began

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Le problème qui nous préoccupe est celui d'actions intermédiaires de moindre envergure pour lesquelles il ne parait pas indispensable de conclure un accord inter-gouvernemental, mais qui nécessitent une assise juridique pour assurer la coordination des recherches et la gestion des opérations.

En voici un exemple : celui de la création d'un Centre européen pour des calculs atomiques et moléculaires, pouvant être implanté près du Centre de calcul du C.N.R.S. à Orsay.

Nous avions pensé initier cette entreprise en constituant une association de la loi de 1901, mais cette solution n'a pas reçu l'agrément de notre Contrôleur financier. Nous pouvons amorcer la coopération grâce à une action spécifique du C.N.R.S., mais il nous faut trouver, si l'expérience se révèle concluante, une solution plus définitive dans les années à venir.

Je vous serais reconnaissant si, ainsi que vous me l'avez proposé, il vous était possible de faire étudier ce problème par vos services."

It is interesting to note that, writing on December 12, Curien says that CECAM "could be installed" at Orsay, while in fact it had actually already been operating there for almost three months.

[16] Explicit reference to the "decision to create a specific action" taken on January 14, 1970, is made in the Convention between CNR and CNRS of May 12, 1970. No document allowing to know what exactly was decided on that day could be found either in the CNRS or in the CECAM archival files. It is also impossible to establish when, and by which body, Moser was officially designated as the CECAM Director.

that led to the participation of ZWO (now NWO) in CECAM, which still exists today." [17] André Bellemans, professor of quantum chemistry at the Libre Université de Bruxelles, and Georges Verhaegen, who had worked for his PhD thesis at CMOA (making good use of the vast amount of computer time that Moser had asked and obtained), played the same role with the Belgian FNRS (Fonds National de la Recherche Scientifique). [18] The "Convention de recherche" between CNRS and the Italian Consiglio Nazionale delle Ricerche (CNR) was signed on May 12 1970, by CNR President Vincenzo Caglioti and the CNRS Administrative Director Pierre Creyssel; it was intended to last for three years, and was indeed renovated on January 1 1973.

CECAM activities in 1971 were directly supported by CNRS (France), CNR (Italy), ZWO (Holland), FNRS (Belgium); in addition, further grants were received from the French Centre d'Etudes de Limeil of the CEA (Commissariat à l'Energie Atomique) and from IBM France and Control Data (France). [19] Control Data soon disappeared, and in the following years the group of the sponsoring partners remained essentially the same: the four national scientific agencies of France, Italy, Holland and Belgium (CNRS, CNR, ZWO, FNRS), CEA-Limeil, and IBM France. They were joined in 1975 by the Belgian Ministére de l'education nationale et de la culture francaise (followed in 1981 by its Flemish counterpart, Ministerie van Nationale Opvoeding en Nederlandse Cultuur), the University of Namur (Belgium), the Centre d'etudes nucleaires de Saclay (CEA, France) and, for a period of two years only, the Délégation générale à la recherche scientifique et technique (DGRST, France). The Namur University withdrew in 1980, and so did IBM France the following year. 1981 saw the arrival of direct funding from the main British agency, the Science Research Council (SRC), that changed name in 1982 to become SERC (Science and Engineering Research Council). Despite this late official

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[17] W. Niewpoort, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, p. 23. The Nederlandse Organisatie voor Zuiver-Wetenschappelijk Onderzoek (ZWO) was the Dutch equivalent of CNRS, established in 1950, whose activity was limited to pure science; in 1988 it was renamed Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), covering both pure and applied science.

[18] The Belgian National Fund for Scientific Research (NFSR) is split in two separate organisations: the Fonds Wetenschappelijk Onderzoek – Vlaanderen (FWO), for the Flemish Community, and the Fonds de la Recherche Scientifique – FNRS (F.R.S. – FNRS) for the French-speaking part of Belgium. In the CECAM Scientific Reports, they are usually designated as FNRS.

[19] This, and most of the information that follows, is taken from the yearly CECAM Scientific Reports. The CECAM archives in Lausanne preserve an almost complete series of these Reports. Unfortunately, no copy is left of the first Report, covering the period October 1969 – September 1970. The second Report is preserved (October 1970 – September 1971), then there is another hole for 1971-1972. From then on the series is complete. The next in line (October 1972 – September 1973) is labelled as being the fifth (it should actually be the fourth). Since 1978 the period covered by the Reports was made to coincide with the solar year.

entrance of Britain in the CECAM membership, British scientists took an active part in CECAM's activities from the beginning.[20] As for Germany, on the other hand, CECAM only attracted a few German theoretical chemists who were in contact with Moser. Moreover DFG (Deutsche Forschung Gesellschaft, the German national research council), was not authorized to grant international funding: this was a German application of the theory of the separation of duties. DFG was solely concerned with research inside Germany, whereas the policy of international research was the exclusive responsibility of Ministries, a circumstance that prevented DFG to participate to an enterprise such as CECAM.

Widening scopes

"Those of you who will have read the first report will note that there is an increase not only in our activity but also in the subjects which have been dealt with in our Centre"; this is the opening sentence of Carl Moser's introduction to the second report of the scientific activity of CECAM, covering the period from October 1970 to September 1971. Unfortunately, the first report not being available in the surviving files of CECAM's early period, it is impossible to judge exactly to what extent the range of scientific subjects covered by the centre's activities had increased from the previous year; for sure, however, already in its second year of operation CECAM had hosted several scientists whose interests were not confined strictly to quantum chemistry. Besides support given to individual visitors, two colloquia had been organized on models for X-ray, neutron and electron diffraction, and on the calculation of the electronic structure of solids. Even more interesting, however, was the invention of a new way to organize and conduct a research project. In 1970 had already appeared the tool that was going to establish itself as the trademark of CECAM's style for cooperative research: the workshop, in the very specific sense that this word acquired at Orsay.

