Multi-scale modelling from first principles

Concluding Remarks

"If you want to understand all the talks, then do not go to a multi-scale modelling conference! "

Overall

- An exciting opportunity to meet and discuss with a broad cross section of the CECAM and Psi-k community and to understand the direction of a wide field of science.
  - Plenty of white space for discussion
  - A good sharing of jargon and vocabulary
  - Lots of pointers to the future directions

- Some real example of multiscale modelling
  - Mainly across on length or time-scale zone
  - Mainly of the parameter passing variety
  - Little dynamic coupling between the length and timescales
  - Hope to see more at the higher end (CFD, dislocation dynamics)
  - More systems biology

- Great poster session

Much has been accomplished but much remains to be done

Stick with the one scale just for now !

- Optical spectra (Claudia Draxl)
  - Both the DFT/GW/Bethe Salpeter and constrained DFT can be used to look at excitions. The jury is till out on the best approach. Difficult to use methods combined with, say, molecular mechanic if the electron hole pair is not localized

- Walking the talk (Ali Alavi)
  - Perhaps the most interesting breakthrough in electronic structure through the birth, death, annnihilation and spawning of walkers in a Slater determinants space. A walking holiday which does not collapse onto a bosonic wavefunction. Chemical accuracy for C_2. 50 electrons can be tackled, less if there high correlation.
  - Improved sampling of Slater determinants, maximally compact natural orbitals and two electron geminals

Stick with the one scale just for now !

- Atto spectroscopy (Alberto Castro)
  - Femto-second laser pulse with atto-second bursts . Linear relationships between the response function and the probe: dipole moments for adsorption spectroscopy; higer harmonic generation; photoelectron spectroscopy. Modelling of non-equilibrium electron dynamics. Quantum optical control theory for steering electronic motion. Ehrenfest model of the electron-ion coupling.

- Damage (Emilio Artacho)
  - Calculation of the electron stopping power dE/dx in complicated materials using time dependent density functional theory and the GCA.
  - The holy grail is accurate non-equilibrium simulations with both nuclei and electrons for a few picoseconds
  - A much better understanding of how the electronic excitation effects the interatomic forces. A deeper understanding of phonon coupling to removal energy
-

Chasing those potentials

- Never mind the potentials go straight for the crystal symmetries. Rule based approximation for crystal energies (Gus Hart).
  - Fast lattice hamiltonians by cluster analysis and compressive sensing rather than GFA

- Neural networks potential builders (Jorg Behler, Christoph Dellago)
  - Building neural network potentials based on the atomic coordinates and DFT calculations for systems such as O_2/Al, H_2/Pd
  - The science is including the permutation symmetry of the system (switch from Cartesian to symmetrized variables)
  - Expect large training sets $2x10^6$ pieces of information.
  - Similar networks can be used **to identify** crystal structures in finite clusters undergoing reversible phase transitions (CuS). Use simulated crystal simulations of particular structures to train the network.
  - Can potentials and structure be done at the same time?
  - Can complete and improved sets of symmetry functions be developed

Chasing those potentials

- Classical pair potential close in and mesoscale potentials at a distance. (Pep Español, Kurt Kremer)
  - Two geometrical zones for the classical and coarse-grained potentials with a transition zone between.
  - Difficulties in keeping g(r)(r) and the compressibility equivalent in the two zones and the same time as keeping the pressure the same in the two zones
  - Compensating forces to overcome this anomaly can be can be calculated from the gradient of μ(z)
  - Interesting applications to proteins in water and to water/ethanol mixtures
  - Possibilities for combining with multiple time step methods

Keep a solid footing

Free energy calculations (Jorg Nugbauer, Luca Ghinrengilli)

Beyond DFT energies to free energies via the harmonic and anharmonic approximations. Free energy differences from histogram reweighting or thermodynamic integration. MD from simpler functionals, accurate energy calculation along the path. Proper inclusion of magnetic and electronic contributions to C_P.

Begin to employ a range of simulation techniques from the stat mech community

Plastic deformation (Karsten Albe)

The physics is in the boundaries and not the grains. Really interesting opportunities of coarse-graining through dislocation dynamics and opportunities for reaching acceptable shear rates some 10 orders of magnitude below the current values). The placement of solutes is a tricky but important problem.

