REPORT OF THE CECAM VISITING COMMITTEE
FOLLOWING A SITE -VISIT TO CECAM-HQ OCTOBER 27/28 2014

1. PREAMBLE

CECAM is a network comprised of HQ (EPFL Switzerland) plus 18 other nodes spanning Europe and beyond, each having a Node-Director who is a member of the CECAM Board of Directors (BOD). The CECAM Director (**Dominic J. Tildesley**) is located at HQ, with a small staff. He receives advice from a Science Advice Committee (SAC) comprised of 10 eminent scientists. The CECAM Council and its President provide oversight of the CECAM network and its activities. Members of the Council cannot be Node-Directors but represent the interests of agencies/institutions who are responsible for paying the annual membership subscription to CECAM; currently a minimum of 30,000 Euros. Each such entity can have two members (an administrator & a scientist) on the CECAM Council but only one vote.

The primary function of the CECAM-Network is to organize Workshops, Summer Schools, Tutorials, and Conferences for a clientele of researchers interested in using Computational Science to solve problems in Chemistry, Physics, Engineering, Applied Math and to some extent Biology as well as Biophysics, Biochemistry, etc. CECAM has aspirations to expand its domain of influence to embrace new and exciting areas of science. CECAM also senses a need to get involved with EU Strategy to be a voice for Computational Science.

Importantly, the small Staff at CECAM-HQ is outstanding, handling as it does all logistical issues (accommodation, travel, remunerations, etc.) associated with the CECAM activities held at HQ (EPFL), as well as those held at ETHZ, and USI-Lugano. The HQ staff is very efficient and effective and has recently been augmented to include a research scientist who acts as a Deputy Director (30% administration).

1.1 CECAM Visiting Committee

The CECAM Visiting Committee composed of the following seven people arrived at CECAM on the afternoon of October 26 and departed the morning of October 29, 2014:

Kurt Binder (Mainz)
Pablo G. Debenedetti (Princeton)
Michael L. Klein (Temple)
Nicola Marzari (EPFL)
Elisa Molinari (Modena)
Peter J. Rossky (Rice)
Marie-Christine Sawley (Intel)

1.2 Charge to the Visiting Committee:
The CECAM Council charged the Visiting Committee to deliver a thorough assessment of and give appropriate recommendations on:

- **Scientific Outputs of CECAM**
- **Added Value of CECAM to EU Computational Research**
- **HQ ⇔ Nodes Balance and CECAM's Overall Efficiency**
- **CECAM's Scientific Strategy**

1.3 Data Provided
- CECAM Self study document
- CECAM Strategic plan 2020
- Various of internal documents

1.4 Data Generated
- Survey of participants of HQ-workshops in the past year (see Appendix 1)
- Informal survey of, and meetings with, selected members of the SAC

1.5 Survey & Outcomes (See Appendix 1)
Overall the HQ participants were all very satisfied on all aspects probed by the questionnaire but responses also identified
- The costs of food at HQ events as being too high for students & postdocs

Others asked for:
- More links to experimentalists and industry

Still others asked for:
- Better interactions with the workshop host institution (EPFL)

1.6 Informal Survey of SAC
- Overall the SAC is very happy with the new CECAM Director
- The number of workshops is about right and quality is very high overall
- Some additional funding would be good for HQ and the nodes since the cost of node workshops is much greater than the amount allocated by HQ
- SAC would like to see improve links of CECAM to workshop host institutions
- SAC feels adding a few more nodes is OK
- SAC suggests monitoring node workshop conduct/quality
- Perhaps explore more innovative workshop formats

2. SCIENTIFIC OUTPUTS

The primary purpose of CECAM is advancement of the scientific enterprise in the general area of computational atomic, molecular, and materials science, and this is accomplished at a high level in a number of complementary ways.

The major emphasis of CECAM since its earliest days has been on its signature workshops. Workshops, as distinguished from mini-conferences, remain the unique product of CECAM that distinguishes its special role in the computational sciences. CECAM hosts an extremely rich program of Flagship Workshops (31 in 2013, 49 in 2014, ~ 56 anticipated in 2015) with a good balance between HQ and node-run events. The number of workshops held at nodes has increased considerably in the last few years, reaching ~ 25 planned in 2015.