"This report includes the first results of our interest in direct methods in crystallography, and these have in large part been obtained from a six-week workshop. We have already organized, and plan to continue to do so in the future, the usual 3-5 days colloquia. The workshop on the contrary means getting together a small number of scientists (the optimum will depend on the

[20] "The UK came into CECAM late when Malcolm Haines and myself wrote a memo to SERC in 1979 [sic: actually, in 1979 SERC was still SRC] pointing out the advantages of membership. However, it is characteristic of the flexible way that Carl Moser organises CECAM activities that in spite of our late membership, the UK community were able to take part in CECAM activities from the beginning." P.G. Burke, *Electron-atom and electron-molecule collision calculations*, in *Perspectives for Computational Sciences in the 1990's*, CECAM, Orsay 1990, p. 5. See also S.J. Smith, B.T. Sutcliffe, *The Development of Computational Chemistry in the United Kingdom*, Reviews in Computational Chemistry 10, 1997, pp. 271-316.

subject matter) who are willing to work together for several weeks on one central theme though each one should be encouraged to try out his ideas. The results of the first workshop have been to my mind sufficiently positive so as to encourage us to organize others." No full report of this first CECAM workshop on "Direct methods in X-Ray crystallography" has survived; for sure, among the participants was Herbert Hauptman, who had laid the foundations of the method and would be awarded the Nobel Prize for chemistry in 1985 for its application to a wide variety of chemical structures.[21]

The experience of the workshop was repeated in 1972, when two such events were organized. Most significantly for the future development of CECAM's activities, one of them opened a completely new field, that would become in later years one of the strong points of the science developed at Orsay. In a presentation of the new centre appeared on the CNRS newsletter in April 1972, Moser anticipated that "a suggestion by a Dutch colleague has led the Scientific Committee to take the decision to organize a new workshop dedicated to Monte Carlo calculations and molecular dynamics of water, to be held in summer 1972".[22] The Dutch colleague was Herman Berendsen, professor of Biophysical Chemistry at the University of Groningen, and one of the pioneers of molecular dynamics in Europe. The ground-breaking paper by Aneesur Rahman and Frank Stillinger on the molecular dynamics of liquid water had just been published the previous year, and Berendsen's proposal to devote a full workshop to the matter couldn't have come at a more appropriate time. Over a period of almost two months, the CECAM workshop collected on the hill at Orsay a good sample of the best experts in molecular simulation (including Kurt Singer and Ian McDonald from Britain), was the starting point for the durable and fruitful relation between Rahman and CECAM, and opened a full new line of development for future CECAM activities, in a way that was just hinted at in its summary report: "This workshop is the first scientific activity of CECAM devoted to computational physics that is essentially classical mechanics. Previous efforts have all been directed to the application of quantum mechanics to problems in atomic and molecular physics. We plan that

[21] In a report submitted to CNRS Moser made explicit reference to this case to underline the significance of CECAM's workshops: "A recent event, the attribution of the 1985 Nobel Prize for Chemistry to Herb Hauptman, shows how influent CECAM's workshops can be. Though the early papers by Hauptman and Carle date back to the mid-fifties, the CECAM workshops in 1970, 1973 and afterwards have largely contributed to make the community of experts in crystallography aware of the potential power of the so-called direct methods. A common interest could develop this way, to a point that would have been unattainable without this workshop programme; moreover, Hauptman has been an active participant to the workshops on direct methods." Report by Carl Moser for the Direction des Relations et de la Coopération Internationales, May 20, 1986, CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[22] C. Moser, *Le Centre Européen de Calcul Atomique et Moléculaire*, Courier du CNRS, April 1972, pp. 26-27.

this workshop is only the first of many where a particular interest will be the applications of molecular dynamics to problems of physics and chemistry and eventually other types of problems where classical mechanics may be of interest".[23] Molecular simulation had come to CECAM, and was there to stay.[24]

Soon a new working tool was tested. The Council agreed that the selection of the topics around which to organize future research activities would have benefited from preliminary debate about the relevance, and the perspectives for future advancements, of the subject matters proposed for the workshops to come. The novel format was announced in the Scientific Report for 1972-1973: "We believe the organisation of workshops is one of the most original features of our Centre and that if these are to be most successful, they should be carefully prepared, if possible, at small preliminary meetings". Two such "discussion meetings", as they came to be usually called, were indeed held in 1973 and led to the organisation of three workshops the following year. "Small" meant in fact that these meetings were supposed to last only a few days, contrary to the long duration of the workshops (between one and two months). By that time, the pattern that would be followed in the future was set: each year CECAM would organize a number of workshops, putting together a limited number of people working on a well-defined subject for an extended period of time and actually doing research making full use of CIRCÉ's computing facilities, and a few short meetings of larger groups of interested scientists to discuss the state of the art in a given research sector, evaluate the potentialities for a successful cooperative effort on that specific field, and submit proposals for further workshops, to be in the end approved or rejected by the Scientific Council.

It is not the aim of this paper to provide a detailed and exhaustive account of CECAM' scientific activity and results. A reasoned and critical survey has been made by Herman Berendsen in his contribution to the booklet produced

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[23] *Molecular Dynamics and Monte Carlo Calculations on Water*, Report of a CECAM Workshop, held in Orsay, June 19 – Aug. 11, 1972, CECAM Archives, Lausanne.

