# Recollections of CECAM For Carl

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**What is computational Science and the purpose of CECAM?**

Carl's definition, as he wrote it in the 1984 Annual Report was:

*"CECAM's purpose in the scientific world is to concentrate on problem areas in which only numerical solutions exist and for which larger and larger scale computing power becomes necessary for progress"*

In 1985 he added to this:

*"A main scientific purpose of CECAM has always been to encourage a cooperative goal towards scientific development"*

Both assertions have formed the heart of CECAM's success in the 20 years that have passed since CECAM became alive in October 1969. Two years earlier, in March 1967, the principles of CECAM were discussed and the foundations layed at a meeting in Blaricum, Holland.

Computational Science has grown to a third discipline next to the traditional theoretical and experimental sciences. Its aim in the molecular sciences, at least – is to compute properties like structure, dynamic and thermodynamic properties, reactivity etc.… of materials in the widest sense, based on first principles. For this purpose one can distinguish various levels of description: elementary particles, nuclei, electrons, atoms and molecules, clusters and aggregates, and finally: continuous media. The involvement of CECAM has focused on the levels ranging from *electrons, atoms and molecules to cluster and aggregates in condensed matter.* In addition and somewhat on the sideline of this general description, CECAM has been strong in *direct methods for X-ray diffraction and evolution of galaxies and interstellar clouds.*

Computational Science is nothing without computers, and big ones too. In fact, as Carl has pointed out, CECAM has always focused on those problem areas where the use of "big" computers is essential. In those areas it is often the case that the method of solution of a problem depends, on the architecture of available computers. More importantly: computer architectures can be developed for specific ranges of computational problems. Since 1984 the study of computer architecture for computational problems has become part of CECAM's activities and has found a fervent stimulator in Carl Moser. Together Carl and I have travelled through Europe trying to generate enthusiasm for a European laboratory where special purpose hardware and software could be developed for the computational sciences. I think we were a bit ahead of time the real developments are still coming with the gigantic growth of parallelism.

**How has CECAM contributed to the development?**

CECAM's activities have been of the following types:

- individual visits and scientific cooperation resulting from these
- specialized discussion meetings
- workshops
- preparatory meetings and workshops

In the course of the years the emphasis on various kinds of activities has shifted. Individual visits were important in the beginning, but declined later. Workshops have been the key activities since the early days, but their character has changed. In the early seventies the usual duration of a workshop was at least one, and often two months, but in later years the enthusiasm to spend such long periods has declined. As a result the emphasis has shifted to shorter meetings, with finally hardly a distinction between short and long meetings, lasting about a week. The character changed too: instead of doing a lot of innovative new work at CECAM, people have generated and absorbed ideas at CECAM and worked them out in their home institutions. In part this change is due to the maturation of the filed, requiring longer and more sophisticated programs that cannot be generated on the spot. Bit another factor has been the relative decline of the computer facilities at CECAM. While in the early seventies powerful computers were not routinely available for most researchers and CECAM could provide this at a high level, more recently computers power has become abundant almost anywhere. In the years that networking facilities were very inadequate, one factor contributing to CECAM's driving force – its computational facilities – became less important. Now things may have changed, because one doesn't need to transfer programs and data but can work at one's own institutional computer from CECAM. This means that being present at CECAM is immaterial for the purpose of using computers, but essential for the exchange of scientific ideas. Thus CECAM's focus must be on the driving force it experts on scientists to achieve new goals by interacting with each other and creating renewing initiatives.

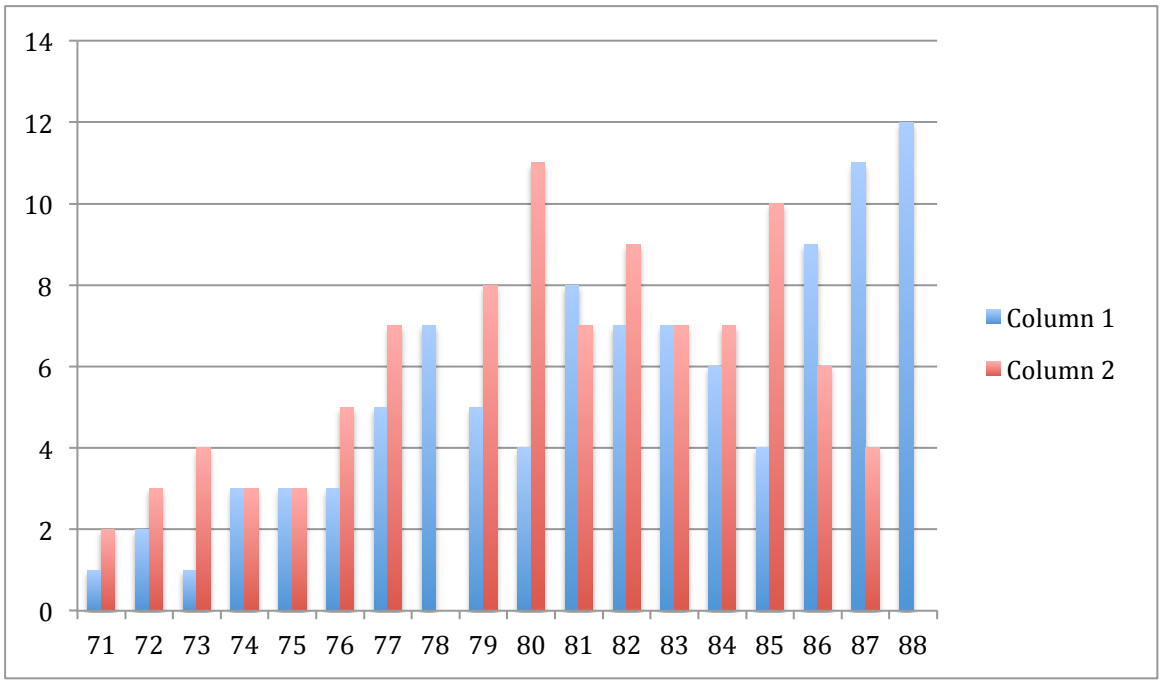


Fig. 1

## Workshops

Preparatory or Discussion Meetings

Figure 1 shows how the number of workshops and discussion meetings has changed over the years. The number of workshops has increased, but their duration declined: From 8 weeks in the period 1971 to 77. Via 4-6 weeks during 1978 to 81, to 2-4 weeks since 1983. The individual visits declined from between 30 and 60 each year sin the period up to 1975 to almost zero since 1982. A slight recurrence can be observed after 1967, when Carl wrote "*We have begun to encourage individual visits".*

## Lines of research at CECAM

Let me try to give a survey of activities at CECAM over the past 20 years. Although many activities seemed unrelated, as they were dependent on what individual scientists were willing to put forward at a given time, it is quite possible to discern major lines of developments. Often one activity followed another as a planned and logical consequence but equally often there is a seemingly accidental, but still logical sequence in the series of activities as a result of the scientific development. In some field like plasma's and laser fusion, CECAM has become a binding force for an adhesive group of scientists, who have cooperated strongly and continuously. In other fields, like molecular dynamics, specifically in biophysical applications, CECAM has been a focal point, without which the scientific developments would not have taken place at the same rate, if at all.

*Direct methods in X-ray diffraction (Table 1)*

The first CECAM workshop was in this filed with Herbert Hauptman of Buffalo (Noble prize winner, with Jerome Karl, in 1985 on direct methods for the determination of crystal structures) being the initiator. Work was extended to proteins by Bricogne and others, but the line was not really continued after.

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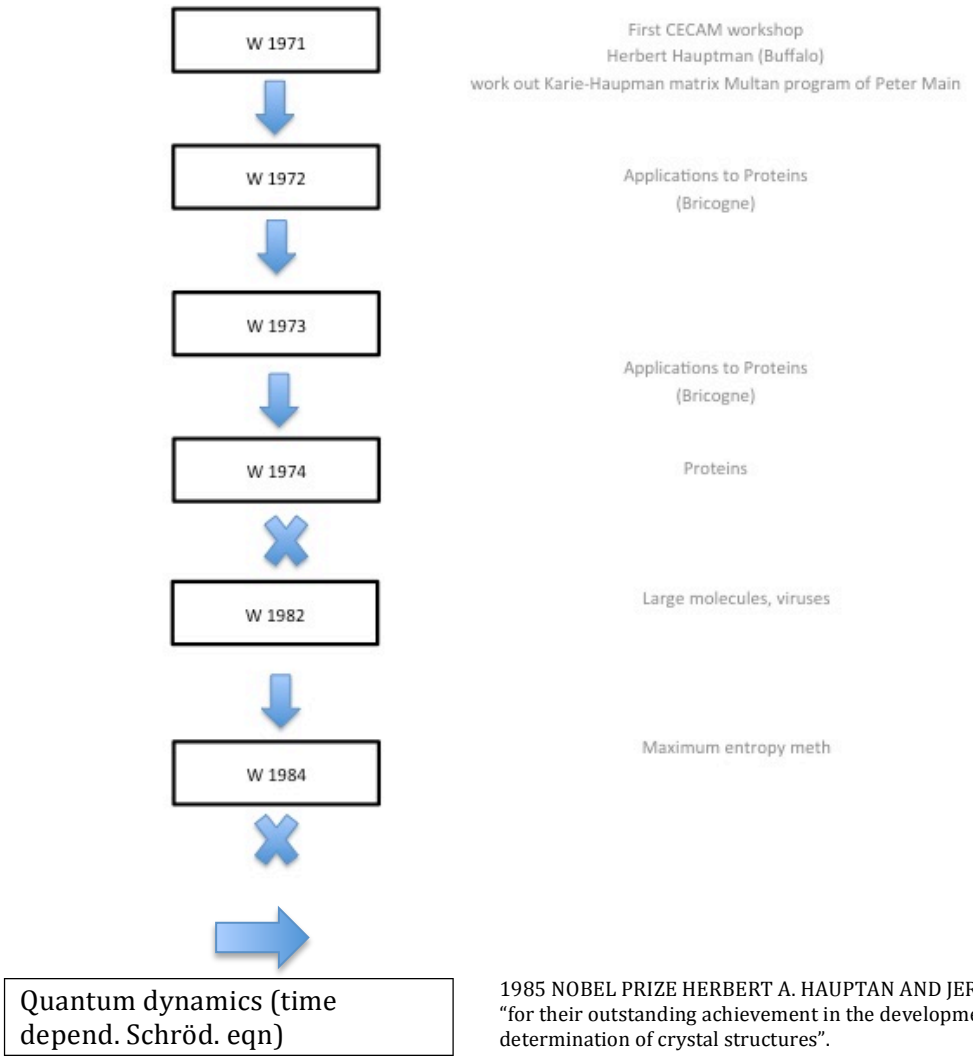
Table 1

DIRECT METHODS IN X-RAY CRYSTALLOGRAPHY

Problem of phase determination of X-ray structure factors by using inherent relations between phases of various reflections (and other information)

Frist CECA Frist CECAM workshop Herbert Hauptman (Buffalo) work out Karie-Haupman matrix Multan program of Peter Main




1985 NOBEL PRIZE HERBERT A. HAUPTAN AND JEROME KARL
"for their outstanding achievement in the development of direct methods for the determination of crystal structures".