The Flagship Workshop program, as well as each individual workshop, is of very high quality, with their main focus on frontier science, as it should be, and a significant effort to balance among subfields.

The following points could perhaps further improve the workshops:

- It is important to consistently refresh the topics within the CECAM domain. Hence, recruitment of a number of exploratory workshops that address new fields or new problems facing a field. Promoting submissions of such proposals could be one of the key jobs of SAC;

- The Director could actively promoting a few leading edge workshops, e.g., by inviting organizers to fast-track submission on 'urgent topics' and by actively encouraging workshops that promote interactions between subfields;

- Workshop organizers could be pressured toward maintaining a program that has ample discussion time and a forward-looking focus, rather than resembling a mini-conference in a conventional field. This notion could be incorporated into the written guidelines for workshop organizers.

The above-mentioned items are designed to help CECAM retain its pre-eminent position as a centre of cutting edge computational science. Another action that might be helpful

- Inclusion of 'discussion leaders' for workshop sessions, similar in style to the Gordon Conferences, to provide a mechanism to involve additional senior scientists in a satisfying but non-presenting role.

There is a positive opportunity to increase diversity in terms of areas and people that are involved in workshops. To this end, the Visiting Committee suggests:

- Discouraging organization of multiple workshops by the same people in close chronology (this should not be a strict rule, some of those are excellent)

- Allow for a number of non-invited participants with an active role (e.g., at least a poster, and possibly a few oral presentations)

- Promote diversity in speakers and organizers, as concerns the role of women and underrepresented minorities (an active effort identifying some targets individuals has been effective in other contexts)

- Promote an active effort aimed at a distribution of participants among universities, national laboratories/agencies, and industrial scientists.

The Committee has the distinct impression that the demand for additional workshops in the area of CECAM's expertise is saturated at the current level of ~70. Hence, any growth of CECAM activities would need to be in other areas, including tutorials and summer schools. These venues are also ideal for collaborative efforts between CECAM nodes. One area where there is opportunity might be a tutorial focusing on the needs and current uses of computational modeling in the industrial sector. Also graduate and postdoctoral students would likely flock to such an offering and would benefit a great deal from such an experience.

As CECAM has evolved to meet the needs of the community, its contributions have expanded to the sponsorship of a number of tutorials in specialized areas of computational science, as well as summer schools that allow for more depth of instruction. These venues fill a very important need in providing the specialized educational opportunities for computational scientists effectively and at a high level not accessible without this cooperative group effort. A recently introduced summer school on software engineering for computational scientists was well received and addresses a critical, but widely overlooked, topic in the training of computational scientists within traditional science departments.

The CECAM-run Electronic Structure Library website appears to be extremely valuable and such innovations deserve increased attention in the future. They will likely also contribute towards building a lively local research environment at the CECAM-HQ.

In addition to these group events, CECAM has always maintained a visitor program where scientists can spend an extended stay of a week to a few months, or more at the HQ site. The Committee recommends that the penetration of CECAM within their hosting institutions, and particularly within the EPFL, could be fruitfully increased through the expanded exposure of eminent visitors to CECAM, whether they are participants in workshops or they are longer-term scientific guests.

The committee urges CECAM to introduce a 'CECAM Lecturer' program, where, perhaps two or three times per academic year, a distinguished CECAM visitor be invited to present a public lecture at the host institution, e.g., EPFL, during his/her visit to CECAM. The format we envision is one that would be accessible to a broad group of the science and engineering

population, so that it might attract and connect with a relatively large cross-section of this potential audience. The lecture might be webcast and/or the lecturer might also visit ETHZ and/or USI-Lugano.

3. VALUE ADDED TO EUROPEAN RESEARCH

3.1 Assessment

CECAM as an Institution can pride itself of a remarkably long history in the scientific landscape of Europe, having been founded in 1969 in Orsay (Paris), moved to Lyon on the grounds of École Normale Superieure in 1994, and to Lausanne in 2008 at the École Polytechnique Federale de Lausanne.