[24] Indeed, molecular simulation had already landed, rooted and developed in Orsay, even before CECAM settled there. At the Theoretical Physics Laboratory on the lower part of the Orsay campus, Loup Verlet and his group had given pioneering contributions to the field since 1967, making use of the Univac computers of the Orsay University Computing Centre, and maintained close ties with several of the same experts which Moser hosted at his Centre up on the hill. For various reasons, in spite of their physical proximity and community of interests, the Verlet group and CECAM "superbly ignored each other" for quite some time. This rather peculiar story is briefly recalled by Jean-Pierre Hansen and Dominique Levesque in their contribution to *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, p. 31. A detailed account of Verlet's contributions to the field is given by the same authors: D. Levesque, J.P. Hansen, *The origin of computational Statistical Mechanics in France*, European Physics Journal H 44, 37-46 (2019).

in 1990 on the occasion of Moser's retirement.[25] Berendsen gives a full list of the workshops and discussion meetings held over a period of twenty years, from CECAM's birth to 1988, arranged in six tables corresponding to six different (though often related) main areas into which he splits the research activity developed at CECAM. These are 1) Direct methods in X-ray diffraction, 2) Plasma's and laser fusion, 3) Quantum mechanics in chemistry and solid state physics, including the study of excited states, 4) Molecular dynamics, 5) Biological applications, 6) Reaction paths and rates. Boundaries between these areas were often not rigid, and indeed fruitful cross-fertilization across different fields was one of the main results of successful workshops. Possibly the best example was given by the celebrated 1976 workshop on "Models for Protein Dynamics", where, in addition to the important results obtained (during the workshop the first protein simulation was carried out, by Andy McCammon), a significant accomplishment was to put effectively at work together for the first time scientists working on molecular dynamics and biological matters: "the accurate simulators and the crude biophysicist formed two groups with highly deviating interests and preferences. But there was a lot of interaction and some could bridge the gap".[26]

The Scientific Report for 1976-1977 provides useful information allowing to trace a summary balance of CECAM's first eight years of activity. In the annual 1976 meeting of the Scientific Council it had been decided to hold in September of the following year a conference to celebrate the tenth anniversary of the Blaricum meeting, where the foundations of CECAM had been laid.[27] In the end, the conference did not take place, but the recurrence was nonetheless duly noted the Scientific Report: "The year of 1967 was the tenth anniversary of the meeting in March 1976 (sic!), which was held in Blaricum, Holland and which led to the organization of CECAM. It seemed to us worthwhile to take stock of the activity of our Centre by compiling a list of those scientists who have actively participated in our Centre's research activities and the publications which have resulted from their stay in Orsay."[28] To sum it up in a few numbers, in eight years 18 workshops and 20 discussion meetings had been organized; 306 scientists from 22 different countries (14 of them European) had spent some time as visitors of the Centre, while 198 papers, more or less directly connected with research conducted at CECAM,

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[25] H.J.C. Berendsen, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, pp. 2-18.

[26] H.J.C. Berendsen, *The Development of Molecular Dynamics at CECAM*, in J.P. Hansen, G. Ciccotti, H.J.C. Berendsen (eds.), *In Memoriam Aneesur Rahman 1927-1987*, CECAM, Orsay 1987, pp. 9-14. A measure of the historical relevance of this workshop is given by the fact that a conference was organized to celebrate its 40th anniversary: *Models for Protein Dynamics. 1976-2016*, held at CECAM Headquarters in Lausanne on February 15-18, 2019.

[27] Compte-rendu du Comité Scientifique du CECAM – 27/11/76 à Orsay, CECAM Archives, Lausanne, Box 050.

[28] Rapport d'activité scientifique du CECAM, 1er Octobre 1976 au 31 Décembre 1977, CECAM Archives, Lausanne, p. 4.

had been published in the scientific literature. Clearly, the impressive list of over three-hundred names (which anyhow does not include scientists who attended only discussion meetings) does not allow to distinguish between those who just paid a short visit to Orsay, and those who went there repeatedly and were actually residents for an extended period of time. Nor can be exactly told which of the listed papers were actually written during CECAM stays, thanks to the availability of the computing facilities there. Most of all, what impresses is the extremely wide range of countries represented among visiting scientists. Already in its early years of operation CECAM had succeeded in establishing itself as a genuine international pole of attraction for researchers working in fields that were no longer restricted to quantum chemistry, but covered an expanding and broad spectrum of interests. And the attraction worked for the younger people at the beginning of their career and for the senior scientists; both found at CECAM working facilities often unavailable at home and a stimulating intellectual environment. Daan Frenkel gives a lively description of the "atmosphere of structured chaos" reigning in Orsay when he first arrived there in May 1975 from Amsterdam as a young PhD student: "The atmosphere at CECAM was truly international: a constant flux of Gods and semi-Gods in science, people whose names I had thus far only read in awe, appeared in person, gave seminar, stayed for dinner, and by large changed perception of science".[29] And he goes on with an appreciation of the "style" that allowed that atmosphere to survive and provide the proper environment for intellectual creativity: "I consider it the lasting merit of Carl Moser that he has managed to keep this spirit alive in this time of "business-like" science management, where the average administrator wants the scientific discoveries of the next five years to be written down in advance and in triplicate. Carl never joined the paper-shuffling game. The impact of CECAM can therefore not be gauged by reading the annual CECAM reports. Unless you simply look at the list of names, and count the number of European scientists who, effectively, started their computational work at CECAM. Then the picture becomes very clear".

Into the 80's

While CECAM was performing successfully on scientific grounds, thanks also to his director's pragmatic behaviour and disregard for the "paper-shuffling game", the persisting lack of a clear definition of its legal status continued to be a source of uneasiness for the top CNRS officials (and, to some extent, for the partner institutions). The "more definitive solution" that Curien was invoking in 1970 had not seen the light over ten years later. To maintain a high level of autonomy and operational flexibility, Moser refrained from creating rigid bureaucratic norms, while the peculiar character of his centre made it hard for

[29] D. Frenkel, in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, p. 30.