*Plasma's and laser fusion (table2)*

Here we list lines of activities with separate organizational schemes, but with closely related subjects plasma research in Astrophysics and plasma research related to laser fusion. The activities in both fields have continued almost throughout the existence of CECAM.

Table 2
PLASMAS, LAZER FUSION

P73, P74, W75 Atom-electron collis, energy transfor (Asytrophys.)
P75-W76 UV spectra of hot dense plasmas

| | | |
|---|---|---|
| | P75 | MHD applied to active phen. On the sun |
| | W76 | Plasma physics on the sun |
| P77 | | Transport phenomena in laser fusion plasmas |
| W78 | | Transport in laser fusion |
| | W79 | Solar flare physics |
| W79 | | Fast electrons in laser fusion plasmas |
| P80 | | Laser-plasma interactions |
| P80 | | Heavy ion fusion |
| W81 | | Laser fusion plasmas |
| W82 | | Flux limiter & heat flow instab. |
| W83 | | Laser fusion plasmas |
| | P83 | Energy part it-in astrophys. plasmas |
| | W84 | Radiative prop. of hot dense matter |
| W84 | | Interact. & transp. in laser plasma int. |
| | W84 | Energy conv. in active astrophys. plasma |
| W85 | | Interaction & transp. in laser plasmas |
| | P85 | Non-linear methods in astrophysics |
| W86 | | Int. & transp. in laser plasma |
| P87 | | Int., transp. & hydrodyn |
| | P87 | Non-linear MHD in stellar atmosphere |
| W88 | | Rayleigh-Taylor instab. In laser plasmas |
| | W88 | Photoabsorption by astrophys. Plasmas |

Important and substantial activity
in the filed of laser fusion;
rather isolated in CECAM

*Quantum mechanics in chemistry and solid state physics including the study of excited states (table 3)*

While quantum-chemical methods were central to CECAM's activities in the beginning years, and many individual visits were devoted to such topics in the early seventies, the importance of quantum mechanics for small molecules has declines. In the course of the years interest shifted to larger and more complex systems ("mesoscropic systems") and CECAM activities have covered a wide field of topics, particularly on the new methods, as soon as they became available. It seems that a number of "subcultures" exist that not even CECAM is able to unite. Putting related topics on one list, as in table 3, does not mean that everyone agrees on what the best method is for certain class of problems, and there still is important work ahead for CECAM in the future.

Table 3

QUANTUM MECHANICS IN CHEMISTRY AND SOLID STATE PHYSICS,
INCLUDING THE STUDY OF EXCITED STATES

| | | |
|---|---|---|
| | <73 | Main activity by many individual visits |
| | M73 | Many-electron interactions in solids |
| | M74 | Ab-initio one-electron potentials for solids |
| → | W75 | Local potential methods |
| | P77 | Electron-phonon interactions |
| | P77 | Inner shell excitations in atoms, molecules and solids |
| | P77 | Electronic str. of actinides and lanthanides |
| | W78 | Selective exc. of atoms and molecules by laser |
| | W78 | Inner shell excitations |
| | W78 | Many body problems in actinides and lanthanides |
| | P79 | Correlation energy on ground state of polymers |
| | P79 | New models for intermol-interacctions |
| | P79 | Photoionization of small molecules |
| | P79 | Ployatomic photoionization |
| | W80 | Laser excit and dyn. of high excited polyatomics |
| | W80 | Intermolcular potentials |
| → | P80 | Generator coordinate methods |
| | W81 | Correlation energy on ground state of polymers |
| | P81 | Ab initio calc. of phonon spectra |
| | P82 | Electron correlation in molecules and solids |
| | P82 | Force fields in transition metals |
| → | P82 | Monte Carlo methods for many fermion systems |
| | W83 | Intermediate valence |
| | W83 | Interatomic potentials |
| | P86 | Atoms in strong light filed |
| | P86 | Interatomic forces in semiconductors and transition metals |
| | P87 | (idem) |
| | W88 | Semiconducto interfaces and superlattices |
| → | W88 | Spectral grid methods in QM calc. |

+several activities on surfaces
+ helium in metals

*Molecular Dynamics (table4)*

Simulation of atomic and molecular systems in the condensed phase started in 1972 at CECAM with a workshop on Molecular Dynamics and Monte Carlo methods on water. This grew out to one of the most elaborate activities of CECAM with a considerable spin-off in other areas. The 1972 workshop was also the first activity worth the name. It lasted a full two months and set an example for later workshops. It should be mentioned here that the CECAM development in molecular dynamics has depended in a critical way on the presence of Aneesur Rahman in many activities: his sincere personality and scientific depth have set an example to all. We miss him with deep sorrow.

Molecular dynamics has developed along two lines, with often different people, but never out of touch of each others the "exact" treatment of simple systems meant to test and enlarge methods of statistical mechanics, and the approximate treatment of models of the real world meant to understand and predict properties of realistic systems. Along the first lines were many activities on simple liquids, ionic liquid, stochastic dynamics and non-equilibrium behavior. There is an important spin-off toward reactions in general, where approaches from different sides have merged (see below). Along the second line, the main application area has been the study of biological macromolecules as proteins and DNA. It is not an exaggeration to say that CECAM has created the molecular dynamics of proteins, and certainly in aqueous environment. It was during a crucial workshop in 1976 on Protein Dynamics that people from very different background came together for two months. The first simulation of a protein was carried out during that workshop by Andrew McCammon, using programs already prepared in Martin Karplus's group at Harvard.

More recently two developments have taken place that we can be found in recent CECAM activities: Quantum Dynamics and Cellular Automata. After classical Hamiltonian molecular dynamics had matures and shifted from methodological development to applications, interest has grown in the study of real quantum dynamics. The methods in this field are still under development and CECAM will undoubtedly see itself involved in this process in the near future. The other development – cellular automata – makes use of extreme simplifications of interatomic interactions that allow fundamentally different computational techniques to be used. By applying proper conversation laws macroscopic propertied (as flow) can be studied on the basis of interacting particles (or lattice points) rather than on continuum differential equations such as the Navier-Stokes equations.

Table 4

MOLECULAR DYNAMICS

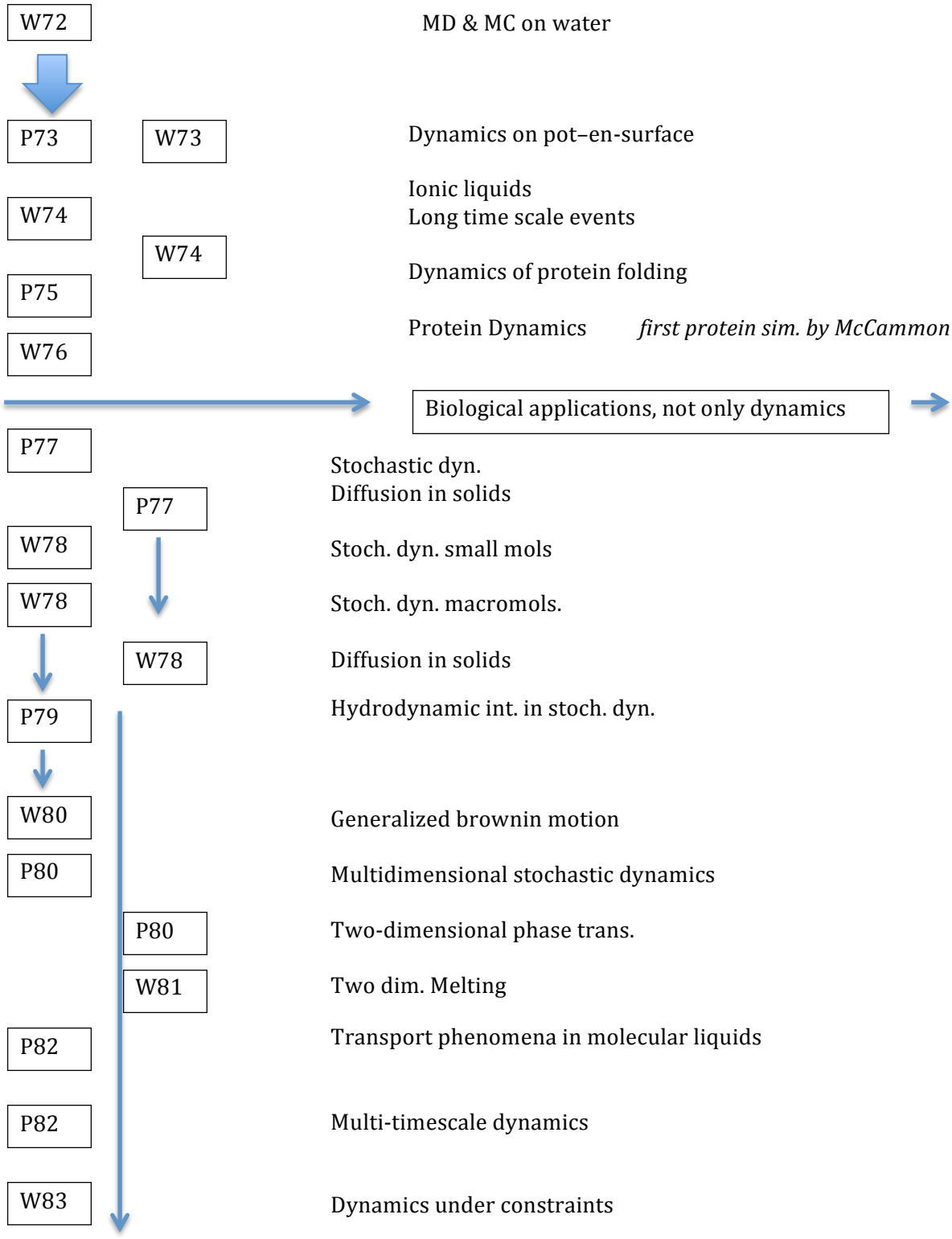
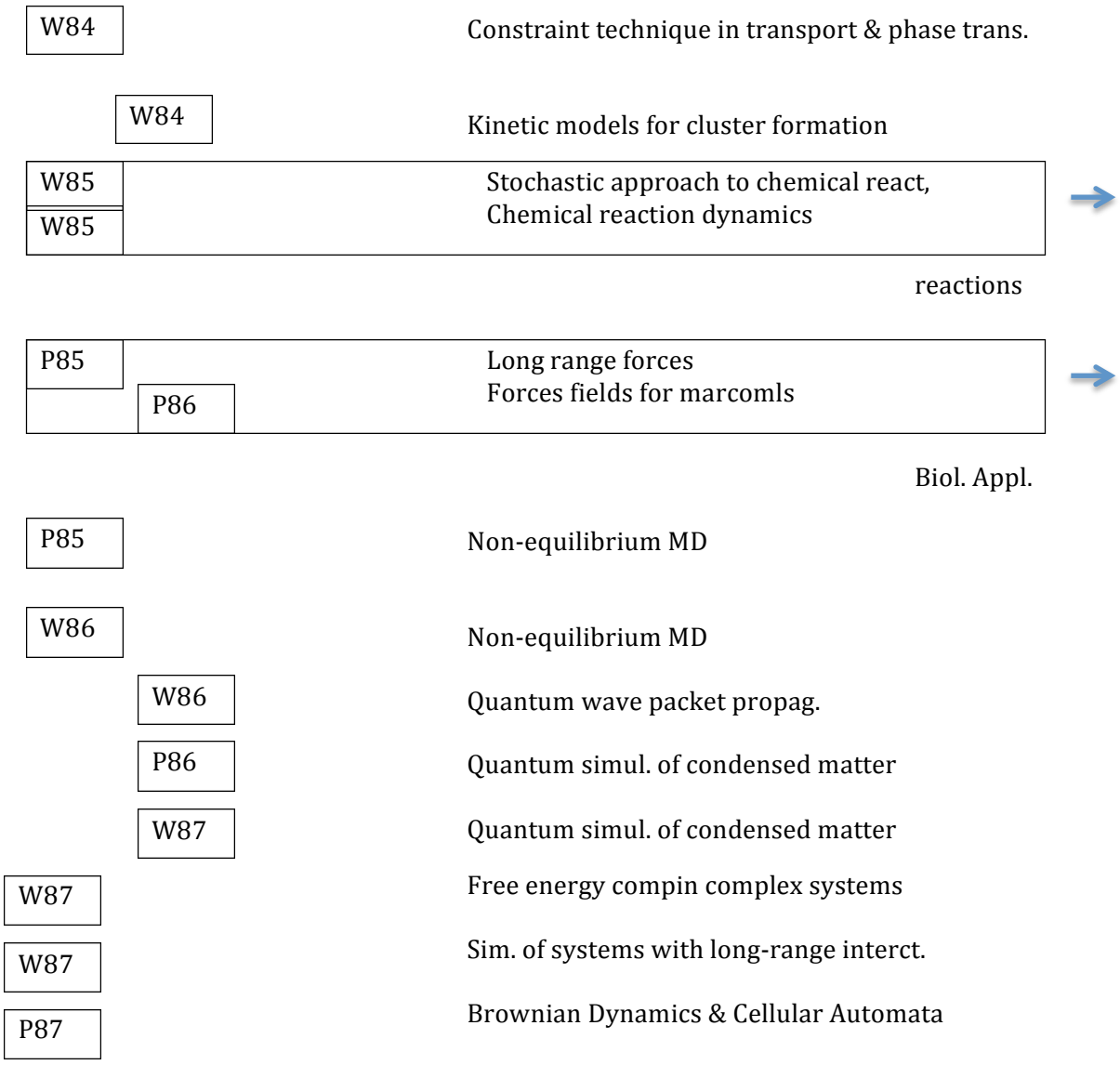


