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CMST COST Action D23

Metachem

Descriptions are provided by the Actions directly via e-COST.

The main objective of D23 was the exploitation of the potentialities of meta and grid computing for developing computational applications, connecting the know how distributed among several research laboratories and sharing the related computer resources, which would not be possible otherwise, due to the complexity and innovative content of this task. The sharing of machines on the network has been boosted by the dramatic development of grid technologies in recent years and by the emphasis given by the 6th European Framework Programme. The further added value of D23 is to be seen in the use of grid computer systems to build the so called European Meta Laboratories (clusters of geographically distributed Laboratories working in a co-ordinated way on a common project by sharing manpower, hardware and software), fostering innovative solutions for chemical applications and a new paradigm for collaborative research. This made it feasible to develop new a priori realistic simulations for several scientific, technological and environmental applications. Likewise, the extension of traditional quantum chemical schemes to the four component regime, although straightforward in principle, was still posing major technical difficulties which could be overcome in the last years thanks to the contribution of this Action. One of the working groups addressed a serious problem that arises when different quantum chemical codes are used on the same target, namely when the internal representation of quantum chemical data is largely incompatible. A standard database format has been developed to solve this, which is accessible by a set of library routines. As an additional benefit the emphasis given to e-learning has to be mentioned. Metacomputing in computational chemistry is still at its beginning. COST Action D23 has put the initial momentum into this development, which will become increasingly important in the future.

This COST Action has allowed the collaboration between 46 research groups from 19 different countries. Deepening these links within Europe is particularly important to establish a competitive scientific landscape which is not hampered by national borders. The scientific results have been presented in a multitude of research papers in refereed journals and are thus publicly accessible.

Chemistry and Molecular Sciences and Technologies COST Action D23

- ▶ **Description**
- ▶ Parties
- ▶ Management Committee



General Information*

- Chair of the Action:**
[Prof. Hans Peter LUTHI](#) (CH)
- Science officer of the Action:**
[Dr Lucia FORZI](#)
- Administrative officer of the Action:**
[Ms Svetlana VOINOVA](#)


Downloads*

- Action Fact Sheet**
[Download AFS as .RTF](#)
- Memorandum of Understanding**
[Download MoU as PDF](#)
- Final Report**
[Download Final Report as PDF](#)

Websites*

- Domain website:**
<http://www.cost.eu/cmst>

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