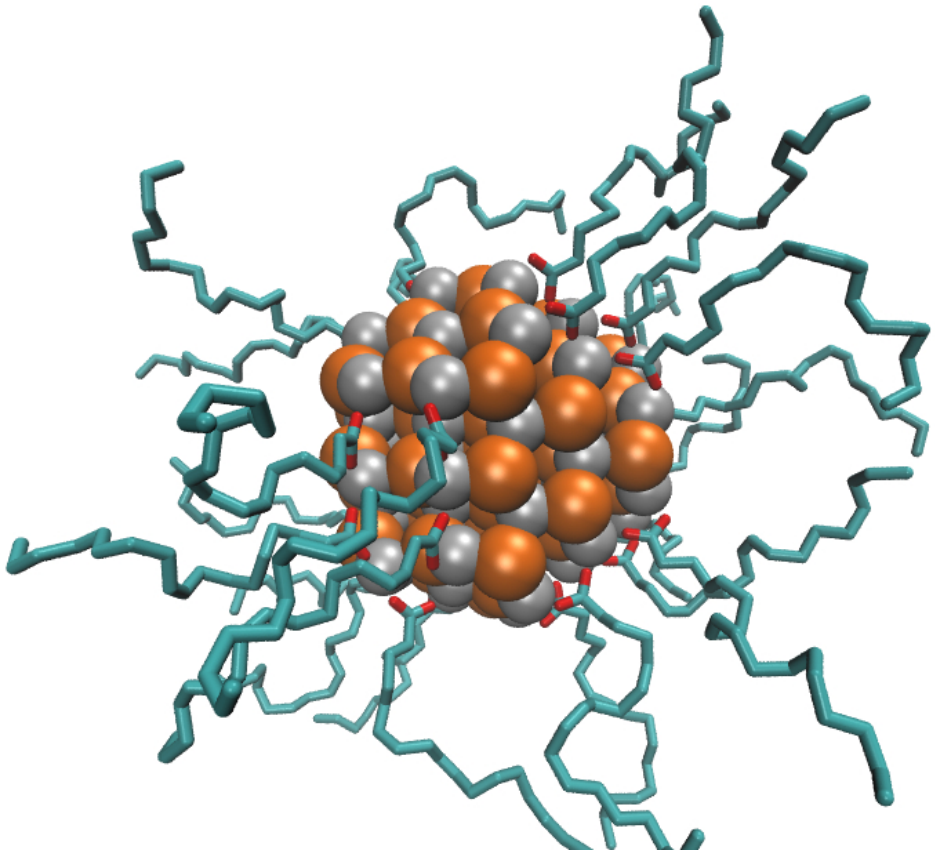
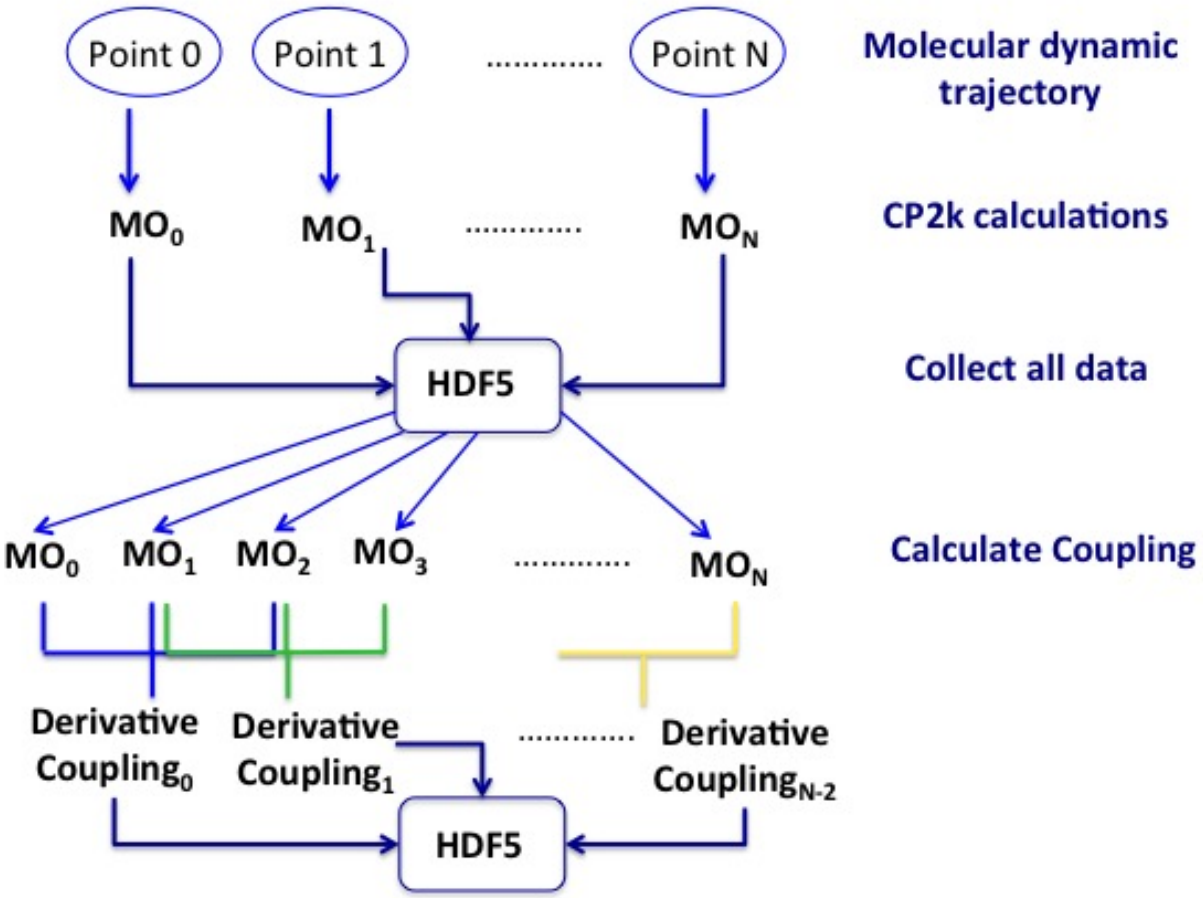
# Quantum Dots