Table 4 (continued)

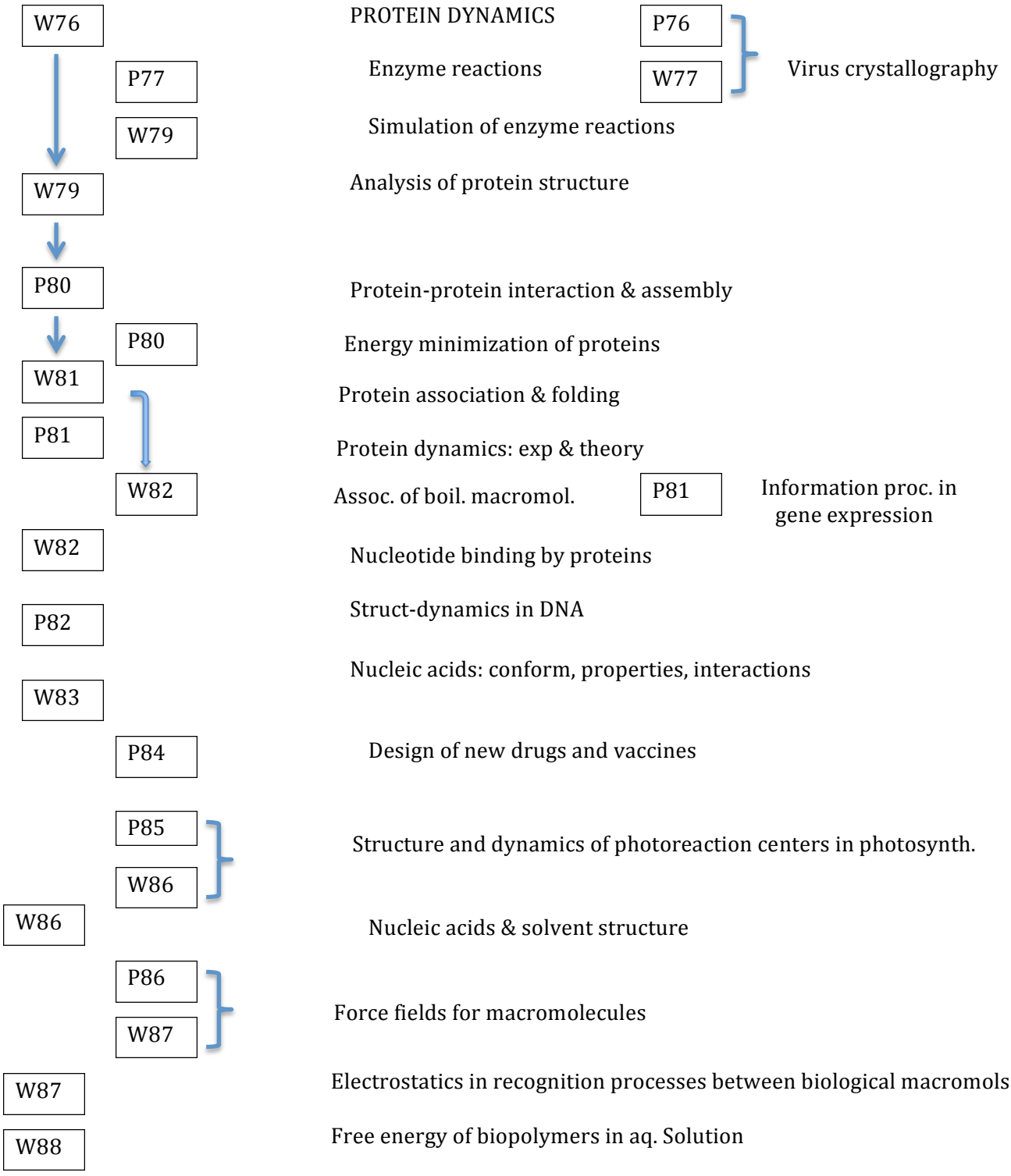


*Biological applications (table 5)*

After 1976 biological application have boomed. Not only dynamical simulations, but many questions about the relation between structure and function of biological macromolecules have been addressed at CECAM activities. The focal point was the 1976 workshop on protein dynamic, but activities diverged eater to include protein and DNA folding and association, enzyme reactions and electrostatistic fields around macromolecules. A number of discussions were held on force fields, the stumbling block for reliable simulations of complex chemical systems. The last word has certainly not been said.

Table 5

BIOLOGICAL APPLICATIONS

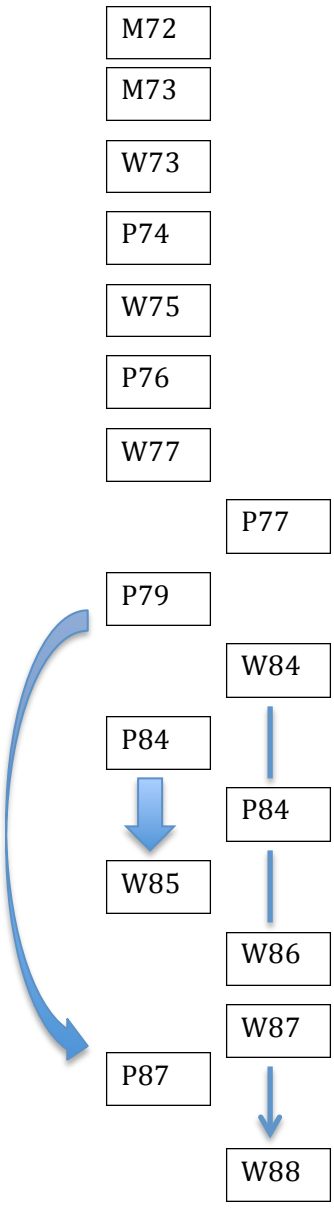


*Reaction paths and rates (table 6)*

Starting from a quantum-mechanical approach to reaction paths and mechanisms, several CECAM activities have followed on reactions. There are separate lines that were not related in organization and people: electron-molecule or atom collisions on the one hand stochastic approaches to solution reaction dynamics on the other hand. CECAM could play an important role in the future by strengthening its activities in this filed and reconciling the various approaches. Simulation of reaction dynamics is an increasingly important filed where quantum mechanics and classical mechanics, including stochastic treatments, must merge. Applications range from "simple" reactive collisions to complex catalyst and enzymes. The study of the first reactive steps in photosynthesis is one of the most challenging in the biophysical filed.

Table 6

REACTION PATHS AND RATES




Reaction paths and reaction mechanisms

Atom-electron collisions (astrophys.)

Dynamics on potential surfaces

Collisions on excited state pot. Surf.

Collisions involving excited states

Electron small mol. collisions

Electron molecule scattering

Stochastic dynamics

Decoupling meth for low energy mol. collis.

Kinetic models for cluster form.

Chemical reaction dynamics

Reaction dyn. in condensed phase

Chemical reaction dynamics

MD of chemical reaction rates

Solution phase chem. react.

