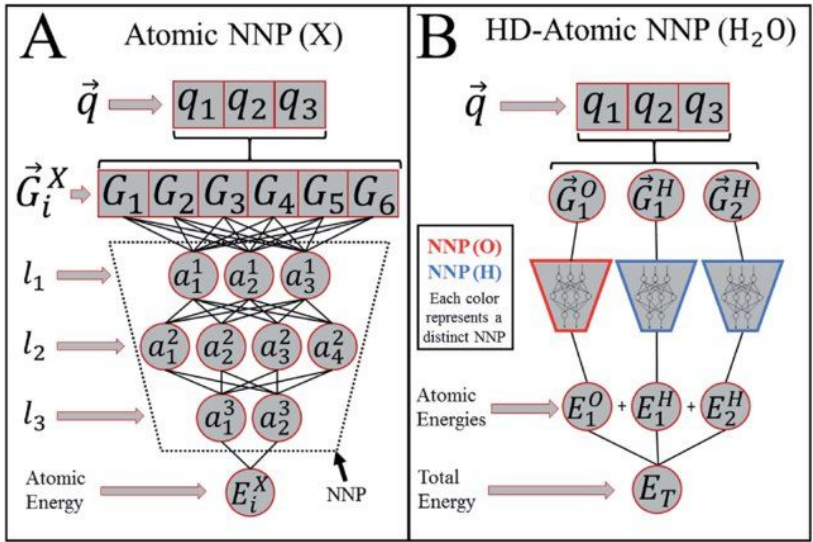
Breakout session: Neural network potentials

Literature discussed

ANI-1 NN potential: http://xlink.rsc.org/?DOI=c6sc05720a
GitHub: https://github.com/isayev/ASE_ANI

Algorithm:
- for each atom:
    compute a feature vector from close atoms
    add atomic energy contribution from NN

Using active learning to build ANI-1 with less
https://aip.scitation.org/doi/10.1063/1.5023802
Includes examples of MD with NN potentials



What can we do to enable research on NN potentials?

Example experiment:

Can we use a NN model like ANI-1 for short-ranged interactions, together with more traditional Lennard-Jones and electrostatics for long-ranged interactions?

Implement SMIRNOFF experimental extensions for using a TensorFlow compute graph potential via ONNX format
- implement common featurization strategies
- expose NN weights as parameters to optimize
- generalize element-directed NN selection to SMIRKS-based selection, or featurize atoms based on SMIRKS

What can we do to enable research on NN potentials?

Example experiment:

Can we use a NN model to compute partial charges?

Implement SMIRNOFF experimental extensions for using a TensorFlow compute graph charge model via ONNX format
- expose NN weights as parameters to optimize
- implement common featurization strategies

Action items

We created a new Slack channel to continue the discussion: **#machine-learning**