Hybrid Molecular Dynamics (HMD): coupling atomistic and continuum descriptions on the GRID

G. De Fabritiis, *R. Delgado-Buscalioni and P.V. Coveney*
Centre for Computational Science, Department of Chemistry, University College of London,
20 Gordon street, WC1H 0AJ, London, UK
g.defabritiis@ucl.ac.uk, r.delgado-buscalioni@ucl.ac.uk, p.v.coveney@ucl.ac.uk

Hybrid molecular dynamics simulations

interface molecular and continuum descriptions in such a way that mass, momentum and energy are correctly exchanged across the domains [1-2]:

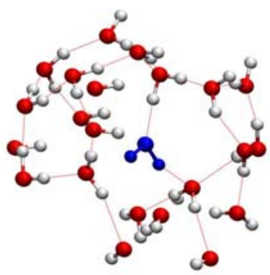
1) *Molecular -> continuum*, a simple local average to obtain density, pressure, temperature, etc.
2) *Continuum->molecular,* **possible only with a method for fast, energy controlled molecule insertion in dense liquids**

Equilibrium and non-equilibrium conditions

1) the continuum plays effectively the role of a boundary condition, e.g. spherical open boundary or driving flows may be imposed

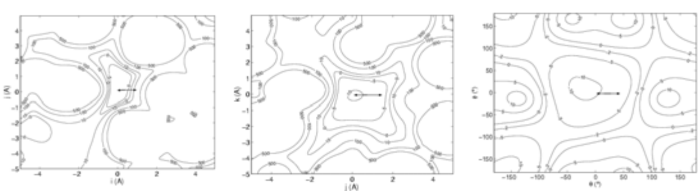
2) coupling both ways, the continuum provides a boundary condition for the molecular description and *vice versa*. The continuum is spatially resolved as well (fluctuating hydrodynamics).

Insertion of water molecules in dense liquids



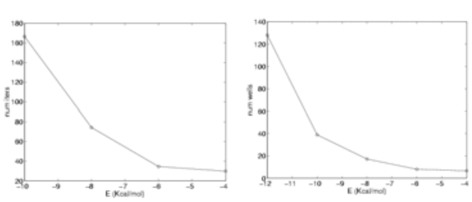
TIP3P water model. The local structure of liquid water at equilibrium presents a hydrogen bond network formed by oxygen and hydrogen atoms of neighbouring water molecules.
This configuration makes it very hard for an incoming water molecule to find low energy configurations.

On the potential energy surface, low energies are located inside energy wells whose local minima span a relatively large range of energy values.



Contour diagram of potential energy landscape for an equilibrated water molecule. (i,j,k) reference system solid to the water molecule, i is the dipole axes. Useful information on sizes of the potential energy wells can be extracted and used by the energy minimization method to constrain the search inside the energy well.

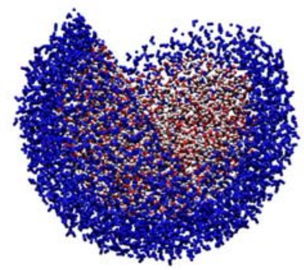
The main idea of our method is to reconstruct the energy landscape with a limited number of probes by constraining the search inside energy wells.
The minimization is performed via a combined steepest-descent and Newton-Raphson iterator which is tailored on the structure of the potential energy landscape [2-3].



Number of iterations and number of searched wells per water molecule insertion

The insertion of a water molecule requires **35 iterations** at the target energy equal to the chemical potential (-5.4 Kcal/mol) and **166 iterations** at the mean energy per particle (-9.6 Kcal/mol) [3].

Spherical open boundary



A cross-section of the water shell. Molecules are removed outside the sphere and inserted in the blue external region where a constant potential is applied to confine the water molecules.

No thermostat is required because the energy released to the system is carefully controlled by the insertion algorithm. The spherical boundary is maintained at a **negligible cost (<3%)** compared to the associated molecular dynamics (MD) simulation [3]. Applications and advantages:
1) grand canonical MD simulations
2) interface continuum fluid dynamics and MD
3) remove finite size effects due to periodic boundaries
4) reduce amount of explicit water needed for atomistic simulations

Coupled models on the GRID: RealityGrid architecture

RealityGrid

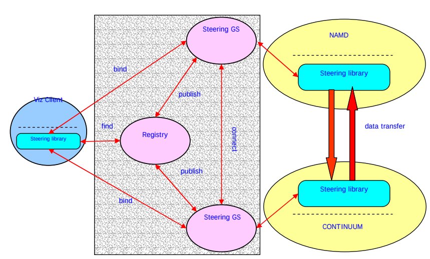


FIG. Architecture showing middle (Grid Services) layer in the grey box, molecular and continuum descriptions and optional visualization client to monitor the codes (figure from Andrew Porter).

Molecular and continuum models communicate via the ReG library which provides a “GRID aware plumbing” for data transfer between one model and the other. This allows to move codes around where resources are available in the GRID while ReG takes care of maintaining the communications.
Official site: www.realitygrid.org

[1] R. Delgado-Buscalioni and P.V.Coveney, *Phys. Rev. E* **67**, 046704 (2003)
[2] R. Delgado-Buscalioni and P.V. Coveney, *J. Chem. Phys.* **119**, 2, 978-987 (2003)
[3] G. De Fabritiis, R. Delgado-Buscalioni and P.V.Coveney, preprint (2004)

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