Electron- molecule collision

Chem. reactions in solution

Table 6 (continued)

REACTIONS

isolated simple systems — (complex) systems in complex environment

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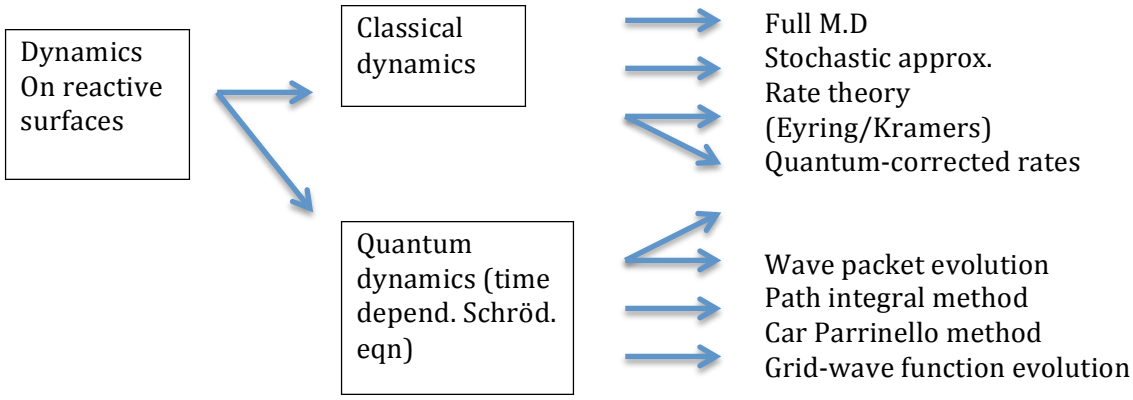
1) QU. MECH. — Reactive surf. (Schrod eqn) — Modified by environment (incl. statist. averaging) potential of mean force

2)



*A new future*

After 20 years, CECAM has established its place in computational science without doubt. It has been Carl's family, no doubt, and it has been through his stimulants and persuasion that things have happened. But he always gave the scientists the freedom the need to dream up something entirely new and then realize it too. CECAM has been a place where many of us could concentrate on science without the burden of daily duties in our own institutes. It has been the community of scientists, vigorous and competitive but open and trusting, that has made CECAM special and productive. No international meeting of any kind approaches this and achieves anything similar. I wish to thank Carl for his total commitment to CECAM over all those years and wish the new Director all the wisdom he needs to keep CECAM in shape. Let us grant him our trust.

# Lia Berendsen

Dear Carl,

I will not forget the many times you stayed in our house with our family. There was more than science! You shared our family matters with all kinds of advice, I remember, for instance, how Hermans first son-in-law was quite an item of discussion. We got many educational tip: how to treat our daughter-teenagers and how to educate our dog. The free education our dog had received must have been apparent when you took him for walks in Zuidhorm.
It is all past now, but we will keep these little events as dear memories.
With my warmest regards,
Lia Berendsen

# Franco Bassani

Scuola Normale Superiore
Piazza dei Cavalieri, 7
56100 Pisa, Italy

I was responsible for the Collaboration between the Italian C.N.R (Consiglio Nazionale delle Ricerche) and CECAM in the early seventies, and I wish to acknowledge the enormous usefulness of CECAM to the development of computational physics in Italy.

In those days everything was rather informal, as Carl Moser liked, and I am grateful for that. Decisions were often taken on the telephone, with a minimum of bureaucracy, and then approved at an official meeting in Paris, where most of the time was spent in discussing physics. And some decisions were taken. Among them, I wish to recall the decisions to support the collaboration with Andreoni, Jacucci, Resta and Ciccotti. This started the filed of electronic state calculations, model cluster calculations and lattice dynamics, and was seminal to a very fruitful research, which is still continuing today. The Italian condensed matter theorists wish to express to Carl Moser their appreciation and their thankfulness.

# Jan J.C. Mulder

Gorlaeus Lab. – University of Leiden
Leiden/ The Netherlands

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 – in fact the first calculation on the first computer at Leiden University in 1962 was a Hückel matrix diagonalisation – 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. Gunter van Sachsenberg was there too. 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 abinitio quantum-chemical calculations.

My arrival in Paris on the 1st of October led me to the Rue du Maroc, where Carl was packing. In a few days I was sharing a room in the Aimee Cotton laboratory (in the cellar) with Simone Jasper from Brussels and Marguerite Cornille who was local. It was extremely beneficiary for my French as well as most enjoyable. Together with Jim Wright, a post-doc with Lionel Salem we worked on $CH_5^+$ and $CH_5^-$ using Steven's abinitio programs that had come to Orsay from the Lipscomb group at Harvard. Eventually this led to a paper in Chem. Phys.Letters in 1970, which was probably one of the first mentioning CECAM support. It also became part of my thesis, and Carl became a member of the committee. He and I had our discussion at the public defense in French, which we found rather amusing.

In the fall of 1970 I went to IBM – San Jose on a fellowship. No doubt Carl had acted as a reference; he knew of course many people in the department of Large Scale Computations, in particular Bob Nesbet and Paul Bagus. After coming back to an associate professorship at Leiden University, it did not take me very long before I went to Orsay again. In 1972 Paul Warmer from Nijmegen and Marc van Hemert and myself from Leiden cooperated in construction CI and 4-index transformation programs to be connected to the SCF routines that we had obtained.

In the mean time CECAM had introduced the concept of the workshop and its preparatory planning meeting, which would become a corner-stone of its policy in the years to come. Participating in the three scattering workshops that were held on the summers of 1973, 1975 and 1977 has been one of the best scientific experiences that I have had. One got to know a large group of people active in that area. In particular there were Paul Brumer and Moshe Shapiro in the first workshop "Dynamics of Reactive Collisions on Potential Energy Surfaces"; then Tome George and Keiji Morokuma in the second: "Collisions on Potential Energy Surfaces of Excited States", and finally John Light and Bob Walker in the third workshop "Reactive Collisions". Furthermore I met Jonathan Cono, Eric Heller, Philip Pechukas and of course renewed my acquaintance with William Miller and William Lester. The last one I had worked for while at IBM. In 1977 we celebrated 10 years of CECSM during the first two days of September. Apparently it has always been ambiguous whether CECAM should be dated back to its birth in 1969 o to its conception in 1967.

In summer of 1979 I participated in the "Sudden Polarisation" workshop, organized by Lionel Salem. The length of the workshop had gone from two months to four weeks, but the atmosphere was pleasant as always. We had a planning meeting in Orsay in January with Martin Karplus and Koutecky's present and participating in lively discussions. During the workshop I interacted especially with Alain Sevin and Jonathan Tennyson and I wrote a paper that later

appeared in Nouv. J. de Chimie. Very appropriately it was born in Paris Café on a corner of Bd St Michel near Jardin de Luxembourg.

By far the best memories are connected to the two planning meetings that I organized in the Gorlaeus Laboratory of Leiden University during September 1976 and September 1978. The first one was concerned with the preparation of the 1977 workshop on “Reactive Collisions”, and the second tackled the difficult subject of “Transition States in Enzymatic Reactions”. On both occasions we had most enjoyable informal parties at our house.

The story continues: after a number of quiet years we meet again in 1989 to look into the 90’s after 20 years of CECAM. Moreover Joe Gerrat, another old friend from earlier days convenes a planning meeting for a workshop on Valence Bond Theory. And this we may conclude: If CECAM without Carl Moser is unavoidable, computational physics and chemistry without CECAM is unthinkable.

# Wim Nieuwpoort

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**Carl and CECAM** or how to create approximate order out of chaos.

I met Carl for the first time in 1964 ant the end of an iterative process aimed at finding integral programs running at a CDC 3600. The process had started at Philips Research in Eindhoven where as a side line to my main work I had continued developing and applying abinitio electronic structure methods that I had learned about some years earlier at Purdue, Argonne and the University of Chicago. Convergence took place after a far from monotonic path in Paris at Daudel's Centre de Mécanique Ondulatoire. There, in an unlikely street called Rue du Maroc, I found Carl. The setting was appropriate, slightly chaotic offices and people, stacks of cards and listings spreaded out over desks and tables in rooms and corridors.

Carl was busy, writing letter, talking to someone at the telephone and trying to operate a card punch by a terminal or PC, add a few Pekinese dog-like creatures and a secretary and you will agree that not much has changed in essence. Well, not quite, there is CECAM after all. Having completed my mission – worth a separate story- we stayed in contact and 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 Suttcliffe to mention a few. The reception was mixed. I remember my own reaction. As a true Dutchman I favored a careful start through bilateral cooperation, rather than an all out multilateral organization.

How he did it I do not know, but in 1968 I got word that an organization called CECAM was brought into existence under his directorship and located at Batiment 506, Campus d'Orsay. Interested scientists were invited for research stays during which they could use computational facilities of CIRCE with generous limits. Several of my students and I made use of this opportunity to do work we could not do at home and to learn about theory, methods and programs from pioneers on the filed lured by Carl (and Paris) for an extended stay. An invaluable experience! In the meantime 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 to ZWO, the Dutch science foundation. Shortly after negotiations began that led to the participation ZWO (now NWO) in CECAM, which still exists today.

The development if CECAM is fortunately not without serendipity. Personally I think that Carl attracts this phenomenon. One morning in the early seventies my colleague Groningen Herman Berendsen had talked to me about ways to solve many-body Schroedinger equations (in fact an early suggestions to approach them as diffusion equations and perhaps apply the then emerging numerical integration schemes for molecular dynamics). Quite by chance Carl came to visit me in Groningen that day when Herman came by I introduced them to each other. They talked about biomolecules, molecular dynamics and computational possibilities. And out of that grew the tremendously successful and fruitful cooperation between Carl, Herman and many others in the field of molecular dynamics that has seen so many CECAM workshops and discussion meetings since that time.

This is only one example of Carl's gift to recognize fruitful new ideas and equally important, the people that can develop them. It has always been somewhat like a mystery to me how he managed to stimulate so many different scientists in so many different fields to get together under the auspices of CECAM, often with important follow-ups. But he did ! CECAM will never be the same without him. We have seen each other more frequently in the seventies than in the eighties, but my wife and I kept the fondest recollections of our more personal meetings at our respective homes as well as at a variety of eating establishments, of Carl's choice of course! We wish him best of luck, convinced as we are that there must be a life after CECAM.

# Graham Richards

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I joined Carl Moser as a port-doc in 1965 when he was still at the Centre de Mécanique Ondulatoire Appliquée in the rue du Maroc close by the still functioning abattoir of the Villette.If CECAM was born in 1969 then the period when I was with Carl was certainly the copulation and lengthy gestation period while the embryo grew.

Already at that period I went to work with Carl because he was providing unequalled computer power at the time – on an IBM 704, soon to be replaced by a 7090. This made it the best possible location to do the then unfashionable ab initio molecular orbital calculations and Carl also not only had a copy of Bob Nesbet's program, but almost uniquely, he could enter the data (which required the use of octals and hexadecimals). Above all, however, 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; much to the benefit of myself and Goerges Verhaegen. 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. When taking Gunther for a walk his collar was tied around his middle and his rear end was held suspended by the vertical lead. 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.

As well as cheek and charm, Carl also possessed instinctive vision. Like many computational chemists I have consistently been surprised by the rate of hardware advances. So often things which I never dreamed would be done in my lifetime have come to pass a couple of years later. Carl always saw these futures quicker than anyone. By providing the best facilities he enabled many of us to forward our own scientific careers.

