Poster presentation

# SOMA2 – open source framework for molecular modelling workflows

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During the last five years, we have developed and deployed a molecular modelling workflow environment at the Finnish IT Center for Science CSC. The SOMA2 environment [1-3] is a web server based system offering a framework for integrating molecular modelling applications, including molecular data exchange. SOMA2 allows users to combine software available in the computing system into unique workflows, which are automatically executed. Recently, the SOMA2 source code was released under GPL license [4].

For end users, SOMA2 offers a secure and personalised web browser operated environment for inputting molecular data, submitting and controlling jobs and analysing the results. In SOMA2, parameters of the scientific applications are presented and configured via uniform web forms. The web forms guide the users to correctly configure a program by supplying default values, thresholds, runtime help and content verification. For experts, SOMA2 provides a framework to make virtually any command-line application or combination of applications easily accessible to the (naïve) users. The system enables communication and data exchange between molecular modelling programs on different computing platforms by employing a general data exchange format, CML (Chemical Markup Language) [5].

SOMA2 framework has a modular design where the third-party scientific applications are described as pluggable capsules with generic interfaces to manage the data. The description of a scientific application in SOMA2 facilitates the transfer of technical know-how from experts to service users. A SOMA2 capsule consists of an XML description, used e.g. to automatically generate a web form for the program, and scripts & configuration file templates to enable automatic program execution and processing of the program output. The XML descriptions are based on a schema, which we have developed. No programming skills are required to create a SOMA2 capsule.

A demo installation of SOMA2 with limited features is available [6].

## References
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