

**PACE-ECLT Integrated Twin Workshop**  
**Multiscale Molecular Simulations and Stochastic Feedback**

**November 22 - December 5, 2004**

**ECLT, Venice, Italy**

## **Organizers**

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## **Location**

European Center of Living Technology, Palazzo Giovannelli, Venice, Italy

## **Workshops**

### **Multiscale molecular simulation**

Date: Nov. 24 - Dec. 5

Organizer: Steen Rasmussen

This workshop will focus on molecular dynamics and self-assembly simulation methods at different time- and length-scales. The format will include both presentations and 'hands-on classes'. The hands-on classes consist of experts guiding students through the implementation of their simulations (mostly open source/publicly available software) on the participant's laptops and helping them use these simulations. Who the experts and students are will change depending on the specific type of simulation. Tasks include:

- Multiscale representation of oil/water droplets, micelles and emulsions, membrane systems using MD, DPD, MD lattice gas, lattice Boltzmann, LGA, CA, Navier Stokes, Ginzburg Landau and related methods.
- Introduction of chemical reactions into the self-assembly process, e.g., (i) template (e.g. PNA, RNA) or metabolic aggregate interactions with oil/water interfaces or amphiphilic aggregates; (ii) template melting in different phases and environments; (iii) reaction diffusion kinetics, e.g. Gray-Scott.
- Presentation and development of methods to 'glue' together the different time- and length-scale simulations.
  
- Review how to apply the presented methods to key PACE molecular systems and problems in future collaborative projects with both PACE participants and external experts.
  
- Design interfaces of simulation tools for communities both inside and outside PACE: brainstorm with TILS (Telecom Italia Learning Services).

## Statistical experimental design and stochastic control

Date: Nov. 22 - Dec. 5

Organizer: Norman Packard

This workshop will focus on the following issues:

- Ion dynamics, and the problem of electrophoretic control of ion dynamics with pulses on electrodes. Goals: Establish a model that can predict properties of flow control realized in micro-reactors. Design of experimental sequences to provide data for model validation.
- Inclusion of reaction and diffusion into the experimental model. Develop PRESS model (from BioMIP group) for integration into modeling. Connect with TCIL for standardization of interface using SBML (Systems Biology Markup Language cf. <http://sbml.org>).
- Statistical experimental design. Use time scales of flow, reaction, diffusion, observational noise levels, to design data gathering protocols for a micro-reactor array. Goal: Take the first steps of designing the framework, without details of chemical reaction rates, etc. This latter phase will be followed up in subsequent workshops with specific involvement of chemists.
- Other questions to be addressed: How can spatially extended data be used to increase resolution of chemo-fluidic dynamics? How may experimental perturbations (addition of noise) be designed to increase resolution of chemo-fluidic dynamics?