Now that, thanks to him, and the facilities he provided, I have moved from diatomic molecules to drugs and onto biological macromolecules and the inclusion of solvent, I still wryly remember this comment (in his inimitable French) made about colleagues who worked on what were big molecules in the 1960 "grands molécules: petits esprits".

# Mario Tosi

Physics Institute
University of Trieste
Trieste/Italy


My first contact with Carl Moser goes back to the early seventies, when I was a newly appointed professor of Solid State Physics at the University of Messina. Carl wanted at that time to stimulate the great potential usefulness of the computer in learning about many-electron interactions in the quantal electron gas and in the electron theory of metals and semiconductors, and proposed that we pull together the leading theoreticians in these areas through a CECAM Colloquium to be held in Sicily. The Colloquium, which was held in Taormina in September 1973 (see Nuovo Cimento 23B, ni1, 1974), is still memorable for lavish Sicilian hospitality that we enjoyed and for the warm discussions that enlivened it between exponents of such different theoretical viewpoints as Albert Overhauser and Walter Kohn, rather than for the computer work that it inspired in the immediate sequel. Of course innumerable developments started to take place somewhat later, culminating in the work of Ceperley and Alder on the phase diagram of the degenerate electron gas and more recently in the Car-Parrinello method.

My further professional relations with Carl in the seventies again bear witness to the fact that his ideas for new areas to be stimulated through CECAM's activities have consistently run at the forefront of things. These concerned preparatory symposia on computer simulation of structure, dynamics and transport in molten salts and on computer simulation, with great enjoyment of us theoreticians.

My contacts with Carl have faded in the eighties. I think of him from the seventies as an exquisite gentleman and friend with a warm concern to bring the Italian scientific community into the activities of CECAM, in the midst of the administrative vagaries of the Consiglio Nazionale delle Ricerche. I feel that our national community owes him a great deal and wish him all the best in his retirement.

# Wanda Andreoni

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My recollection goes back to April 4, 1974, the day when I first landed at CECAM while an enormous crowd in Paris was accompanying Pompidou to his last home. I was enormously disappointed when, instead of a big center full of computers and people that I expected, I realized that CECAM was only a corridor with offices mostly empty, and more densely populated with dogs than scientists. Clearly this was NOT the ideal place where to go work after my studies at the University of Rome where the distinction between colleagues and friends did not exist, and after a whole long life-time spent in the warm protecting ambiance of my wonderful family: away from Paris, away from the main life-center of the Université d'Orsay, directed by the most peculiar fellow I had ever met, who seemed to be more interested in his odd little dogs than in the progress of my research.

For months I has as only creature to love "the program" I was working on. Nevertheless, I kept waking up at 6am (a habit that left me for good only a few days later), running to the train and to the navette which would take me to Orsay-Plateau, where only after passing my deck of cards on the computer-reader, I would finally have breakfast at the small nice café of the unforgettable Mme Clouzeaux.

It was only after some time that some people started to enter my lonely daily life. I remember Pino Suffritti who was always fascinated by his "rotating" molecules and cooked very good "risotto" to make me feel better sometimes, Girolamo ??? who used to listen for hours my complaints about CECAM (with sympathy) and to my enthusiasm (not shared) about Wannier functions. M. Rao who introduced me to the Kohn method for Wannier functions, to the computer program, and also started to illuminate me about the mystery of some strange character going around the place, Giovanni Ciccotti who, expected by several people with curiosity and/or suspicion, after some time spent exclusively to work hard on his mathematics in orthogonality with the whole world around him, started to show his pleasant human side. I remember in particular how enthusiastic he became about the power of the computer and how we all shared his happiness about the success of his work.

Later that summer, there started to be sunshine again: Walter Kohn came and taught me a number of things, giving also meaning to my solitary work on Wannier function. Smiles also came my way from the Director, owing to the presence of Walter Kohn and also the birth of a few more dogs in his family. From that time on, life went on essentially fighting on two fronts: with the computer on one side and with the Director on the other. The former struggle brought me victory and satisfaction at the end. The latter aimed to convince the Director of my value, cost me a lot of energy and surely I was defeated. But… how can you give eyes to somebody who is blinded by congenital misogynism?

At the same time I enjoyed the company of my Italian friends and the contact with several people who were visiting CECAM especially at the time of workshops (Art Williams, Mario Raimondi, Werner Hanke, to mention some of them).

It was at CECAM that I first learned (in a probably too-harsh way) a number of things which turned out to be useful for making me stronger in confronting my subsequent life in the physics community. I learned that even on our wonderful world of Science, success is not reserved to great scientist.

Unfortunately, also mediocre people who know how to steal ideas and profit from the naivety of good colleagues, may become famous and respected. This was a shock to me, and I was only in part consoled by the fact that some great scientist I met there were also nice people. I learned that even for good and honest scientist, character is as important as knowledge and ability to help you survive in the jungle.

At CECAM I worked alone most of the time, apart from the rare and beautiful moments I spent with W. Kohn. I learned that, although it is important to struggle alone with problems, it is not so good for your own education to have so little opportunity to collaborate with others as was my case. This was the reason why after, two years, (in May 76) I definitively left CECAM taking back huge piles of punched cards, with the help of the indefectible Mme. Calvié, and joined with enthusiasm again the group in Rome.

At CECAM I also learned how to use an IBM machine: something that I soon forgot, but one day, 10 years later, this past experience of my youth turned out to be useful. In My ’86 I started to use again MVS system!

# Simon De Leeuv

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The first CECAM workshop, in which I participated, was organized by K. Singer in 1974. The subject was "Computer simulation of Ionic Liquids". I still remember this workshop as a very successful meeting. What struck me most at the time was the intensive interaction between various participants of the workshop, which made scientific progress almost inevitable. I believe this workshop was one of the most successful in CECAM's 20 years of existence. A short list (from personal memory) of scientific contributions arising from this workshop:

1. Calculation of transport coefficients and response functions with applied field simulations using subtractions techniques.
2. Development of Brownian or stochastic dynamics.
3. Molecular dynamics simulations of polarizable ions using the shell model.
4.

These contributions have made a lasting impact on the art of computer simulations and the techniques developed here are widely used today by practitioners in the filed. The subtraction technique, for example, has recently been applied to the calculation of the electron mobility in quantum molecular dynamics simulations.

The format of the CECAM workshops lasted for 6 weeks or so and the actual computing was done on machines available at the computing center in Orsay. For someone like me, just entering the filed, this was an ideal opportunity to learn. Other participants were generally very helpful. In particular I would like to mention A. Rahman and K. Singer, who always shared their insight and ideas with other participants. It is precisely this interaction and exchange of ideas, which led to the success of this workshop.

Since then I have participated in a few other workshops. Nowadays the format is changed considerably, the typical length of the workshop being reduced to about two weeks. The calculations are now mostly carried out at remote sites. Nevertheless, an intensive interaction between participants is still a key ingredient to a successful workshop. This is clearly understood by Carl Moser, who stimulates this as much as possible. CECAM workshops provide the right climate for fruitful scientific cooperation. Such cooperation have often lead to significant contribution in computational science. As a result the contribution of CECAM workshops to the filed of scientific computing is much larger than the size of the organization would indicate. To a large extent it has been Carl Moser's effort over the past two decades, which made all this possible.

# Daan Frenkel

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The first time that I heard about CECAM was during a meeting on Liquids at Royal Holloway College in September 1972. Herman Berendsen had just attended the first CECAM workshop on Molecular Dynamics and at Royal Holloway he gave a talk to preach the gospel of computer simulation. After that date, I heard more and more about CECAM, but always from a distance. Until one day in April 1975, when Gianni Jacicci visited our lab in Amsterdam. Gianni gave a talk in which he explained the recently invented substractions technique. After having thus completely overwhelmed us, he enquired if any of us graduate students would be interested in working at CECAM for a few months, starting May 1st. Although I would dearly have liked to go, I knew that it was not my "turn". Other graduate students had traveled less that I, and it only seemed fair that they should have a chance to broaden their scientific horizon. To my combined amazement, joy and, in retrospect, luck, none of my fellow students was willing to lease the pleasures of Amsterdam behind for an expedition to the uncharted territory of Orsay.

Barely two weeks later I arrived at CECAM. At first, I had the naïve idea that I would meet French scientists there. This turned out to be a serious misconception: the only French citizen that I met during my stay at CECAM, was Madame Calvie. Then there was Jean-Paul Ryckaert who was, if not French, at least Francophone. And finally there was Carl Moser, who, together with his 3 dogs were the only remaining inhabitants of the CECAM premises who steadfastly refused to speak Italian. In short, CECAM, at that time, was nothing else than an Italian enclave. But 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. The atmosphere at CECAM was actually international in a second respect: the political sympathies of most of the Italian graduate students ranged from Stalinist through Maoist to anarcho-syndicalist. And nevertheless Carl managed to keep his kingdom peaceful, happy and, most surprising of all, working. This was no small achievement considering the barriers that the IBM system posed for the uninitiated: the combination of the JCL operating system with manuals in Franglais must surely have been the invention of a sick and perverted mind.

The attitude of the computer-simulators at CECAM, in particular of Giovanni Ciccotti and Gianni Jacucci, was on of exhilaration: all the hitherto abstract, concepts of statistical mechanics had come alive due to the computer, they had become computable and thereby very real. With great recklessness, Gianni Jacucci and I started writing programs to do path-integral Monte Carlo simulations of many-body systems. In one month we had tried it out on a number of "sub-trivial" systems: an ideal gas of Fermions, Bosons and Boltzmann particles, and on a linear harmonic chain. We expected to be doing quantum dynamics in another month or two. Carl was more realistic: he was keenly interested in what we were doing but, at the same time said: "By all means, go ahead. And, as soon as you can compute the attractive well of a pair of He atoms, let me know…"

I have returned to CECAM many times since, and I have always enjoyed the opportunity to interact with many of the best computer-simulators in an atmosphere of structured chaos. 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 lists of names, and count the number of European scientists who, effectively, started their computational cork at CECAM. Then the picture becomes very clear.

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In the late sixties, at the time when Carl Moser created CECAM, Loup VERLET was the dominant figure in Europe in the filed of Statistical Mechanics simulations. At that time VERLET headed a small group at the Theoretical Physics Laboratory on the lower past of the Orsay campus, and he was also in Charge of the Orsay University Computing Center, which was equipped with UNIVAC computers, against CIRCE's IBM machines. Around 1970 the group hosted several leading foreign colleagues, including Berni ALDER, Mal Kalos, Ian McDONALD, Anees RAHMAN and John VALLEAU. Trouble began when CECAM started a series of workshops devotes to Molecular Dynamics and Monte Carlo simulations, attracting much the same people. It is fair to say that the VERLET group and CECAM superbly ignored each other, partly due to personal incompatibilities and to the orthogonality of the IBM and INIVAC computer worlds. The story went that it was cheaper for some American colleagues to fly from the UD to have free access to the CIRCE computers rather than to pay for domestic computing time! In any case we were genuinely disappointed to receive less frequent visits from our friends who were very busy at workshops "sur le plateau". The "conflict" culminated in a somewhat painful climax when some CECAM workshop participants published a paper based on a Molecular Dynamics code entirely developed by the VERLET school, and forgot to include the person responsible for the code in the list of authors.