CNRS to find a satisfactory solution to its institutional status. Was CECAM a CNRS structure, or an independent body? On one hand, from the institutional point of view, CECAM didn't even exist: the visitor entering building 506 in Orsay wouldn't find a single indication that the offices of something called CECAM were located there on the sixth floor.[30] On the other hand, the heading of the official correspondence sent from those offices read: Ministère de l'Education Nationale/Centre National de la Recherche Scientifique/Centre Européen de Calcul Atomique et Moléculaire, showing a hierarchical sequence that presented CECAM as a subordinate body to CNRS. Even on the official birthdate of the Centre there was no agreement; while Moser declared it to be October 1969, CNRS documents postponed the event to 1970. A different perception of the true nature of the Centre was developing: Paris administrators regarded CECAM as a CNRS laboratory open to European collaboration, while the "Moser family" thought of it as an independent European organization that happened to be hosted by a CNRS facility.

Besides the formal side of the question, CNRS felt that its own share of participation to the overall budget of CECAM was growing out of proportion compared to the real benefits for France. The amount of the yearly contribution of each of the member institutions was of the order of 2- to 300.000 French francs; CNRS gave about the same in terms of direct funding, but was burdened with further contributions given by salaries of director and staff, lodging, and, most heavily, computing hours at CIRCÉ that were offered to CECAM users at a very convenient discounted price. At the end of 1979 the CNRS representatives in the Scientific Council estimated that the real financial participation of CNRS to CECAM expenses had been "in ten years oscillating between 50% and 85%".[31] Foreign partners, on the other hand, were at times complaining about the way in which the overall budget of CECAM was administered, and wished for a tighter control of the Council over the Centre's financial management.

The issue was explicitly raised when, at the end of 1976, the convention between CNR and CNRS defining the Italian participation to CECAM had to be renovated. Apparently, CNR proposed to modify the previous rules and establish that Italian funds would only be used to pay for the visits to Orsay of Italian scientists. Moser's reaction was that "if that same rule applied to all partners, there would be no CECAM". He insisted on the policy that "an international organization, even a small one like CECAM, can only work efficiently if there are common research programmes and a common financing

[30] "CECAM occupies a part of the building which houses the Computing Center of the French National Science Foundation (CNRS). The building has a number and the name of the Computing Center (CIRCE) but CECAM' name does not appear"; C. Moser to J.B.H. Otker (Z.W.O.), September 16, 1985, CECAM Archives, Lausanne, Box 043.

[31] Compte-rendu de la réunion du Comité Scientifique du CECAM, 30 novembre 1979, CECAM Archives, Lausanne, Box 050.

of these projects".[32] Writing on that matter to CNR's President Ernesto Quagliariello he made this point clear: "It has never been contemplated that each one pays for his own scientists. I'm convinced that up to now the present formula has been beneficial for everybody, and most of all for Italian scientists".[33] And then he played his winning card: "If we propose that each partner covers only the expenses of his own researchers, this should apply to all partners in our Centre, including French bodies such as CNRS and CEA. One should therefore foresee that the cost of the computations made at CECAM would be supported by each body, according to the use made by his own scientists. In that case, the amount of your contribution to CECAM for 1977 would be much greater than the present estimate of 50 million lire!" An agreement was in the end reached, and the new convention with CNR signed, only in October 1978, for a duration of three years.[34]

A report sent in March 1981 to CNRS Director General Jacques Ducuing summed up the situation and the pending problems regarding the functioning of CECAM.[35] It stated that, "created in 1970, CECAM has never been given a legal structure"; that an RCP (Recherche Coopérative sur Programme) du CNRS had been created to that end in 1978, but had just been abandoned; that a structure of the kind GIP (Groupement d'Interet Scientifique) had been envisaged as a possible way to solve the problems related to CECAM administration. For the financial side of the matter, the report underlined the amount of the double (direct and indirect) contribution by CNRS. The provisional financial balance of 1980 gave an overall expense of about 1.500.000 FF (covered by the direct contributions of the partner institutions); about half of that sum was what CECAM paid to CIRCÉ for computing time. This was actually a limited portion of the real cost of the computing time used by CECAM (it used to be around 20% in the early years and had grown up to 60% by 1980). The estimated "indirect" CNRS contribution to the real total CECAM expenses amounted to about 500.000 FF.

The report went on presenting the preoccupations of (some of) the

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[32] C. Moser to Mme Mirabel, CNRS Relations Internationales, 2 décembre 1976. CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[33] C. Moser to E. Quagliariello, 2 décembre 1976. CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001. Moser had a point in claiming that Italy had possibly benefited from CECAM more than any other partner country. This was, at least, the feeling of visitors to Orsay. According to Daan Frenkel and Jean-Paul Ryckaert, CECAM in the mid-seventies was "nothing else than an Italian enclave", and "an Italian colony": see their contributions in *Recollections of CECAM – For Carl*, CECAM, Orsay 1990, pp. 30 and 34 respectively.

[34] At the end of 1981, however, due mainly to internal tensions about its overall scientific policy, CNR withdrew its participation as a partner member, until in 1986 the Convention defining the CECAM status was approved. Nonetheless, between 1982 and 1986 Italian scientists took part in CECAM activities, their expenses being directly covered by their institutions.

[35] W. Mercouroff (Direction des Relations Exterieures), Note à l'attention de Monsieur Ducuing, Paris, 20 mai 1981. CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

foreign partners: "Since several years, the main CECAM foreign partners, namely M. van Lieshout, Director of ZWO, and the representatives of the Italian CNR have communicated to CNRS that they consider CECAM's activity as being of particular interest, but that they are not satisfied of the way it is administered... The foreign partners wish that M. Moser could no longer make uncontrolled handling of the credits at his disposal, and think that a well-established structure would allow to solve these difficulties".

