The CECAM Node at Sapienza
Supplementary Sapienza-Node Agreement

1 Purpose

This agreement between *Università degli Studi di Roma "La Sapienza", Sapienza in short,* and CECAM establishes a CECAM node within *Sapienza*. The Agreement forms a supplement to the Convention of CECAM and is subject to the provisions in that Convention. In particular, Articles 1, 4 and 5 of the Convention describe the multi-nodal structure of CECAM and define the roles of the headquarters and nodes within that structure. *Sapienza* is a Member Organisation of CECAM.

2 Duration

This Agreement will apply for the 4 years between *November 2012* and *November 2016*. During the final year of the Agreement, the CECAM Council and *Sapienza* will review it, consider any proposed modifications to its present form and agree either to extend it for a further 4 years or to terminate it.

3 Objectives of CECAM

The general purpose of CECAM is to organize and promote the range of activities listed in Article 1 of the Convention in order to enhance European cooperation in computational research in biology, chemistry, engineering and physics.

4 Objectives of Sapienza

Sapienza is a large University with sixty-six departments spanning Science, Engineering, Medicine, Law and Humanities. A significant number of them are directly involved in advanced computation, either as a basic research interest or as a tool used in a wider context. The Sapienza node is instituted with the principal aim of developing leading-edge fundamental research on advanced computational methods at national level. The node will operate in strict interaction with the other existing CECAM nodes both as concerning collaborative funding strategies and technical aspects of numerical modelling. A distinguishing mission of the node is fostering the cooperation between different fields of application of advanced numerical simulations. To this aim, beyond the Physics, the Chemistry and the Mathematics Departments that are traditionally involved in CECAM initiatives, several engineering departments will be active in the node, including Mechanical and Aerospace Engineering; Chemical Material & Environmental Engineering; Information Engineering, Electronics and Telecommunications; Computer, Control and Management Engineering; Structural and Geotechnical Engineering; Civil, Building and Environmental Engineering, Basic and Applied sciences for Engineering (SBAI); Drug Chemistry and Technology.

Typical in-house computational research interests and capabilities of *Sapienza* are as follows. Computational Condensed Matter Physics (Physics Dep., SBAI), Quantum Chemistry (Chemistry Dep, Drug Chemistry and Technology), Computational Biology & Bioinformatics (Physics Dep.), Soft Matter Physics (Physics Dep.), Computational Statistical Mechanics (Physics Dep.), Lattice Gauge Theories (Physics Dep.), Density Functional Theory (Physics Dep., SBAI), Applied

mathematics and Numerical Analysis (Mathematics Dep.), Transport Processes and Surface Engineering (Chemical material & Environmental Engineering), Electromagnetic fields (Information Engineering, Electronics and Telecommunications, SBAI), Theoretical Informatics, Information Infrastructures (Computer, Control and Management Engineering), Solid Mechanics (Structural and Geotechnical Engineering), Fluid Dynamics & Turbulence (Mechanical and Aerospace Engineering), Combustion and Aero-Space Propulsion (Mechanical and Aerospace Engineering), Geodesy and Geodynamics (Civil, Building and Environmental Engineering), Plasma Physics (SBAI), Drug Design (Drug Chemistry and Technology).

The node will organize and contribute to organize local and international workshops and discussion meetings in the diverse research topics of interest for the node. Local and international advanced schools and training will be planned in order to enlarge the community involved in advanced modelling and computation.

As for the support of computational research within a wider scientific community, the interests and capabilities of *Sapienza,* through its departments joining the initiative, concern:

The development of innovative research through international cooperation; Advanced Education and Training in the different fields involving intensive computations; Computing-software maintenance.

The infrastructure available at *Sapienza* for CECAM activities is as follows:

Administrative support will be provided by one of the joining departments. Similarly, rooms to host guests and visiting professors and seminary rooms will be available at Sapienza's departments involved in the node. Several local computer servers and small clusters are available within the different Sapienza departments and research groups that collaborate in the node initiatives.

These interests, capabilities and infrastructure are the basis for the establishment of a CECAM node within *Sapienza*.

5 The Director of Node Sapienza

The Director of *Node Sapienza* (that is, the CECAM node within *Sapienza*) will be Carlo Massimo Casciola. By this Agreement the Council of CECAM endorses this appointment, having followed the procedure for doing so laid down in paragraph 6.9(ii) of the Convention.

The duration of the appointment of the Director of *Node Sapienza* shall be a maximum of four years. In the event that the Director of *Node Sapienza* has to be replaced, *Sapienza* will identify a successor by the same procedure, and the appointment will be subject to the endorsement of the Council of CECAM.