Despite repeated invitations from Carl, no member of the VERLET team ever attended a CECAM workshop (despite geographic proximity!) as long as LOUP led the group. After 1975 VERLET gradually left the filed of Physics to explore other domains of research, Dominique Levesque and Jen-Jacques WEIS carried on in Orsay, while Jen-Pierre HANSEN started a new group at Pierre et Marie Curie University in Paris-Jussieu. As more and more faces showed up at CECAM workshops, relations gradually warmed up. Complete reconciliation came after the time of the meeting in memory of Anees RAHMAN which took place in September 1987. We had no difficulty convincing Loup VERLET to attend the meeting in honor of his old friend, and Loup gave a very remarkable talk about the origins of molecular Dynamics, of which Anees, Berni and himself had been the pioneers. Since that time CECAM workshop participants could easily come across members od the VERLET team inside CIRCE building and even inside Carl Moser's office! This habit will certainly continue under Carl's successor Giovanni CICCOTTI. "Tout est bien qui finit bien".

# Antonio Lagana

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The first time I visited CECAM was in June 1975 during the three month long workshop on the "Dynamics on electronic excited states". The workshop was my first real impact with the world of the theory of reactive scattering. Since then I went back to CECAM many times away finding the same stimulating scientific environment.

At the time of the workshop, I had just been hired (my first full time job at the University started on April 75) by the Department of Chemistry of the University of Perugia. Because of my previous experience in computing and in (approximate) adinitio calculations my job was to carry out calculations useful for the interpretation of scattering experiments performed at the "Dynamics of elementary chemical progresses" group of Perugia. These experiments were dealing with atom-ion charge transfer processes and rare gases elastic scattering collisions.

Participating to the workshop was like splashing down into the rapidly growing filed of numerical applications to the solution of the equations governing the motion of heavy particles on accurate or model potential energy surfaces. At the workshop, there were every day exciting discussions on the most appropriate ways for implementing related quantum, classical and semiclassical numerical procedures on available mainframes.

We were still working on cards. Therefore discussions were followed by lengthy sessions in the punching room rythmed by the card feeder noise. The purpose was to write programs and collect numerical evidence for the discussed problems. The few available video terminals were dedicated to supply on line information on the job situation. After running the jobs (sometimes till very late in the night) and collecting results preliminary subgroup discussions were taking place at dinner to make ready the ammunitions for the next day discussion.

The workshop, however was not only that. It was for most of us invaluable school on how to get equipped for working in an international research context. Having no idea about what the workshop was, I still remember arriving at CECAM (carrying tow heavy cases) and asking Carl what to do. The answer was "Now go to Paris and get an accommodation. Tomorrow come back and bring interesting problems". I was very lucky to find a nice accommodation in one of the "Maisons" inside the "Cité Universitaire" I was even luckier to meet the following day a lot of people proposing several problems related to the different theoretical approaches to the scattering dynamics. All those problems were interesting and motivated by recent literature. Yet, not only problems. Those people were brilliant scientist and truly motivated investigators having all the qualities of a distinct theorist. Just to mention few of them: Carl was always suggesting to look ahead for new scientific targets, Michael Baer was always having an additional question (and very often disagreeing with the given answer), Keiji Morokuma was always improving the computational strategy of his computer codes, Bill Lester was always launching new ideas, Paolo Palmieri was always able to reconcile different new points of view into a more general design.

And more than that, I met also good friends. Sharing day by day the same life as well as the same work during say-time, continuing quite often the discussion in the evening at a Chinese or Greek restaurant, wandering around the several cosmopolitan corners of Paris made all of us enjoy unforgettable common experience and build up a long-lasting friendship.

# Ian McDonald

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It was my great good fortune to be associated with the first two CECAM workshops to be devoted to molecular dynamics and Monte Carlo simulation. These were the meetings on water in 1972, organized by Herman Berendsen, and that on ionic liquids in 1974, organized by Konrad Singer. At least insofar as developments in Europe are concerned, the importance of these two events in establishing the status of simulation as a legitimate scientific tool can scarcely be overstated. They were also the first of a long series of similar workshops, covering all aspects of molecular simulation, and CECAM meetings in this filed have become a more-than-annual event. Both workshops were organized by chemists, and the attitude that dominated was one that saw computer simulation as providing a unique method of probing the microscopic behavior of real (and therefore complicated) systems. The workshop on water was directly inspired by the famous paper of Rahman and Stillinger (A. Rahman and F.H. Stillinger, "Moleccular Dynamics Study of Liquid Water, "J.Chem. Phys., 53, 3336, 1971), which had appeared less than a year earlier. Anees Rahman was, of course, a participant in the workshop and, indeed, in one on ionic liquids, and much of what I remember of the proceedings is colored by memories of that remarkable man. I worked with Anees during both workshops and I am proud that some of the work we did together on ionic polarization, in collaboration with Gianni Jacuccim was later published in Physical Review. Anees' skill at turning scientific ideas into computer code was unsurpassed. It must be said, however, that he would undoubtedly have failed to satisfy most teachers of computer science: his programs were about as unstructured as one could imagine, the use of subroutines was considered a luxury, and he had apparently never heard of comment lines!

It easy to forget that to many people the Rahman-Stillinger work appeared at the time to be hopelessly overambitious, but molecular dynamics calculations on complex systems now appear almost daily, with applications in biology, engineering and applied science, as well as in pure physics and chemistry. I still have my copy of the report we prepared on the progress that was made during the workshop on water. This has as its frontispiece a copy of one of Herman Berendsen's very elegant figures, in which he sketched out the way in which he believed the simulation would progress particularly in areas near to his own heart, notably the structure and dynamics of systems of biological interest. This figure was the main item in a talk that Herman gave during the workshop to what, I suspect, was a somewhat skeptical audience. I seem to remember the same figure appearing at several of Herman's talks in later years, which perhaps indicated that things did not move quite as fast as he had hoped. How the situation changed! Now, almost every problem touched upon in Herman's figure (nucleic acids, proteins in solution, chemical reactions, and so on) has been treated by simulation with some measure of success, success often triggered by discussions at subsequent workshops and helped along by the many long-lasting scientific collaborations that CECAM meetings have engendered. This is as good an example as I can find of the outstanding role that CECAM has played in the past twenty years. Looking back over that period, Carl Moser has every right to feel proud of his creation.

# Jean-Paul Ryckaert

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## Child of CECAM

How could I possibly deny that CECAM and its living incarnation, I mean its Director for more than 20 years, have not affected my scientific career? With the retirement of Carl Moser, I realize today how closely my scientific childhood has been associated with CECAM. In a way, I am a child of CECAM: what follows should convince you!

Back from Orsay where he attended the 1972 workshop on water organized by Herman Berendsen and where he had met Anees Rahman, André Bellemans suggested to the freshly graduate student that I was, a PhD subject on the equation of state of normal alkanes. The proposed tool was a molecular dynamics simulation technique which had proven to be so much successful for water. The chain model would be a set of Lennard-Jones beads modeling methyl or methylene groups connected by rigid bonds and rigid bonds and rigid bending angles.

The next day, John Orban of our department, offered to help me as I had absolutely no experience with computers. IN front of me, in just a couple of hours he wrote a MD Fortran program on chains modeled as Lennard-Jones beads connected by harmonic springs. Convinced that both Fortran and simulation were easy matters but not much convinced by the too simple classical harmonic springs, I started struggling with the derivation of the equations of motion of semi-rigid chain of arbitrary length in generalized coordinates and with its Fortman translation. At that time, a photocopy of the 1971 paper of Stillinger and Rahman, the book of Flory on Chain Molecules and the book of Goldstein on Mechanics were lying permanently on my table.

In 1974, a CECAM workshop on long-time events was organized by Herman Berendsen for a period of 6 weeks (!). Thanks to the impossibility of my supervisor to leave Brussels for such a long time, he went to Orsay only for the first few days of the workshop while I was invited to replace him for the full period. On that occasion, for the first time I presented some preliminary results on liquid n-butane obtained with semi-rigid model allowing for conformational changes. Quite naturally, the program had been written in generalized coordinates and was based on the Gear integration algorithm. A discussion followed in which it appeared useful, when going to longer chains, to adopt a Cartesian coordinates approach and incorporate constraint forces explicitly. Suggestions about how to evaluate the magnitude of these forces which were supposed to act along the bonds were made, and this helped John and myself to make progress. At the end of the workshop, a MD program of alkanes with rigid bonds and rigid bending angles was working in Cartesian coordinates: it was thus possible to treat longer chains: we selected decane. At the final dinner of the workshop, which took place in a Chinese restaurant, I was seated quite timidly at the end of the table and the discussions were going on quite smoothly. We were having our dessert when a fellow, who had just arrived in Paris to participate to the workshop on molten salts starting the following week, entered to the restaurant and joined us. The center of animation moved to “my” end of the table where he came to sit. I remember two uncorrelated details: I had to narrate to him my life story (fortunately I was young) and the scientific discussions we had, convinced me that he was an Ising model specialist: later I learnt that his name was Giovanni Ciccotti.

At that time, CECAM was supporting long scientific visits of young researchers. Carl Moser asked me to stay for a few months at CECAM to continue my PhD in Orsay using the computer facilities of the CIRCE, ten times more powerful than in Brussels. This was a new chance from me and in October 1974, I started a stay of nine months in Paris. During that period I met my wife in Paris, indirectly another influence of CECAM on my life!

The working conditions were quite good at CECAM: this was great punching cards period from me. We were however continuously controlled by Carl: every morning, he was informed about our computer consumption of the previous night and about the disk space we were occupying. Inevitably, he would remind us rather rudely not to save big files on the disk, not to use all the budget too fast as there would be no extra,…. To me, this was told in a French carefully colored with a non-European accent. Although three barking dogs were giving an official and executive character to these recommendations, it must be said that, of course Carl would always give you extra time if you asked for it!

CECAM was in 1976-1977 an Italian colony, contrary to a well established opinion spread in Belgium, I discovered that Italians were not all ice cream sellers, gangsters or rapers. Among these exceptions, Gianni Jaccucci and Giovanni Ciccotti were working at that time on the subtraction method. One day, probably at the CIRCE cafeteria, Giovanni started questioning me about what I was doing. As usual, after an hour of extensive and detailed explanations, he had just learned from a chemist that some molecules have more than one atom and that some of them, typically the alkanes, are partly rigid and partly flexible.