Focusing here on the latter period from 2008-2013, the assessment on the impact that CECAM has had on European research is outstanding, supported by sheer numbers of workshops held at headquarters and the regional nodes. In total there have been 13,109 participants, of which ~25% come from outside CECAM member countries (i.e., Australia, Brazil, China, Czech Republic, Denmark, Greece, Hungary, India, Norway, Poland, Portugal, Russia, South Korea, Sweden, Turkey, US, etc.), with most notably 1712 participants from the US.

There is no doubt in the view of the committee that such activities have had and will continue to have a profound and long-lasting impact in shaping the intellectual landscape and the research efforts, first and foremost in Europe, but with worldwide resonance. It could even be stated that CECAM has the highest profile and most consistent effort worldwide in supporting Computational Science through the organization of conferences, workshops, and tutorials.

The nodal structure, started with the move of HQ to EPFL, also highlights the Institutional support and pan-European CECAM mandate.

3.2 Suggestions for the future

While the research activities have been and are accomplishing above and beyond their goals, it is notable that other opportunities are becoming worthy of consideration (or not) depending on the strategic direction that CECAM plans going forward. Directions in particular can be identified regarding the role of CECAM as a *policy maker,* and the role of CECAM as a *leading house for EU proposals,* on the broad themes of simulation and modeling. One could also add industrial engagement for simulations, and/or perhaps big-data for simulations.

CECAM as a *policy maker*:

At variance with e.g., the US, funding in Europe is largely in the hands of state-funded national agencies, or European bodies, most notably the European Commission and the European Research Panel. Interactions with those bodies have been sporadic, but an opportunity (and a threat) is arising with the recent creation of the *European Materials Modelling Council*, which already includes participants of very diverse backgrounds.

Notably, Computational Science is largely absent in the ERC and EU panel descriptors in physics, chemistry, and materials – these are essential when creating review panels for e.g., ERC or Marie-Curie grants, or address grants of a certain content to a given panel. This

under-representation makes it more difficult across the board to have Computational Science properly represented.

The intersection of Material Science with the national economies in Europe is also a relevant issue. This is one sector in which the demand for skilled computational physicists, scientists or computer science experts in parallel programming, as well as access to powerful computing facilities, will grow significantly during the next few years. Simulation as a pillar of innovation has already proved that it is a valuable component in the area of Oil/Gas exploration and the pharmaceutical industries. There are new areas that will need to gain competences and experience due to new policies, such as for example the vast domain of cosmetics, as the animal testing capacity is becoming more and more restrictive. In addition, society will need new materials for construction, battery development and power production to cite a few examples.

Some major industrial players (L'Oreal, as an example) will be looking to develop competences in areas such as soft matter modelling and biologically induced phenomena such as skin reaction. They will be looking for access to enabling technology and to relevant competences in material modelling. This could be a sizeable opportunity for CECAM groups to outsource their experience and accelerate uptake of their research and of their young graduates.

Thus there could be roles for CECAM as:

- Provider of the scientific advances and of expertise on numerical applications, as a source of new talent, and as a policy maker to sustain this effort.

- Technology partner for the enabling technology, IT, ISV, sensors, network, etc.

- Provider of new talent and the new results for industrial users needing to increase their capacity in numerical simulation to model inorganic, biology inspired or biological tissue for industrial usage.

CECAM could kick off such opportunities by for example running/producing:

- A roundtable each year inviting highly regarded representatives in each of the roles identified above.

- White papers on selected topics relevant for new industrial usage; identifying crowd funding opportunities; giving directions for new educational needs

CECAM as a *leading house for EU proposals or other crow-funded research*:
This opportunity is now at the forefront of CECAM's attention, and the proposed e-INFRA bid is a very timely and central opportunity. CECAM could play a major role both as a leading house for large EU proposals, but also very effectively propose itself as an outreach partner for education in many of the focused proposals that are submitted by the computational community in Europe every year.