The note that Ducuing sent privately to Mercouroff upon receiving the report leaves no doubt about the feelings prevailing among the upper echelons of CNRS: in the benefit-to-cost competition between the several partners of the collaboration, the French scientific community felt distinctly to be by and large the most disadvantaged, to the point that CNRS Director was considering the idea of "putting an end to that all", unless the situation be substantially redressed.[36]

Five years later, a similar report (indeed essentially the same, with some minor modifications required by the few novelties occurred in the meantime, such as the entrance of Great Britain in the group of the foreign partners) was sent to the CNRS Financial Controller, with an urgent request to evaluate the attached proposal for the creation of a Groupement Scientifique.[37] This was the final outcome of a project that "had been elaborated in several occasions with our foreign partners since 1982". In fact, over a period of five years a dozen different versions of that proposal had circulated among the various actors, each time introducing slight modifications to reach an agreement that would satisfy all demands. The definitive version of the convention was signed on October 24, 1986 at the CNRS Chateau, Gif-sur-Yvette. It formalized the creation, by the institutions signing the agreement, of a Groupement Scientifique, the "Centre Européen de Calcul Atomique et Moléculaire", with seat at CIRCÉ in Orsay, having as its aim "to promote the exchanges and contacts inside the international scientific community, to promote scientific collaboration between the main research bodies at the European level, and to set up and coordinate seminars and workshops in those fields where the methods of numerical simulation play a dominant role". The agreement was signed by representatives of CNRS (France), CEA-DAM (France), CNR (Italy),

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[36] "L'interet pour le CNRS et la communauté scientifique francaise du CECAM n'apparait toujours pas nettement. Aussi suis-je, actuellement, défavorable à la création d'une structure internationale impliquant le CNRS. J'avoue d'ailleurs ne pas tres bien voir la justification du cadeau de 500 KF en heurs de calcul. Pour te livrer le fond de ma pensée, je mettrais bien un terme à tout cela, à moins qu'on ne me montre un bénéficiaire francais." Note by J. Ducuing to W. Mercouroff, April 16, 1981, CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[37] J.F. Miquel (Direction des Relations et de la Coopération Internationales), Note à l'attention de Monsieur J.F. Heyman, Contrôleur financier, Paris, 25 avril 1986. CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

ZWO (Holland), SERC (Great Britain) and FNRS (Belgium). It was meant to be valid for a period of three years, and it was intended to be renewed by tacit agreement unless explicitly denounced by one or more of the member parties.

In its essence, the convention just limited itself to formalize the existent situation, and not much changed afterwards in the usual functioning of CECAM; however, by putting explicitly on an official document the rules of the game, defining the composition and the functions of the Scientific Council, the tasks and prerogatives of the Director, fixing the annual contributions to be versed by the member organizations, the convention finally gave CECAM the legal structure it had been lacking since its foundation. The main innovation concerned the Director: he (or she) was to be designated by the Scientific Committee, and would stay in charge for three years, with a possibility for a second mandate. This condition wiped out any problem potentially arising with CECAM's founding father and eternal Director, Carl Moser, who would in any case be forced to retirement in 1990. At the first meeting of the Scientific Council of the "new" CECAM, held on March 20, 1987, Moser was confirmed in his function of Director, for three years starting January 1, 1987, "under reserve that it be consented by the law regulations on the age of retirement".[38]

Continuity and changes

In 1990 two CECAM publications, of quite different character but in some sense related, saw the light. One was a collection of personal reminiscences by some of the protagonists of the Centre's life during the "Moser kingdom", prepared as a tribute to Carl Moser on the occasion of his retirement.[39] Daan Frenkel had circulated the proposal of producing such a collective memory during a special meeting held at Orsay in October 1989 to celebrate the twentieth anniversary of CECAM. The proceedings of that meeting were also published in 1990.[40] Though the meeting was intended to provide insights for the future, looking forward to potential developments, the list of the subjects covered give a fair representation of the impressive expansion in the range and scope of the scientific fields covered by CECAM's activities since its creation as a centre solely oriented to quantum chemistry. And some of the authors, before discussing future possibilities, introduced their talks by a retrospective look at the way in which CECAM had contributed to the development of their specific field.

In fact, all along the 80's CECAM's scientific activity had kept expanding, both in the number of initiatives and in the range of subjects covered. Here

[38] Compte-rendu de la 1ère reunion du Conseil CECAM qui s'est tenue au siège du CNRS à Paris le mardi 20 Janvier à 14h30. CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[39] *Recollections of CECAM – For Carl*, CECAM, Orsay 1990.

[40] *Perspectives for Computational Sciences in the 1990's*, CECAM, Orsay, 4-6 October 1989.

again, for an accurate evaluation the reader is referred to the reconstruction provided by Berendsen. A few numbers give an idea of that growth: while in the decade 1970-1979 CECAM had organized 30 workshops and as many discussion meetings, these numbers grew in the following decade (1980-1989) respectively to 80 workshops and 72 discussion meetings (that sometimes also took the name of preliminary, or planning, meeting). Such had been the growth of the different subjects covered, far away from the original confinement to computational chemistry, that Moser was led to comment that "There are some who feel that the program of CECAM workshops doesn't have nearly enough "chemistry" subjects. We seem to be concerned only with physics, astrophysics and molecular biology".[41]

There were, however, a few novel problems arising along with this enlargement of activities. One was a crude problem of space. If in 1969 CECAM could be happily hosted in Building 506 thanks to the amount of free space there, by the late eighties the increasing need of more room for the expanding computing facilities of CIRCÉ came into conflict with the growing number of workshops and related activities, requiring seminar rooms that were no longer easily available. Moser had to raise the issue with CNRS Scientific Director and ask for his intervention to define "the rules of "cohabitation" between CIRCÉ and CECAM in this building" when the director of CIRCÉ planned to appropriate one of the two CECAM seminar rooms and convert it into offices for his group.[42] Cohabitation, somehow, continued.