He understood what I was doing by looking later at the program and my notes: my program was using a Runge-Kutta algorithm to integrate the Cartesian equation of motion of the LJ beads subject to constraint forces. There were two reasons for the choice of this algorithm: a) the magnitude of the constraint forces were velocity dependent b) it was easier, in comparison with the Gear algorithm, to readjust the constraints empirically from time to time: the C-C bond lengths (supposed to be constant) were indeed slowly increasing with time as a result of the finite precision of the integration algorithm. A slight total energy drift, which is now known to be usual with such algorithm, was worrying me at that time. Giovanni declared that I was a “pig” and a “cook” (this was unfair as the same method would be published by another group more than ten years later in the Journal of Chemical Physics): first, he said, I should know that mechanics is a well founded theory: 200 years ago, the Cartesian equations of motion of a set of interacting point-masses subject to arbitrary holonomic constraints were derived by Lagrange they are now baring his name under the denomination “Lagrange equations of the first kind”. Second, computer simulation is a statistical mechanics method and is not a recipe which can be adjusted according to your taste!

In Groningen, H. Berendsen was thinking of the application of the same kind of technique to incorporate bond constraints in proteins. While in CECAM, Giovanni and myself were filling pages of calculations to derive the explicit dependence of the Lagrange multipliers on the positions and velocities for most general molecule, subject to the most general constraint, to be applied to the most general numerical integration algorithm, Herman, who was probably too busy to do explicit calculations, treated the Lagrange multipliers as ad-hoc parameters in the simple Verlet algorithm! These parameters would simply be determined by imposing that the bond constraints would be satisfied exactly at the next time step. This procedure was extremely simple for a diatomic but was leading to horrible coupled non-linear algebraic equations for any other molecule. So, Herman decided that a protein with bond constraints was just interconnected diatomics and bypassed the problem by iteratively treating each bond in succession, and this for about ten to twenty times: SHAKE was born. Being in contact with him, we stopped our calculations and tried another more classical interative technique. To Herman’s relief, tests on decane indicated that SHAKE was converging to the right solution and, moreover, we were able to show theoretically that the replacement of the Lagrange multiplier by ad-hoc parameters was not affecting the Verlet algorithm precision! We then decided to combine everything in a single paper [1] which, although much referenced, should be even more referenced in pedagogical science as an example of what style to avoid when writing scientific papers.

[1] J.P.Ryckaert, G. Ciccotti, H.J.C Berendsen, J. Comp. Phys. (1977), 23, 327

# Konrad Singer

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At the time of the foundation of CECAM many onlookers may – like me – have expected that this was to be a center where scientists interested in quantum chemical calculations would hold meetings or work individually. In the 21 years of it's life CECAM has been a unique center from which advances in a wide range of topics in theoretical physics, chemistry, materials – and computer science have originated.

This is the merit of its first director.

Short meetings on relatively narrow topics are often called "workshops", although they amount to no more than the presentation and brief discussion of papers.

The CECAM concept of a workshop was different: a fairly small number of scientists should meet to interact and work intensively on problems where significant progress depended on innovative thought. The close contact of leaders in the field with young scientists would make it likely, if not certain, that advances would be made and that participants would learn a great deal from each other. They were true workshops.

Essential ingredients helped the realization of this idea: Through his remarkable intelligence network in American and European laboratories Carl Moser pinpointed promising topics: preliminary meetings decided whether a useful (but not narrowly defined) program for a workshop would emerge: and the collaboration of Carl with the organizer(s)led to the smooth day-to-day running of the workshop.

There cannot have been many similar successful scientist enterprises in the last few decades.

Carl Moser deserves credit and the gratitude of the (scientific) community for this achievement. Many colleagues helped to make the CECAM venture a success.

In the filed of computer simulation there are two "founding fathers" who deserve special mention:

- Aneesur Rahman was "the soul" of workshops which he attended; anyone coming into contact with him benefitted as a scientist and probably as a human being.
- Herman Berendsen's scientific judgment and energy has been a pillar of CECAM from its beginnings until now.
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Let us hope that CECAM will continue to prosper on the foundations laid by Carl Moser.

# Giuseppe Suffritti

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When I went in Paris to work at CECAM in 1974, I was just at the beginning of my research career. It seemed to me a good opportunity for developing my work about lattice dynamics to have a “large” (3 MB storage!) computer available, but later it resulted that life at CECAM would be unexpectedly fruitful. During the year I spent in Paris, I met many other workers, and the friendly team led by Dr. Moser gave good opportunities to promote contacts, collaborations and discussions.

Dr. Moser encouraged the visitors on their own work and introduced them to the academic French world. The frequent workshops stimulated interest and knowledge in the fields connected with my work, opening new perspectives of investigation.

In particular, I discovered Molecular Dynamics, that was practiced in that period by G. Ciccotti, J.P Ryckaert, A. Tenenbaum, G. Jacucci and A. Rahman, and which eventually has become my research field. Ina a word, my stay at CECAM was a fruitful and pleasant piece of my life shared between the green plateau in Orsay and a microscopic and doubtful “studio” in Rue St. Sulpice in Paris.

# Alexander Tenenbaum

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In the early spring 1974 I met again Giovanni Ciccotti, whom I knew since the years of my study at the University of Rome, at a congress of condensed matter physics in Bologna. He told me of his recent experience at CECAM in Paris, where he had joined Gianni Jacucci (also and old friend of mine) a few weeks earlier; he was learning the molecular dynamics technique and leading gipsy-like life.

At that time I was working at the Physics Institute of the University of Padua; I had just finished a work on conformational transitions in macromolecules, where I had been confronted with the limits of a purely analytical approach in studying complex structures. Therefore, the proposal to join Gianni and Giovanni and learn the techniques of computer experiments attracted me immediately. In a short time they arranged things with CECAM and already in April I moved to Paris, participation in the "Italian connection" of numeric simulation. Carl Moser (and his dogs) received me very friendly and helped making the transition to the new work rapid and smooth.

Gianni and Giovanni were applying molecular dynamics to liquids, so I was "assigned" to solids. This new line of research was indeed born under the mark of collaboration between CECAM and the Section de Recherches de Métallurgie Physique (CEN-Saclay); the head of the latter. Yves Addam very soon recognized the power of the simulation techniques for tackling the complicated special dynamical structures encountered in physical metallurgy. In this work I collaborated with Gianni and Roger Taylor – who visited CECAM from NCR (Ottawa) -, with Yves Adda and Nguyen Van Doan, also of the SRMP.

During the first months I lived with my two friends on the ground floor of a nice small villa in Sevres, with a lovely garden. Above us lived Madame Hirovo, a kind old Russian lady and owner of the villa. She used to involve me in long discussions about golden age of the tsars, but I am afraid she didn't feel very happy about my response to her arguments. In October 1974 Sylvia, my wife–to –be, moved to Paris and we took an apartment in the 14$^{th}$ arrondissement, a nice quarter and at one end of the ligne de Sceaux, the railway connecting Paris to Orsay. In the following years, when we went again to Paris, we always looked for some place in the same quarter.

Altogether, I spent between 1974 and 1979 about three years at CECAM, much of this time was a common venture with the SRMP, where interest in the simulation of material was always alive. I worked on point defects and on low energy radiation damage in metals; later I collaborated with Giovanni Ciccotti in elaborating new non-equilibrium molecular dynamics methods. I profited from contacts with many of the visitors of CECAM. I remember here only Charles Bennett, Bill Kerr and, with particular gratitude, Anees Rahman.

Those years were demanding and rewarding and life didn't lack charm. I remind that we used to work from time to time during the whole night, when the big computer at our disposal was almost empty and we could perform in one night a work which would otherwise have requested a week. I remember, coming back to Paris with a very early train, that a red and violet band broadened the bottom of the dark sky, announcing the incoming dawn. The roofs of the little houses bordering the railway drew a sharp black zigzag profile on that vivid strip.

We enjoyed several times parties at Carl's home and, a couple of years later after we left Paris, he visited us in our home in Padua. Carl appreciated Sylvia's aubergine dish (melanzane alla parmigiana) to the point that he warmly suggested to abandon her University career in order to open a Restaurant…

The time I spent in Paris has been very important in the development of my professional profile. I became a “simulator” at a time when the question whether this kind of research could be a general purpose tool was still controversial.

Things are nowadays quite different, and computer experiments have been widely recognized as an important branch of physics. CECAM and Carl Moser have definitely given an important contribution to this positive evolution.

# Pierre Turq

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I was an isolated postdoctoral student lost in an experimental lab, without any connection with a modern laboratory in the field of computational statistical mechanics, having no possibility to go abroad. I entered in relation with CECAM and my scientific life changed:
All top level scientists in my filed were reachable for some moths each year, at car distances.

As an example of such possibilities let me just recall briefly my encounter with Giovanni Ciccotti. It was at one of the parties organized by Carl Moser. We were both looking for rare things: cheese, ham and the rarest occurring event in a free seat. By chance I won the competition for the seat. After the liberation advertisement: "party over", we decided to have a drink together and so started our collaboration.

Thanks will be given to CECAM and its director Carl Moser to offer us this extraordinary opportunity.

# Mike Allen

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I first visited CECAM in 1978, as a graduate student and it would be an understatement to say that this was a formative experience. I must have been the most junior and inexperienced participant in a fairly lengthy workshop- four or six weeks I think – and I had never before been amongst such a concentration of specialist in my filed, but everyone made me feel at home. I arrived eager but uncertain, learned a great deal, and left feeling that I had made a contribution, and also that the direction of my research was much more well-defined. I was fortunate to have the opportunity at that stage to spend such a period of time with colleagues from so many different countries, each one with different perspective and background. The atmosphere was stimulating, with endless informal discussion groups, seminars, visitors dropping by, and late-night sessions on the computer. And behind it all, the presence and personality of Carl Moser: welcoming, encouraging, cajoling, threatening (sometimes), and generally making sure that we continued to concentrate on the matter in hand.

I am still impressed by the organizational skills and motivation which led all these people to come together for several weeks; to sustain such an effort year after year is a remarkable feat. I returned several times in the following decade, indeed I seized every opportunity I could to visit CECAM and benefit from its unique qualities. These later trips were shorter and more structured, but the workshop format suited me and provided a welcome opportunity to bounce ideas around, experiment with new techniques, and keep in touch with developments elsewhere.

It goes without saying that Paris is a nice place to visit. Naturally there was a certain culture shock at first. There was the challenge of grappling with foreign language for example: I refer to IBM JCL of course, compared with which French was child's play. In any case, almost any language would do at the Cité Universitaire, and life in Paris quickly became familiar and always enjoyable. Travelling to work seemed like entering a different world: a half-hour journey on the RER from busting city to the sleepy stations of Le Guichet, followed by a brisk climb up the hill to CIRCE. There was plenty of time to meditate on the work in hand while gasping for oxygen and gulping down "un petit café" in the Cafeteria. Much of the discussion took place here, and it continued over lunch, and in the bars and restaurants in the city in the evenings. We were scientists and tourists at the same time, a very pleasant arrangement. I should pay tribute to a few of my colleagues, who toured the Latin quarter with me night after night in search of restaurants that served vegetarian food. I think that we all enjoyed these explorations, but I'm still surprised they didn't charge me for shoe leather.