More dislocation dynamics

.

Surface chemistry and surface growth

- Surface chemistry (Karsten Reuter) and the growth of nanowires (Peter Kratzer)
  - Kinetic Monte Carlo models with transitions probabilities from DFT. Integration into macro-scale fluid dynamic. Uncoupled CFD and KMC for real processes (see poster of Nicola Kleppmann on C_{60} surfaces)
  - Inclusion of diffusion through the growing fluid and along the surface.
  - Solid and liquid diffusion techniques
  - Do not always blame the functional there may be other more important approximations at other length scales (sensitivity analysis) (see the poster of David Membane)
  - See poster on crystal growth (Tongyu Wang)

A good pinch of biophysics

- Mesoscale protein dynamics (Ray Kapral)
  - Cyclic machine processes phosphoglycerate kinase. Treat the amino-acid residues as beads, inject the correct hydrodynamics of the solute by multiparticle collision dynamics. Diffusion in the dense obstacle course of the cell. Flow of Janus particles in an anisotropic atmosphere of chemistry. Heats of reaction as well as particle fluxes must be considered.

- Membrane biophysics à la *Car Parrinello* (Paulo Carloni)).
  - Simulations of protons close to membrane water surfaces. QM/MM methods for studying membrane channels. Simulation of membrane bound proteins (odorant and bitter receptors). Combine with milestoning.

- Multiscale modelling of DNA (Modesto Orozco)
  - Modifications of nucleotides with sulphur produces promiscuous bases (selano-guanine) –the power of QM to calculations to guide the synthetic chemist. Long timescale MD allows for the study of strucutre on positional substitution (folding and unfolding). Mesoscale modelling of the genome based on elastic properties.
  - Prediction of methylation and epigenetic effects

Speed dating

- Milestoning (Ron Elber)
  - identifying milestones in a process and calculating the probabilities $K_{\beta\alpha}(t)$ that the system move from one milestone to the next in a specific time t. Then solving the milestone equation for the flux, demonstrating its relation to the master equation Applications to helix cracking and membrane penetration
- Tipping the barrier (Carsten Hartmann)
  - It is possible to speed up rare events by biasing the probability distribution of the original system, tipping the potential. The no free lunch theorem inducated that ine need the full free energy function to find the optimum bias.
  - Lots of opportunity to develop an anatz for f(R) from the knowledge of f at the mimima and the barriers. Tough problem in many dimensions
- Green-Kubo-Ciccotti (Giovanni Ciccotti)
  - A demonstration of how the perturbation of trajectories technique, which has been used to calculate transport properties in equilibrium simulations, can be extended to non-equilibrium but stationary system (Bernard convection) and constrained non-equilibrium ensembles (interface relaxation). Two interesting new weapons in the arsenal.

MESO-land is less complicated than it used to be

- Coarse-grained molecular dynamics
- Dissipative particle dynamics

  respect for conservation laws (mass, energy, momentum)
- Lattice Boltzmann

  drastically simplified dynamics

Dominic Tildelsey described an attempt to model lubrication using DPD including charge and the conservation of topology (see the poster of Gaëton Maurel)

Gerhard Gommper described the full detail of MCD and its implementation with simulation of the flow of deformable blood cells in narrow channel showing a transition from biconcave disk shapes to parachute shapes (see also the talk of Ray Kapral)

Ignacio Pagonabarraga described the application of the LB method to wide range of flow problems including the spreading of an oil droplet in water on a solid surface. He emphasized and demonstrated the propogation method for calculating autocorrelation functions (see the poster of Francisco Alarcón)

Some more posters

- Sumathy Raman: REAXFF for hydrocarbon cracking
- Henry Heitzer: dielectric response in materials
- Robin Richardson: Engineering strain equations applied to biomolecules

A big vote of thanks to

- Michel Mareschal and Matthias Scheffler
  - A white knuckle ride programme across a fascinating landscape of science
  - An excellent cast list
  - A complete and interesting conference booklet
  - A beautiful hotel in sunny Barcelona (with sunny staff and excellent food)
- Thanks to the session chairs for many outstanding summaries.
- Thank to the speakers and colleagues. Time is precious and you have made the commitment.
- Please consider and contemplate the ideas you have heard here and make them CECAM workshops of the future