

Ref E-054*

CULGI Demonstration.

JanWillem Handgraaf^{a*}, Ruben Serral Gracia^a

^a Culgi BV, Leiden, The Netherlands

The Chemistry Unified Language (Culgi) aims to integrate relevant chemical modelling tools (quantum, molecular, mesoscopic and statistical) into one computational platform, with a focus on soft materials or formulations.

The computational technology, and a real-world application of multiscale modelling in the context of chemically enhanced oil recovery is presented elsewhere at this conference.

In this presentation at the stand of Culgi, we will present and discuss several practical aspects of multiscale modelling in an industrial setting. In particular, the writing of workflows in the CULGI's Graphical Programming Environment, that enables the rapid development of dedicated proprietary applications, and the relevance of Client-Server relations, that enable development in a heterogeneous computational infrastructure, from desktop or laptop, to production runs on a parallel cluster.

Attendees of the presentation will be offered hands-on tutorials, and trial licenses for testing of the software on laptops.

Demonstrated examples range from surfactants and polymers to colloids and actives, and techniques from molecular to mesoscopic, and combinations thereof, such as reactive systems (glues) and emulsion interfaces. Interested attendees are invited to present their own problems, and we could discuss how such system could be addressed by the Culgi modelling approach.

Keywords: Multiscale Modeling, Workflow, Client-Server relation, parallel computation.