More relevant on scientific grounds, a significant change intervened throughout the 80's in the organization of the workshops. While their number grew steadily, their duration was drastically shrinking. On the average, the 30 workshops held in the first decade had kept the participants occupied for a period of seven weeks. Between 1980 and 1989, the 80 workshops lasted on average only two weeks; some of them, more and more as time passed by, only about a week. There were several reasons for that. Besides organizational problems (holding more meetings necessarily meant less time to devote to each one of them on CECAM premises, which also explains why a growing number of workshops did not take place at Orsay), the increasing diffusion of computing facilities throughout Europe made it unnecessary to stay for long periods of time at Orsay to exploit the once unique possibilities offered by CIRCÉ. People could now envisage workshops being just an occasion for theoretical discussions and elaboration of projects, while the actual computational work could be more easily performed at their domestic institutions. The organizers of the workshops had to find the best compromise to lighten the burden of heavy computational costs (in terms of time and money) while keeping the meetings long enough to guarantee effective intellectual

[41] C. Moser to W. Niewpoort, January 20, 1986. CECAM Archives, Lausanne, Box 043.
[42] C. Moser to J.C. Lehmann, July 15, 1987, CECAM Archives, Lausanne, Box 048.

interaction between participants, a characteristic of CECAM workshops regarded by many as the fundamental key to their success, even more than the availability of excellent computing resources. CECAM's "old guard" insisted on keeping workshops as long as possible, and both Moser and his successor Giovanni Ciccotti encouraged the renewal of the former policy of having at Orsay long-time visitors, an habit that had been slowly disappearing.

Computer development was a subject very dear to Moser, who devoted a good part of his personal efforts to that matter. A discussion meeting on "Special Purpose Computational Machines" was held in Holland in 1984. Soon after, in close collaboration with Berendsen, Moser tried for a while, relying on his extended network of personal relations, to set up a joint effort for the creation of a European centre for the construction of special purpose parallel architecture computers. A thick correspondence on the subject is preserved in Moser's files, involving not only scientists of the CECAM inner circle, but the wider community of people working at the time to design new computer architectures tailored for specific scientific tasks. In the end, mainly because of the lack of the necessary industrial support, nothing came out of that proposal; the issue of future developments of computer design, however, remained one of Moser's main concerns.

Among the different research areas investigated by individual visitors and discussed in workshops, molecular simulation may serve as an example to judge the relevance of CECAM related contributions to the advancement of the field. Already in the 70's, following the 1972 workshop on the simulation of water, a workshop held two years later on "Methods in molecular dynamics – Long time-scale events" was the starting point for the introduction of the mass tensor technique by Charles Bennett, while at the same time, during the long periods of time they spent at Orsay, Gianni Jacucci and Giovanni Ciccotti developed their subtraction technique, and soon after Ciccotti and Jean-Paul Ryckaert started the work on constrained dynamics that incorporated the SHAKE algorithm just in time for it to be used during the 1976 workshop on the simulation of proteins. Moving into the 80's, it was during a 1983 workshop that Daan Frenkel and Tony Ladd wrote their paper on the calculation of free energies; in 1984, the encounter between Shuichi Nosé and Bill Hoover at another CECAM molecular dynamics workshop led Hoover to work on his modified version of the Nosé thermostat, while a group of participants, including Nosé and Hans Christian Andersen, produced a detailed report on "New molecular dynamics methods for various ensembles". In the summer 1985, CECAM organized at Orsay the first workshop devoted to a stochastic approach to chemical reactions, a topic that was resumed in three following summer workshops, from 1986 to 1988, all of them dedicated to "Computer simulation and the theory of chemical reactions in solution", whose outcome was the development of the "Blue Moon Ensemble". Some of these results were reached during the workshops themselves, others resulted from further

elaboration of ideas originated in workshop discussions. And, beyond the achievements that were direct results of CECAM activities, there is little doubt that in general CECAM acted throughout this period as an effective "resonance box" for ideas that, even if produced elsewhere, found in the peculiar international atmosphere of the workshops the perfect environment to diffuse and be circulated among the scientific community at large.

The issue of the choice of Moser's successor was discussed by the Council at the 1988 meeting, when the procedure for the appointment of the new director was established. It was agreed that the directorship would be a full-time function, and that the choice should fall on an active scientist, whose administrative duties were to be kept at a minimum, thus allowing him to devote the major part of his time to scientific activities relevant to CECAM.[43] Candidatures were advanced throughout the following year. Following interviews with prospective candidates in June 1990, the final choice of the Council fell on Giovanni Ciccotti, professor of Molecular Physics at the University "La Sapienza" in Rome. As a computational theoretical physicist, Ciccotti was really a "CECAM's child": his long-standing activity in molecular dynamics and statistical physics had started during a stay at Orsay in 1974, at the invitation of his friend and colleague Gianni Jacucci, and since then his achievements, both in research and in organizational endeavours, had been strictly connected to CECAM related activities. Ciccotti was officially designed as Moser's successor on October 1 1990. To give a clear indication of the changing and widening range of scientific areas falling under CECAM related researches, he managed to have them shifted, for the sake of official CNRS evaluation, from section 04 (Atoms and molecules; optics and lasers; hot plasmas) to section 02 (Physical phenomena, theories and models). Ciccotti made a substantial effort to resume the practice of having at CECAM long-term visitors, and, in the course of his mandate, managed to equip CECAM with first-class computer hardware.[44] In the way of managing practices, he definitely shared with his predecessor a nonchalant attitude toward bureaucratic obstacles and a disregard for the "paper shuffling game", that were difficult to reconcile with the rather stiff handling of such matters by French administrators. These peculiar traits of character would soon be put to test by the new institutional crisis that was preparing.

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[43] CECAM Scientific Council, Meeting of 20 September 1988, "Procedure for Appointment of New Director", CNRS Archives, Dépôt de Gif-sur-Yvette, versement 910001.