The Director of CECAM together with all the Node Directors will constitute the CECAM Board of Directors. This Board will be chaired by the Director of CECAM and carry out the tasks assigned to it in Article 6.14 of the Convention. *Sapienza* agrees that Carlo Massimo Casciola will represent *Node Sapienza* on the Board of Directors.

6 CECAM Activities at Node Sapienza

The entire programme of CECAM activities in any given year, that is

(i)activities to be hosted at the CECAM Headquarters in EPF Lausanne plus
(ii)activities to be hosted at the node within *Sapienza* plus
(iii)activities to be hosted at the other nodes

will be agreed during the previous year following discussions in the Board of Directors, as described in articles 6.13 and 6.14 of the Convention.
As for the research program the node intends to develop in the initial phase, a preliminary list of topics is:

- *Chemical and physical hydrophobicity.* Physical hydrophobicity concerns solid/liquid/gas systems (superhydrophobicity for e.g. drag reduction in micro-channels and self-cleaning surfaces). Chemical hydrophobicity exhibited by non-polar molecules in polar solvents determines structure formation and stability in biology. The associated metastabilities call for advanced methods to address free-energy barriers and transition mechanisms, and techniques for bridging the scales from nano to micro.

- *Phase change near to and far from equilibrium conditions of systems of potential technological interest.* Nucleation problems found in applications involve a broad range of scales. Characteristic examples are clathrate compounds formation that can clog oil/gas pipelines, and cavitation in liquids where bubble implosions deteriorate the manufacturing material of, e.g. ship propellers. The inherent multi-scale coupling need smart computational approaches to consistently bridge the variety of involved scale.

- *Modelling of coating built-up in thermal spraying processes.* Droplets substrate and droplet-droplet interactions, deformation mechanisms and kinetics, splats size control and shape need being addressed to study adhesion, cohesion, porosity distributions and surface roughness. The aim is to conjugate the theoretical information with object oriented FEM codes to estimate off-line coating properties depending on adopted processing parameters

- *Soft matter and self-assembly*. Interactions among colloidal particles can be tuned in order to control mechanical, optical, or dynamical properties. Such possibility makes colloidal suspensions very appealing and suitable for technological applications. In this respect, Monte Carlo and molecular dynamics simulations are invaluable tools to understand how microscopic properties of novel soft matter materials influence their macroscopic behaviour.

- *Quantum dynamics of molecular systems in gaseous phase and confined superfluid He clusters.* The numerical simulation of quantum structures allows investigating collisional transfer of molecular energy in the interstellar medium and in low temperature magneto-optic traps, e.g. in dense interstellar clouds, and is becoming crucial in molecular physics given the increasing number of experiments.

- *Ionic Liquids*: *theoretical simulations of their structure and dynamics*. Theoretical characterization and modelling of ionic liquids is essential to understand their behaviour, to tailor the properties of these systems and to optimize their specific performances. Recently

interest raised on their mixtures with molecular liquids and rare earth elements as "solvated" dopants. The investigation requires sophisticated quantum and classical simulation techniques and the exploitation of large scale computational facilities.

7 Financial Arrangements

Sapienza, through its departments joining the initiative, confirms that they are prepared to provide funding of at least 50,000 Euros per annum to support such CECAM activities at *Node Sapienza* as agreed by the Board of Directors according to paragraph 6. This target budget is to be used for planning purposes. The actual Node budget for a given financial year is confirmed in advance in a meeting of the Board of Directors. The minimum Node budget is 50,000 Euros per year (Article 8.2 of the Convention).
This funding will be used and remain in *Sapienza* and will be clearly identified as the CECAM Node Sapienza budget. The transactions within this budget line will be administered by the Director of *Node Sapienza* and will be reported annually to the Director of CECAM who will include the accounts of all nodes in the complete annual Financial Report to be presented to the Council of CECAM as required by paragraphs 6.9(v), 7.3(vi) and 7.6(iii) of the Convention.

8 Renewal or termination of Agreement

This Agreement will terminate on November 21, 2016 having been in force for four years. At least 3 months before the Council meeting immediately preceding the above termination date of the Node agreement, the Node Institution writes to the President of the Council stating its wish either to continue to host a Node or to cease Node activities. In the former case, the Node Institution may propose amendments to its Node agreement for the consideration of the Council. The Council then discusses this statement at its next meeting and decides on renewal or termination.

Signatures:

Rome, _____ (date) _____

Prof. Luigi Frati
Rector of Sapienza University of Rome

Lausanne, _____ (date) _____

Prof. Paul J. Durham
CECAM Council President