Co-design or validation of new HPC architecture, both software and hardware, could be of value for technology partners on a range of issues such as capacity, resilience, flexibility and scalability characteristics based upon the demanding use cases provided by CECAM or enabled by its network; "the take it or break-it test".

- Intersect with ETP4HPC technology roadmap and identify opportunities
- The COE could be a platform for prototyping

4. BALANCE BETWEEN THE CECAM NODES AND HEADQUARTERS

The present number of CECAM nodes outside of Switzerland (18) is considerable, but not too large, and is definitely manageable. For the largest countries (Germany, France, Italy) the present distribution means roughly one CECAM node per ca. 20M people, which seems more reasonable than requesting a rule of 1 node per country.

The geographic distribution of nodes within Europe is reasonable, with the exception that countries from Scandinavia—from which large numbers of participants at CECAM events come (e.g., Sweden, Denmark)—are not represented. The same is true for Eastern Europe (e.g., Poland). We encourage CECAM to make every effort (together with local eminent scientists) to have these countries join. Should this effort lead to an increase in the number of nodes (e.g., 21 instead of the current 18 outside Switzerland), one can envision limiting the number of CECAM flagship events at these new nodes by encouraging joint organization of an event such as a tutorial or a summer school by two nodes. If one then allows a somewhat larger number of participants, it would be justified accordingly to spend additional funds on such a joint event.

Overlap between the topic of a tutorial or a summer school held at different nodes in the same year, is less critical than for workshops, given the larger fraction of local participants at tutorials or summer schools. For CECAM flagship workshops at the nodes, a proper international balance among participants is advisable, to ensure that all workshops maintain the same scientific excellence and are able to impact the frontiers of research. As with all CECAM events, it is very important that the local organizers as well as the leadership at HQ make gender diversity, industry participation, and expanding opportunities for young scientist participation a priority. This requires permanent vigilance and advocacy.

The joint decision by the CECAM Director and node directors regarding events at the nodes (e.g., defining whether a workshop is proposed to Council as a flagship or a local node event without the "CECAM label") is adequate as an organizational procedure. The use of node programmatic funds (50 K€/year) to support a strong visitor program is encouraged. Eminent scientists (especially ones from outside Europe) could be proposed to HQ as CECAM-Visitors, and perhaps visit more than one node in case of extended stays. Regardless, each node should be involved in two flagship events per year (perhaps in collaboration with another node, see above). Spending the program funds solely on local node events and/or visitors should be discouraged. Greater flexibility in assessing node

performance could be beneficial (e.g., giving more weight to the quality of events, rather than simply enforcing the 50 K €/year criterion rigidly).

The Committee applauds efforts made at several nodes to form consortia involving several universities and/or research institutes to ensure the availability of local node funds. The formation of such consortia also has the potential for strengthening existing scientific collaborations among these participating institutions, and/or creating new ones, thereby strengthening computational science activities in that region.

The nodes benefit from the CECAM-HQ by the use of the excellent CECAM website and CECAM's longstanding experience on practical matters of workshop organization. They also benefit greatly from the quality control provided by the well-established CECAM workshop review system, and the advice offered by expert reviewers to improve the scientific quality of workshops. The resulting excellent quality of CECAM flagship workshops at the nodes not only enhances their general scientific reputation, but also helps obtain the desired scientific output, such as new relevant ideas for future research.

Node directors also profit from the advice and experience of the CECAM Director. The latter also conversely profits from the advice of node directors (and the BOD), who are eminent scientists across a broad spectrum of fields. This fruitful exchange as well as input from the SAC should enable CECAM to act as a 'think tank'. In addition, some of the node directors may have contacts with industry, which are useful in establishing desirable stronger links between CECAM-HQ and industry spanning the full spectrum of CECAM activities (workshops, tutorials, summer schools, visitors). Joint efforts between nodes and HQ in applying for EU funding are also clearly worthwhile.

Given the fact that several nodes have only existed for a short period of time, it seems sensible to give the network of nodes sufficient time to develop stronger links, consolidate the focus of activities in each node, and develop more visibility. This will allow the CECAM node network to become gradually established as a vibrant center of competence for computational physics, chemistry, and biology, plus materials science, applied mathematics and engineering in Europe.

