**Rough sketch of LJC summer school content**

First, many thanks to you all for providing your ideas for what you might include in the LJC summer school. As you have probably gathered, the school aims to cover a broad range of topics, ranging from wavefunction methods to classical molecular dynamics. As the school only runs over five days, we are limited in the amount of detail that we can cover on any individual topic. Moreover, we should aim for a degree of coherency rather than a hotch-potch of hastily arranged material.

The purpose of this document is to make an **initial** proposal, based on the material that you have provided, on how to link the different topics. The practicals provide a natural starting point to identify areas of commonality. In addition, if we broadly settle on the practical content, this may help to focus on the key content that needs to be covered in the lectures.

But it is worth reemphasizing that this is an initial proposal – it is very much intended as a starting point for discussion, and the final plan may end up looking very different!

**Where might we end up?**

Aim: to identify one or two systems that are simple enough for students to investigate meaningfully, yet complicated enough to contain physics from each of the individual topics. The idea is that students work toward these systems in stages, using knowledge gained along the way. It seems natural to end up with a dynamical simulation that uses a MLIP (probably MACE) and/or “discovery” of a new material.

**Case study 1:** Liquid water (or aqueous solution) in contact with a metallic surface. Ideally, the water would do something interesting at the surface (e.g., dissociate).

What they might compute:

* Dissociation free energy barrier; dissociated fraction at the surface.
* Density profile for water (ions) from the surface.
* IR/Raman/SFG Spectra (possibly too advanced); vibrational spectra.

**Case study 2:** Materials discovery

I am not the person to attempt to outline this!

**How might we get there? [1]**

Now let’s try and outline the steps that are needed to get to these two case studies. We’ll do this in order of decreasing (system) complexity. The content on molecular dynamics seems to be most similar.

**Case study 1 (water-metal):** Simple point charge model of water in contact with a metal surface. Although dissociation cannot be sensibly investigated, this can be used as motivation for introducing the MLIP. There will also be some other points of contrast (some where the SPC model has an advantage) and commonality.

What they might compute:

* Density profile of water (ions) from the surface.
* Capacitance from charge fluctuations on the electrode. Impedance might also be possible. (If this is the case, better to restrict to pure water).

**Case study 2 (material’s discovery):**

**How might we get there? [2a]**

It seems that DFT calculations of (monolayer) water in contact with solid surfaces would be natural precursor to classical MD of these systems.

**Case study 1 (water-metal):** Identify adsorption sites for a water molecule, and compare whether dissociative or molecular adsorption is favored. Look at dimers etc., building up to monolayers.

What they might calculate:

* Geometry optimized structures.
* Dissociation pathways (or diffusion barriers) with nudged elastic band or something similar.

**Case study 2 (materials discovery):**

**How might we get there? [3]**

Here is where the transition from finite to extended systems might occur.

[Feasibility?] Map out the energy landscape for small metal and metal alloy clusters, and look at the transitions between different minima. If these are catalytic clusters, then binding of small molecules could also be looked at, as could reaction barriers. This could also be a point at which an MLIP could be introduced. After the finite clusters, AIRSS could be introduced.

What they might calculate:

* Disconnectivity diagrams. Transition / reaction barriers.

**How might we get there? [4]**

Wavefunction calculation of single molecules, small clusters of molecules, metal-water clusters.

What they might calculate:

* HF and post-HF of these systems.
* Interpretation of the electronic structure. Thinking ahead to water at metal surfaces, this would also help to interpret why water binds in the orientation it does.

**Global optimisation** – mean first encounter time statistics with GMIN

examples for atomic clusters, Thomson problem, bulk silicon

atomic clusters LJ150,

nanoalloys, generalised basin-hopping Cu8Ag4Au7

NO \*\*\* peptides and DNA/RNA – trpzip, chignolin \*\*\* NO

**Pathways** – single and multi-step paths

ORCA with B97-3c for a hydrocarbon H-transfer reaction in a Pt complex

LJ38 with permutational isomerisation

LJ38 without permutational isomerisation

DP5 peptide beta hairpin to alpha helix

adenine-switch

I will try and connect problems with difficult global optimisation targets with broken ergodicity are rare event dynamics!

The key algorthms are basin-hopping for global optimisation and

doubly-nudged elastic band  + hybrid eigenvector-following + missing connection algorithm for pathways