EUROPEAN SCIENCE FOUNDATION

SETTING SCIENCE AGENDAS FOR EUROPE

FORWARD LOOK

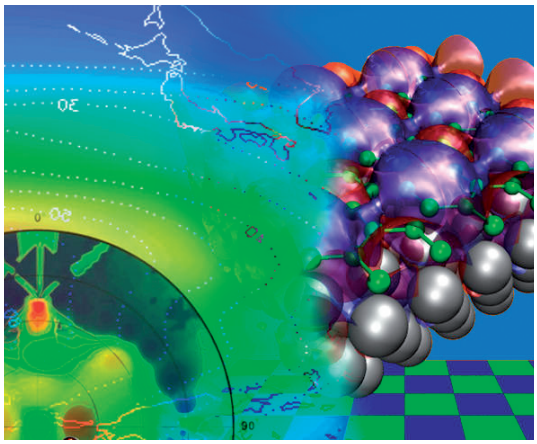
EUROPEAN COMPUTATIONAL SCIENCE: THE "LINCEI INITIATIVE": FROM COMPUTERS TO SCIENTIFIC EXCELLENCE

Computational sciences and computer simulations in particular, are playing an ever growing role in fundamental and applied sciences. The aim of this Forward Look is to develop a vision on how computational sciences will evolve in the coming 10 to 20 years. Based on a scenario of how this field will evolve and on the needs of the scientific community, a strategy will be presented aimed at structuring software and hardware support and development at the European level.

Computational approaches are becoming an increasingly important tool in modern science. Computational sciences have reached such a level of importance as to now be considered the third pillar of science, after experimental and theoretical approaches.

The complexity of the modern codes has caused a transition. A few years ago, each computational group had its own "home-brewed" software. At present, an increasing number of groups rely on the availability of such codes. In the field of computational sciences Europe is playing a leading role, also thanks to the availability of these codes. To consolidate its position, a scientific software must be developed at transnational level, playing the same role as large European facilities (i.e. neutron, X-ray) do for experimental research.

The aim of this Forward Look is to develop a vision of how Computational Sciences will evolve in the coming 10 to 20 years. Based on a scenario of how this field will evolve and on the needs of the scientific community, a strategy will be devised aimed at structuring software development, support and training on computational aspects of Computational Sciences at the European level. The initiative of this Forward Look was originally taken by the atomic-scale materials simulation community, but several communities, ranging from Computational Fluid Dynamics to Astrophysics, from Life Sciences to Environmental Sciences, from Computational Materials Sciences to Computational Chemistry, are contributing to this effort. The outcome of this Forward Look will be of interest to other Computational Science communities as well. Implementation of these recommendations should lead to an advanced cyberinfrastructure that allows Europe to maintain its leading position in this field.



The Organising Committee of this Forward Look adopted web based tools to publish preliminary reports and to organise the day-by-day life of the initiative:

- *Forward Look Portal:* https://cyberinfrastructure.caspur.it: contains information about the Forward Look ongoing activities, and important provisional.
- *Two mailing lists*: cyberinfrastructure-oc@caspur.it, which is used for circulating messages among members of the Organising Committee; cyberinfrastructure@caspur.it, which is extended to everyone who wants to receive news about the Forward Look
- *Document Management System:* https://cyberinfrastructure.caspur.it/kt: all the documents examined and produced in the context of the Forward Look are stored on the document management system (DMS).

ESF Forward Looks

ESF Forward Looks provide medium to long-term authoritative visions on science perspectives in broad areas of research bringing together ESF Member Organisations, other research organisations and the scientific community in creative interaction. Forward Look reports and other outputs such as ESF Policy Briefings assist policy makers and researchers in defining optimal research agendas and in setting priorities. Quality assurance mechanisms, based on peer review where appropriate, are applied at every stage of the development and delivery of a Forward Look to ensure its credibility and impact.

www.esf.org/flooks

Timeline of activities

- **November 2006**
  Six small-scale, parallel, community level workshops.
  The aim of this series of parallel workshops is to define the needs about the software Cyber Infrastructure within each scientific community.
- **January-February 2007**
  Workshop with the aim of defining the common Software CyberInfrastructure.
  The aim of this workshop is to identify the expertise needed to setup the envisioned Software CyberInfrastructure, including those areas which are not available within the scientific communities participating to the Forward Look.
- **February-March 2007**
  Workshop to gather the expertise needed to realise the Software CyberInfrastructure.
  The realisation of a software infrastructure is usually a multidisciplinary endeavour which requires expertise from many different areas such as computational sciences, computer science, software engineering, supercomputing centres, hardware manufacturers and independent software vendors. The aim of this workshop is to gather all these people together to devise an operative plan for the implementation, deployment, operation and management of the Software CyberInfrastructure.
- **June-July 2007**
  General Conference.
  The provisional final report will be presented to a large number of members of target national and international institutions such as EC, ESFRI, National Research Councils, HPCN centres and universities. Participants will be requested to discuss conclusions and recommendations of the provisional Forward Look report, which will be made available prior to the conference.
- **End 2007**
  The final report will be released.

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For the latest information on this Forward Look consult the following website: **www.esf.org/lincei**

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