I have many happy memories of my visits, but I'll just recount one incident. Giovanni Ciccotti was one of my co-participants at that first workshop in 1978. When he learned that O was from Oxford, and that my then-girlfriend Pauline was to visit me midway through, he persuaded me to ask her to buy a few books from Blackwell's on his behalf, and bring them with her. Perhaps not realizing how heavy they were she agreed, and duly turned up at the Gare du Nord, pale, tired, very late but bearing the tomes in question. I was so impressed by her fortitude, muscle development, and perhaps gullibility, that I proposed marriage during her visit, and she, obviously suffering throughout from suspension of the critical faculties, accepted. Giovanni and I are still friends, and Pauline and I are still married, and I hold CECAM in some way responsible.

For me CECAM was always about people: People meeting, talking, exchanging ideas, and opening up new research directions. The contribution of CECAM is frequently acknowledged in published papers, and the annual reports give the bare bones of CECAM's activities, but the real influence I believe is much wider and less tangible. It is a pleasure to have the opportunity to record on paper the debt I owe to CECAM, and the thanks that are due to Carl Moser for making it all possible.

# Madeleine Meyer

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A somewhat impressionistic vision of CECAM

There is, I guess, no originality in telling that for me CECAM means quite essentially CECAM workshops. My participation to these activities is rather recent and one can consider that seven years constitute a short enough period to remind easily the enthusiasm of a neophyte after the first workshop. This meeting on "dynamics of molecular liquids and other complex systems under external constraints" occurred quasi simultaneously with the beginning of my work on molecular systems. I was really delighted to discuss with other physicists sharing the same interest for these exotic systems and I remember clearly tense discussions on MD simulations at constant pressure. The invitation to this workshop was the result of prior collaborations, which were reinforced during this workshop while new ones were initiated.

On this other occasion I also met Carl Moser. Our first dialogue was mainly devoted to the management of the very precious amount of computer time allocated to the participants of the meeting. Since I was a "local" participant I had the "privilege" to know some details about the systems we were using and I thought it was normal to transmit this information to other participants. However I had underestimated the obligations Carl had thought of for me. So at the end of the workshop we had a serious discussion to decide whether or not I should have know if each participant had erased his files.

During the following workshops I was very carful and skillfully avoided this responsibility. Thus I could work without any worry about practical details. As part from this side mark I must emphasize that the participation to the workshops had a positive influence on my research since I have started new themes and efficient collaboration during this meetings. This is mainly the way through which Carl Moser as a Director of CECAM has intervened in my scientific activities. Besides that, we also had many discussions especially about one of Carl's favorite subjects namely the interest of the various computer architectures.

Finally I would also comment on the atmosphere of these meetings, which generally took place in summer during academic vacations. It was a relaxed one, quasi bucolic and this impression was reinforced by the presence of dogs frolicking in the corridors

# Vassilis Pontikis

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Le départ à la retraite de Carl Moser est, pour ceux qui ont connu le CECAM au cours de ces quinze dernières années, une occasion pour se rappeler des moments peut être décisifs dans leur carrière scientifique. Mon premier contact avec cette vénérable institution et son maitre de cérémonies remonte à 1978. Je venais de recommencer un travail de recherche après un détour par le monde français de la technologie qui pourrait se comparer à la descente d'Orphée aux enfers : plein de désillusions.

Sollicité par l'environnement et par l'envie grandissant d'aborder la science des matériaux par la simulation numérique, je tenais in premier contact avec ce que je croyais être l'endroit le plus propice pour rencontrer des spécialistes de la physique numérique. Par la suite, j'ai su que ce n'était pas faux mais cette première entrevue avec Carl Moser a été plutôt déroutante. Il m'a reçu dans ce bureau rempli de désordre, qui ne devait être rangé que par sa secrétaire lorsqu'il était malade ou absent pendant une longue période. Mon entrée fut saluée par un concert d'aboiements et quelques mises en garde maussades : je venais de heurter sans le vouloir une plante d'intérieur, envahissante et objet d'une attention dévouée de la part du locataire des lieux.

Troublé, je ne me suis vraiment rendu compte des trois petits monstres qui ont assisté à cet entretien, qu'une fois installé dans le fauteuil qu'on m'a montré du bout d'une règle. Il s'agissait de trois petits chiens, moches et rares à vous en donner des cauchemars, que tous les visiteurs du CECAM ont du avoir à leurs trousses.

Apres quelques banalités en guise de préambule, j'expliquais la raison de ma présence er subissais un interrogatoire policier détaillé. On m'a expliqué l'intérêt primordial des superordinateurs existant quelque part aux USA et ne valant rien devant la puissance de ceux qu'un scientifique digne de ce nom pourrait construire presque tout seul et avec quelques milliers de dollars seulement. Serait-je prêt à consacrer mes efforts à une telle œuvre ? Devant un scepticisme poli la tactique changea et on me demanda sur quoi bon sang aurais-je pu travailler au cours de ma thèse. J'expliquais inquiet qu'il s'agissait d'une thèse expérimentale et j'essayais de démontrer le caractère primordial du sujet. En vain, le scepticisme avait changé de coté et on accueillit toute ma prose avec un petit sourire accompagné de quelques haussements de tête significatifs. En même temps des coups de téléphone répétés et des coups d'œil discrets pour s'inquiéter de l'heure sonnaient déjà la fin de l'entretien.

Johnie Walker, le troisième petit monstre finissait d'achever son activité destructrice sur ma chaussure de gauche lorsque le jugement dernier arriva : Mon cher dit-il, vous êtes fou de vouloir vous lancer dans une telle aventure, un expérimentateur ne fera jamais un bon spécialiste de physique numérique, je vous conseille de retourner à vos occupations expérimentales.

J'ai pris congé déçu du temps ainsi perdu. Je ne pouvais alors imaginer que par la suite, je retournerais souvent au CECAM et qu'une partie des rencontres qui allaient influencer l'orientation de mes recherches allaient y avoir lieu.

Carl Moser, avec de l'esprit critique et sans hypocrisie, m'a fait part durant ces douze années, d'opinions, critiques et commentaires portants sur mes activités mais aussi sur les personnes que ces dernières m'ont amené à connaître et à fréquenter. Je pense qu'il s'est quelquefois trompé mais ce que j'ai apprécié c'est son courage de vous dire sans détour ce qu'il pensait et sa capacité de changer totalement d'attitude, sans complexes, en constatant s'être trompé.

Si d'aucuns prétendaient qu'il ne fut pas le meilleur directeur que le CECAM pouvait avoir j'observerais que si ce dernier existe ce n'est que grâce à son directeur. C'est l'avantage de l'histoire sur l'explorations inutile de que le passé aurait pu être….

# Bernard Silvi

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I began to participate to CECAM workshops very recently, maybe three years ago. However, I know Carl Moser and CECAM for a long time, since the beginning of the seventies. At that time, I was experimentalist in the filed of vibrational spectroscopy. In order to improve the assignment of my spectra, I carried out force filed calculations at CIRCE. It was the days of cards and to be efficient you had to go at the computer centre. The CIRCE users were all gathered in large rooms formed a friendly community.

The CECAM people belonged to a mostly English peaking subset of the CIRCE users. Their number was fluctuating, perhaps correlated to the weather in Ile de France. I was amazed to see so many big names of Chemical Physics crowded around the printer of the “self”, as I could recognize them thanks to the headers of their jobs.

Sometimes Carl and his dogs were here. Usually he punched two or three cards, ran a thin deck and went back to the third floor.

In the Computational Chemical Physics game, I was a Corinthian and I was very impressed to see the professionals at work. Later I shifted from experiment to Quantum Chemistry at work. Maybe this CECAM atmosphere at CIRCE was one of the reasons of this choice.

# Michiel Sprik

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I learned about CECAM during my extended period as a European postdoc in North America- After finishing my Ph.D. and leaving the Netherlands, I changed fields and lost all contact with the Dutch physics community. Having been admitted to one of the CECAM meetings meant the restoration of this contact and much more than that, since most of Europe was included now too.

In fact I have met all my European colleagues for the first time in one of those rooms in the Orsay building. In this way, CECAM was vital in my decision to return to Europe because it convinces me that there did exist an active community of computational scientists in Europe, where I could be part of and which, helpfully, would help me finding a position. I was not disappointed in this expectation and, without exaggeration, I can say that CECAM has been, and still is, very important to me.

The face of CECAM, in particular for junior scientists like me, was very much determined by the person of Carl Moser. We were somewhat in awe of him and realized, since he evidently know each and everybody, he must be the heart of the organization. Since, certainly in my own perception, the organisation and the man were almost identical, much of what I have just said about the significance of CECAM for me extends to the role of Carl Moser as well.

# Wilfred F. van Gunsteren

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For me CECAM marked a change of direction in my career, one that I have ever enjoyed since.

In the winter of 1976 I was writing my thesis concerning the nuclear quasiparticle model, when Herman Berendsen invited me to become post-doc in Groningen and to participate in the CECAM workshop on Molecular Dynamics of Proteins that was held for eight weeks from May till August 1976. Herman took me in his car and gave me a 7 hours introduction – the length of the trip from Groningen to Orsay – into biophysical chemistry. Needless to say that I enjoyed very much to be introduced to IBM job control language using French manuals. After a few days I just relied on the small card decks that were assembled and handed out by Anees Rahman for various purposes like tape reading, writing, initializing etc. This workshop was a typical CECAM one, bringing together scientists from a wide variety of areas to induce cross fertilisation. Much time was spent to understand each other's ideas and work. I still remember my admiration for Herman when he managed to understand taped English lectured of a Japanese scientist, who, while the tape was running on a small low sound quality tape recorder, gave synchronous comments in Japanese English to clarify his taped lecture. The 1976 workshop made the transition from nuclear physics to biomolecular chemistry particularly easy for me and resulted in my first paper in this area.

The location of CECAM in Orsay was a perfect one. The train rides from and to Paris enabled or rather forced participants to discussions in an informal and ad hoc manner. During 1983 Workshop on Nucleic Acid Structures and Dynamics the basic idea of refinement of protein structures by MD using 2D-NMR proton-proton NOE distance restraints came up in discussions with Rob Kaptein in the daily train trips.

For me CECAM, its Discussion Meetings and Workshops, with their atmosphere of exchange of ideas, of different fields, has been very important stimulus. Let me assure you that I look back to my various CECAM activities with very good memories.