[44] A detailed list of the equipment owned, or on leasing, by CECAM "thanks to Giovanni Ciccotti's far reaching policy", is in a report "Computing at CECAM", undated and with no signature, but most likely compiled by Stefano Baroni and dating from the very early days in Lyon. CECAM Archives, Lausanne, Box 124.

Leaving Orsay

In 1992, the CNRS Director General François Kourilsky launched MIPS (Moyens informatiques pour la science), a large project aimed at an upgrade and a full renovation of the national resources for computational science. Charged with the implementation of the project was Victor Alessandrini, an Argentinian born theoretical physicist, professor at the Université Paris XI in Orsay, who was since 1988 one of the CNRS representatives in CECAM's Scientific Council. Within the larger MIPS project, the creation of a new supercomputing centre was envisaged, endowed with the best available machines and coupled to a research laboratory, originally designed to be located as a brand-new institution in Marseille. This option revealed itself too ambitious to be realized, and it was decided that the new centre would be installed at Orsay, replacing CIRCÉ that was going to be dismantled. Creating such a supercomputing centre and research laboratory at the Orsay site implied for CNRS reconsidering its relationship with CECAM. At the end of 1992 Kourilsky sent to the President of CECAM's Council an official letter denouncing the convention, effective December 31, 1993. Kourilski suggested that to "optimize our interface with CECAM"..."it seems desirable to us that CECAM becomes the European component of this laboratory, the ensemble of these activities being placed under CNRS responsibility".[45] A more detailed proposal would be soon circulated to SC members.

The CNRS proposal, specifying at which conditions CECAM would be "the European component of this laboratory", was addressed by Alessandrini to the SC members in January 1993. In the accompanying letter, he commented that "we should be able to maintain a reasonable amount of independence in the management of the traditional CECAM activities",[46] but this was not enough to dispel the feeling that in the proposed scheme CECAM would be in some sense a subordinate body to the CNRS laboratory. This perception was manifest in the commenting letter sent to SC members by the Council President, Daan Frenkel: "Although the CNRS plans are, at present, still in a preliminary stage, it was clear from the briefing that we received from Victor Alessandrini that it is envisaged that the present CECAM activities would be incorporated in this novel scientific computing center. This would have consequences for the way in which CECAM operates as the presence of the new super-computer necessitates the CNRS to have more direct control over

[45] Letter by F. Kourilsky, December 17, 1992, CECAM Archives, Lausanne, Box 122. The proposed CNRS laboratory was called ICI (Institut de Calcul Intensif); it was to be part of the large supercomputing centre, which was actually inaugurated in December 1993 as IDRIS (Institut du developpement et des ressources en information scientifique), still its present denomination.

[46] V. Alessandrini to CECAM Council members, January 25, 1992, CECAM Archives, Lausanne, Box 122.

personnel working in the same building. In particular, it was explained that, in the new structure, there would be only one director who would be appointed directly by the CNRS. This director would be in charge of both the national and the European scientific activities. Moreover, long-term visitors would also have to be approved by the CNRS".[47] Frenkel asked the Council members to be informed on their views on the matter, to be discussed at the extraordinary Council meeting scheduled for March 8, and in particular "to consider explicitly how much of the independence of CECAM your organisation is willing to trade in exchange for the possibility to have access to the super-computer(s) at Orsay".

The reactions of the representatives of CEA, CNR, FNRS, NOW and SERC to the CNRS proposal were enclosed in the preparatory material for the March meeting. In the joint SERC-NOW discussion paper it was explicitly stated that the Council faced three options: a) closing CECAM on Dec. 31, 1993, b) moving CECAM to a different site, c) retaining CECAM at the Orsay site, in symbiosis with the ICI. Frenkel made it clear that at the meeting only option c) would be discussed; other options would be considered only if "unexpectedly, no satisfactory arrangement for option c) can be found". Nonetheless, already at least two different informal proposals to host CECAM were advanced before the meeting took place, by Michel Mareschal from the Université Libre de Bruxelles, and by the director of the Italian computing centre, CINECA, near Bologna.[48]

At the March meeting, a consensus was reached that "it should be possible to arrive at a new CECAM convention that would be satisfactory both to the CNRS and to the other partner organizations". A hectic period followed, with several drafts of the new convention being circulated and going back and forth, but no satisfactory solution was found. Another note by Alessandrini further clarified the viewpoint of CNRS: he stated clearly that "maintaining in our Orsay site an organisation with uncorrelated European and international policies, whose main concern would be to drift away from CNRS as much as possible" was an option that could not be considered. He reinforced his point asserting that "CNRS management of CECAM is required by the very strong coupling we intend to set up with the future supercomputing centre", and claiming that "CECAM has always been a CNRS laboratory with an European projection".[49] Clearly, the circumstance that Alessandrini happened to be at the

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[47] D. Frenkel to CECAM Council members, January 29, 1992, CECAM Archives, Lausanne, Box 122.

[48] All the relevant documentation is preserved in Box 122 of the CECAM Archives in Lausanne.

[49] V. Alessandrini to CECAM Council members, April 20, 1993, CECAM Archives, Lausanne, Box 122. Regarding the last statement about the CECAM status, it can be interestingly confronted with what Moser was explicitly stating on that same point: "CECAM is a European organization and is not a laboratory of CNRS": C. Moser to K. Morakuma, July 23, 1987, CECAM Archives, Lausanne, Box 048.

same time the CNRS representative in the Council conducting the negotiations on the CECAM matter, and the designated director of the future CNRS supercomputing centre, did nothing to ease the relations. In May, Frenkel informed the Council members that no consensus had been reached yet on a possible compromise, given the essential differences between the draft conventions prepared by Leech and Bertoni (SERC-CNR) and by Alessandrini, mainly related to the role and management of research to be conducted at CECAM.