5. SCIENTIFIC STRATEGY

5.1 Planning Exercise

A planning event was held at the Lugano workshop in October 2013, involving some of the SAC members. The outcome was a vision for CECAM 2020 (see Roadmap below) plus suggestions for workshops and tutorials. Issues involving computational infrastructure were also addressed.

5.2 Scientific Roadmap for Simulation and Modeling for 2020

Key areas of focus:

- Multiscale Modeling in Materials Science

Microscopic grain boundaries, dislocation dynamics, crack propagation, tribology and lubrication**;** Soft matter and active matter

- Predictive Biology

Systems biology, computational therapeutics, long time-scale dynamics of proteins, bioinformatics, computational drug discovery

- Molecular Dynamics and Monte Carlo

The time- and length-scale problems; rare events, electronic structure for ground and excited states, beyond Born-Oppenheimer

- Computational Infrastructure

HPC computing; big data, software development, networking, training skills, security, working in PRACE

The above list is fully endorsed by the Visiting Committee but there should also be ample room for new and emerging activities.

5.3 Additional Thoughts/Suggestions

- CECAM should bridge from molecular to supramolecular – from nano scale to micron scales – to emergent phenomena – from cells to cellular tissue & immune response

- CECAM should also reach out to neuroscience & brain research, especially linking to the molecular level events and processes involved in function and diseases.

5.4 Strategy to Enhance the Brand

- There is a clear need to modestly augment the budget to better support for young participants but, how to do this? One method is to encouraging new EU members to joint the CECAM network and another is to attempt to secure funds via joint proposals

- Non-EU attendees – e.g., US - should seek support from NSF to sponsor young scientists to better access the 70+ CECAM workshops

6. ACTION ITEMS

- Introduce annual lectureship under the sponsorship of CECAM.

Aim here is to expose EPFL community to high profile participants / visitors to CECAM. One could imagine at least three lectures per year: Physical Sciences; Bio-Life Sciences; Engineering; perhaps also Applied Math and Computer/Information Sciences.

- Use the SAC to help identify 'hot' areas for 'fast track' proposals

- Work to move the 'completed' review of proposals to end of the summer.

This will make for easier planning/organization for workshop slated for the January – March window. It might also in exceptional cases allow for a possible iteration of a few rejected/marginal proposals.

- Track issues relating to the diversity of workshop participants.

This will help build ways to encourage the participation of young researchers as well as enhancing the participation rate of female scientists, which is currently around 10%. It was encouraging to see that the 2014 list of CECAM workshops indicates about 16% of the organizers were female.

- Extend the survey of past workshop participants to the 2015 workshops, schools and tutorials

The exercise will enable real time monitoring of quality/satisfaction issues, especially with regards to the enforcement of adequate discussion periods

- Visiting Committee fully endorses and encourages building on initial efforts to engage with industry

There is an excellent opportunity to capitalize on the longstanding tradition of CECAM schools and tutorials in the domain of computational science to bridge to industry.

APPENDIX 1: SURVEY OF CECAM-HQ WORKSHOP PARTICIPANTS

Thinking about the last CECAM flagship workshop that you attended

1. At the workshop did you
   - Given a presentation Y=63%/N=33%
   - Provide a poster Y=30%/N=66%
   - Lead a discussion session Y=10%/N=86%
   - Organize a workshop Y=5%/N=91%

2. Was the hotel accommodation arranged for you at the workshop of a sufficiently high standard for this type of meeting?

The accommodation provided was

1. poor
2. Below average = 2%
3. Average = 29%
4. Above average = 33%
5. Excellent = 28%

Please add a comment: 26%

3. Was the information provided in advance on the arrangements for the meeting useful?

The information provided was

1. Not helpful
2. Below the standard required
3. What I would have expected = 43%
4. Better than I would have expected =18%
5. Excellent = 29%

Please add a comment: = 6.5%

4. Was the workshop booklet of a sufficiently high standard?

The booklet was

1. Of a poor standard
2. Below average
3. What I would have expected =52%
4. Better than I would have expected =19%
5. Excellent = 18%

Please add a comment = 6.5%

5. Were the workshop facilities (lecture rooms, discussion rooms, offices, computing facilities) of a sufficiently high standard for this type of meeting?

