Presentation Preparation Points

*1) What is the problem tackled by your paper: a high-level introduction to the physics discussed in the paper and the computational challenge it intends to overcome.*

* Discussion of the ‘electronic structure problem’
  + Schrodinger’s equation?
* Other recent solutions – the *ab initio* calculations for 1) specific atomic species 2) hand-selected geometric features and 3) using artificial NN to map position to wavefunction given a potential (NOT transferable though) – highlight the problem
* Problem – simplifying the need for solving several PDEs to simply using a deep NN; specific problem of **1 electron in a confining potential**
* More physics background...?

*(2) How does the paper solve this problem using machine learning: a summary of the machine learning models or learning paradigms used by the paper and how the proposed methods solve the problem stated in (1).*

* Paper focuses on generating features AND the mapping necessary to produce output – ‘featureless learning. Same data provided to deep NN and numerical method
* Algorithm is more scalable to large applications
* Mapping a electrostatic potential to ground state energy, KE and 1st excited state of bound electron
* **What problem does it solve? How does it do so?**
  + In this case, solving for these quantities is simple (especially for SHO and IWs since they have analytic solutions)
* Describe the 4 potentials – SHO, infinite-well, double-inverted Gaussians and random; difficulty of each component
* Numerical solver (finite-difference method) for each potential – SHO analytic solution used to verify accuracy of the solver 🡪 this is the method for solving DE
  + Are these the “true” values for the training data set?
    - **FOR SHO and IW there are equations for E0** – can compare to true value
  + If so, how do we do this to find energy eigenvalues? And KE?

*(3) Summary of original and final-project numerical experiments: a summary of the experiments done by the paper. Show the tables, figures, charts, etc. reported by the paper and explain what is reported/claimed in each figure on the assessed application of ML to solving the problem stated in (1).*

* Their focus in on identifying the 3 energies state above – ground, 1st excited state and KE – main focus seems to be on ground

*(4) What you'd be doing: a clear presentation of what parts of the paper you intend to focus on for your final project. How you'd generate training/validation data; how you'd implement the experiment; what reports you expect to be able to generate/reproduce; what challenges you think you might be facing; and how you'd break the upcoming month into milestones to ensure your project stays on track.*