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## **SOMA2 – Open Source Gateway to Molecular Modelling Workflows**

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SOMA2 gateway is a WWW-browser operated molecular modeling workflow environment developed and deployed by CSC. The SOMA2 environment allows users to control and combine scientific applications available in the computing system into unique application workflows, which are automatically executed. SOMA2 offers a flexible framework for integrating and executing molecular modeling applications, including molecular data exchange. SOMA2 source code is distributed under the GPL license.

### **Detailed analysis**

For end users, SOMA2 offers a secure and personalized environment for inputting molecular data, submitting and controlling jobs and analyzing the results. In SOMA2, scientific applications are presented and configured via web forms, which guide users to correctly configure a program by supplying default values, thresholds, runtime help and validation. For experts, SOMA2 offers a framework to make virtually any molecular modeling application accessible to the end users.

SOMA2 has a modular design where third-party scientific applications are described as pluggable capsules with interfaces to manage the data. A capsule consists of an XML description, used e.g. to generate an application web form, and scripts & file templates to enable program execution and processing of the program output. The XML descriptions are based on an original schema. SOMA2 enables communication and data exchange between applications by employing a common data exchange format, CML (Chemical Markup Language).

### **Conclusions and Future Work**

At CSC, SOMA2 is available as a service for CSC's academic users providing access to 14 different molecular modeling applications, which are seamlessly integrated within the system. System is fully integrated with the local computing infrastructure.

In addition to UI enhancements, SOMA2 development plans include DCI-integration by making use of grid middleware. SOMA2 framework is fully compatible for this approach. Technical challenges mostly concern with grid authentication and authorization components.

### **Impact**

SOMA2 gateway provides an easy to use and intuitive single user interface to scientific applications and it hides all technicalities from end users. The system automates repeating tasks and eliminates redundant work so that end users can focus in the actual scientific task instead of dealing with technical issues requiring manual work. SOMA2 does not only integrate applications but also different computing platforms connected to the system making the whole infrastructure easily reachable for all users.

The framework for describing scientific applications in SOMA2 facilitates transfer of technical know-how from experts to service users so that everything remains in machine readable form. In addition, core SOMA2 software is separated from the program descriptions and basically no real programming skills are required to

create a SOMA2 capsule. Flexibility, application oriented approach for abstract level reusable workflows and open source license make SOMA2 system unique in its domain.

## **Keywords**

gateway, user environment, open source, molecular modeling, workflow, CML, XML, knowledge transfer

## **URL for further information**

<http://www.csc.fi/soma>

**Author:** Dr KINNUNEN, Tapani (CSC - IT Center for Science Ltd.)

**Co-authors:** Dr LEHTOVUORI, Pekka (CSC - IT Center for Science Ltd.); Dr NYRÖNEN, Tommi (CSC - IT Center for Science Ltd.)

**Presenter:** Dr KINNUNEN, Tapani (CSC - IT Center for Science Ltd.)

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