The peak of tension was reached in June, when it became clear that a solution of the "stalemate" (as Frenkel evaluated the situation) that would allow CECAM's permanence at Orsay, was not possible. An irritated long letter by Alessandrini, containing harsh judgements on CECAM's management, reaffirmed the points on which CNRS had no intention to compromise, stated bluntly that "CECAM, in its present form, comes to an end at the end of this year", and basically gave an ultimatum to the Council, directly asking the question "whether the organisation you represent is willing to pursue an active cooperation with CNRS at the Orsay site".[50] Frenkel let Kourilsky know that he was "personally worried by the deteriorating atmosphere of the negotiations". Whatever the outcome of the issue, he added, any attempt to diminish CECAM's relevance as a research institution was out of the question: "Let me conclude by stating that I feel that the CECAM collaboration has been extremely successful and is worth continuing. In the 25 years since it was founded, CECAM has developed into an institution with a great international reputation that attracts a constant stream of top scientists in the field of computational science. The research experience at CECAM has been a crucial formative experience for many of the leading computational physicists and chemists in the CECAM member countries. In fact, without CECAM, Europe would never have developed into world leader in the field of computer simulation. It is clearly important that this leading role be maintained and strengthened".[51]

The final decision to leave Orsay was taken by the Scientific Council at the extraordinary meeting held in September. It was agreed that the conditions allowing to take what seemed to many the most desirable solution, i.e. to maintain CECAM at Orsay, could not be satisfied, and that the remaining alternative option was to move CECAM to a different location. A vote was taken in that sense, and the resolution to move passed with the favourable vote of the representatives of CNR, SERC, NWO and FNRS; CEA abstained.[52] Proposals to host CECAM (due to leave Orsay by the end of the year) rapidly

[50] V. Alessandrini to CECAM Scientific Council members, June 2, 1993, CECAM Archives, Lausanne, Box 122.

[51] D. Frenkel to F. Kourilsky, June 18, 1993, CECAM Archives, Lausanne, Box 122.

[52] Minutes of the extraordinary meeting of the CECAM Scientific Council held on 9 September 1993, CECAM Archives, Lausanne, Box 122.

came from ten different sites, alongside with requests to enter as member of the CECAM partnership by the Swiss FNS (Fonds National Science), the Greek FORTH (Foundation for Research and Technology – Hellas), and the Université Libre de Bruxelles, the École Normale Superieure in Lyon, and SISSA (Scuola Internazionale Superiore di Studi Avanzati) from Trieste, these latter in case their proposal to host CECAM be accepted. At the regular annual meeting of the Council, in November, the site of Lyon was selected: the future CECAM would be hosted by the École Normale Superieure at Lyon. Instrumental in the matter was the role played by Jean-Pierre Hansen, a computational theoretical physicist who had been a member of Loup Verlet's group in Orsay and had developed friendly relations with the "CECAM family"; he had moved in 1987 from Paris to Lyon, as research director, to help establish there the new École Normale Superieure, and had founded its Physics Laboratory. The convention defining the status of the new CECAM was elaborated by Carlo Maria Bertoni from CNR and Mme Simoen, general secretary of FNRS. CECAM was an independent association between the member institutions, constituted as a laboratory with the aim "to promote cooperation amongst European research organisations and their scientific communities in furthering research involving computationally intensive methods".

The new premises of CECAM in Lyon were officially inaugurated with a ceremony on April 8, 1994. In the morning of that same day, the Scientific Council had held its first meeting in the new location, and selected as CECAM future Director Stefano Baroni, from SISSA. In his inaugural speech, Council President Daan Frenkel gave his personal evaluation of the state of health of the Centre: "In 1993, when it became clear that the old structure of CECAM had to change, we had to ask: is there still a need for CECAM? I think that this question was convincingly answered by the fact that CECAM received truly excellent offers for new premises from all member countries and even from several countries that had not yet joined CECAM". Indeed, the succession of events originated by the 1993 "crisis" turned out to be a positive indicator of the persisting need of CECAM as an aggregation point for European science. The "CECAM family" was further expanding, and seemed to enjoy good health.

Acknowledgments

This paper was produced following the suggestion, by CECAM Director Ignacio Pagonabarraga, Deputy Director Sara Bonella and former Director Giovanni Ciccotti that it would be desirable to provide the CECAM community with a sketch of the Centre's early life, on occasion of the 50th anniversary of its creation. It is essentially confined to the institutional side of CECAM's history, and even so it has by no means any pretention to be exhaustive or definitive; most likely, the reader will find that important issues are missing, incorrect details are given, and debatable interpretations are suggested. While apologizing for such deficiencies of the present work, I can only express the wish that it may serve as a starting point for further, more complete and extended researches. In preparing the text I have profited, besides the very scarce literature on the subject, of the documentation deposited at the CNRS Archives at Gif-sur-Yvette, thanks to the efficient services of Mme Loïse Scherer, and, most of all, of the CECAM papers that have been in recent times the object of an important archival intervention, and are now properly arranged and deposited at the CECAM headquarters in Lausanne.[53] Among the several persons that have helped me in various ways I want to express my warm appreciation to Victor Alessandrini, Carlo Maria Bertoni, Sara Bonella, Daniel Borgis, Monique Butin, Giovanni Ciccotti, Janine Connes, Antonio Di Carlo, Denis Giroud, Jean-Pierre Hansen, Dominique Levesque, Michel Mareschal, Ignacio Pagonabarraga. It goes without saying that, for all the useful information they provided, any incorrect statement or factual error in the final text are my own responsibility. Finally, I wish to thank warmly CECAM Director Ignacio Pagonabarraga for the support given to this work, and the whole CECAM staff for their hospitality and assistance during my visits in Lausanne.

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[53] C. Abt-Müller, *Organisation et valorisation du fonds du Centre Européen de Calcul Atomique et Moléculaire (CECAM)*, Travail de Bachelor realisé en vue de l'obtention du Bachelor HES, Genève, August 2017.


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