20th Anniversary of CECAM – October 1989

Invitation letter

Dear Colleague,

C.E.C.A.M. will celebrate its 20th Anniversary of scientific activity on October 4-6 by organizing a colloquium in Orsay on **"Perspectives for Computational Science in the 1990's"**.

The format chosen for this meeting will be a series of short papers on several different fields in computational physics, chemistry and biology. About half the time will be devoted to discuss on the talks.

In order for the participants to be able to prepare their contributions to the discussion part of the meeting, abstracts of the papers will be distributed to the participants before the meeting.

A special C.E.C.A.M. report will assemble the papers presented at this colloquium and reflect the impact of the discussion.

I want to invite you to come to Orsay to participate in this meeting, which we hope will be an important stimulation to guide European action in Computational science in the coming decade. We will provide 400 Frs per day as a living expense allowance.

Please inform me as soon as possible if you will be able to attend.

Sincerely,

Carl Moser

C. E. C. A. M.

Perspectives for Computational Science in the 1990's

Preliminary Program

Seminar Room 300, Bldg. 506, Université Paris-Sud, Orsay

Wednesday, October 4

8.45 – <u>Registration</u>

9.15 – **Welcome**

9.30 – **P.G. Burke,** Belfast
> *"Electron-atom and electron-molecule computations"*

10.10 – **J.M. Launy,** Meudon
> *"Reactive scattering calculations in the gas phase"*

10.40 – Pause

11.00 – **C. Leforestier,** Orsay
> *"Grid methods for calculating accurate WF"*

11.40 – **G. Bachelet,** Trento
> *"QMC methods for calculating accurate WF"*

12.15 – Lunch

14.00 – **P. Hiberty,** Orsay
> *"New chemistry by old methods – VB revisited"*

14.40 – **G. Ciccotti,** Rome
> *"Simulation of chemical reactions in solution"*

15.20 – **B. Sutliffe,** York
> *"Parallel architecture and chemistry"*

16.10 – Pause

16.30 – **J. Harding,** Harwell
> *"Modelling of mesophysical systems"*

17.10 - * J. De Hosson, Groningen
> *"Predicting properties of materials through computer simulations"*

Thursday, October 5

9.15 – G. Parisi, Rome
> *"Building your own parallel processor"*

9.55 – D. Frenkel, Amsterdam
> *"Using cellular automata methods to solve algorithms"*

10.35 – Pause

11.00 – M. Parrinello, Trieste
> *"Simulation of electronic structure in condensed matter"*

11.40 – R. Laverie, Paris
> *"Simulation of DNA dynamics"*

12.15 – Lunch

14.00 – S. Wodak, Brussels
> *"Computer modeling for bio-technology"*

14.40 – M. Haines, London
> *"Laser-plasma simulations"*

15.20 – M. Mareschal, Brussels
> *"Microscopic vs. macroscopic representation of condensed matter"*

16.10 – Pause

16.30 – H. Heermann, Saclay
> *"New representation of fracture"*

17.10 – N. Sourlas, Paris
> *"3-D spin glasses"*

*not confirmed

Friday October 6

9.30 – **Round Table**
    *"Influence on new computer architecture from algorithmic
    needs"*
    Chairman, **W. Nieuwpoort**, Groningen.

11.00 – Pause

11.30 – Looking back over 20 years
    *"What has been the contribution of C.E.C.A.M. to
    computational science?"* **H. Berendsen**, Groningen

12.45 – Birthday Party