The facilities provided were

1. Poor

2. Below average
3. Average = 27%
4. Above average = 36%
5. Excellent = 26%

Please add a comment = 8.5%

6. Was the science presented at the workshop of sufficiently high quality?

On average, the science presented was

1. Dull and pedestrian
2. Ordinary
3. Of a reasonable standard = 6%
4. Of a really good quality = 46%
5. Leading edge = 39%

Please add a comment: =9%

7. Did the meeting provide sufficient opportunity to discuss and debate important scientific issues?

At the meeting was

1. Little or no space for discussion
2. There was limited discussion after each talk = 16%
3. There was extensive discussion after each talk = 39%
4. There were separate discussion sessions = 7%
5. Important topics were extensively debated throughout the workshop = 30%

Please add a comment: = 10%

8. Did your attendance at the CECAM workshop influence your research programme after the meeting?

My attendance at the meeting

1. Had no effect on the research I am doing
2. Had a minor effect on my research = 12%
3. Triggered some interesting new approaches = 59%
4. Caused a significant shift in my thinking and approach = 12 %
5. Provide ideas that have had a major influence on my research= 8%

Please add a comment: = 6%

9. Any other comments and/or suggestions for improving CECAM Workshops?

Please add your comments/suggestions: = 27%

APPENDIX 2: EU PANEL DESCRIPTORS

Condensed Matter Physics, Chemistry, and Materials Science

PE3 Condensed Matter Physics: Structure, Electronic Properties, Fluids, Nanosciences

1 Structure of solids and liquids

2 Mechanical and acoustical properties of condensed matter

3 Thermal properties of condensed matter

4 Transport properties of condensed matter

5 Electronic properties of materials and transport

6 Lattice dynamics

7 Semiconductors, material growth, physical properties

8 Superconductivity

9 Superfluids

10 Spintronics

11 Magnetism

12 Electro-optics

13 Nanophysics: nanoelectronics, nanophotonics, nanomagnetism

14 Mesoscopic physics

15 Molecular electronics

16 Soft condensed matter (liquid crystals...)

17 Fluid dynamics (physics)

18 Statistical physics (condensed matter)

19 Phase transitions, phase equilibria

20 Biophysics

PE4 Physical And Analytical Chemical Sciences: Analytical Chemistry, Chemical Theory, Physical Chemistry/Chemical Physics

1 Physical chemistry

2 Spectroscopic and spectrometric techniques

3 Molecular architecture and Structure

4 Surface science and nanostructures

5 Analytical chemistry

6 Chemical physics

7 Chemical instrumentation

8 Electrochemistry, electrodialysis, microfluidics, sensors

9 Method development in chemistry

10 Heterogeneous catalysis

11 Physical chemistry of biological systems

12 Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions

13 Theoretical and computational chemistry

14 Radiation chemistry

15 Nuclear chemistry

16 Photochemistry

17 Corrosion

18 Characterization methods of materials

PE5 Synthetic Chemistry and Materials: Materials Synthesis, Structure-Properties Relations, Functional And Advanced Materials, Molecular Architecture, Organic Chemistry

1 Structural properties of materials

2 Solid state materials

3 Surface modification

4 Thin films

5 Ionic liquids

6 New materials: oxides, alloys, composite, organic-inorganic hybrid, nanoparticles

7 Biomaterials synthesis

8 Intelligent materials – self assembled materials

9 Environment chemistry

10 Coordination chemistry

11 Colloid chemistry

12 Biological chemistry

13 Chemistry of condensed matter

14 Homogeneous catalysis

15 Macromolecular chemistry

16 Polymer chemistry

17 Supramolecular chemistry

18 Organic chemistry

19 Molecular chemistry

20 Combinatorial chemistry