## Molecular dynamic simulations

1. Calculate the nonadiabatic coupling matrix using a 3 point approximation.
2. feed the coupling to PYXAID.

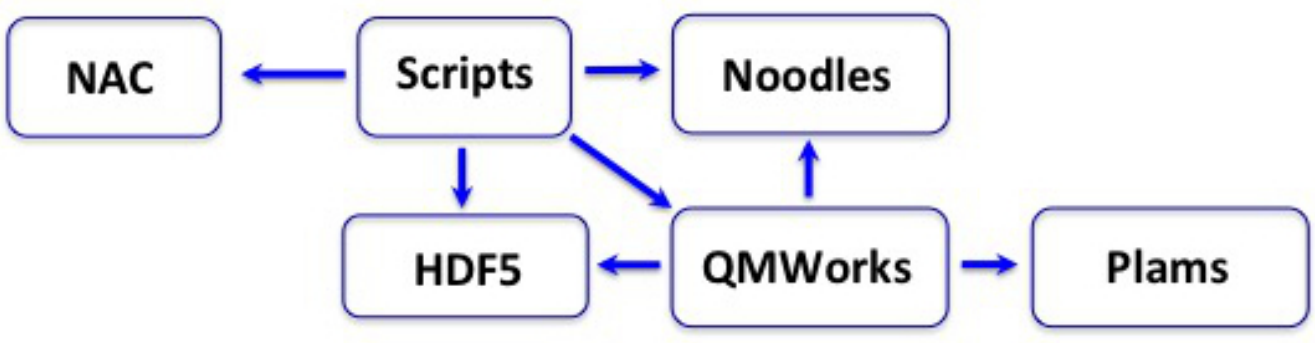


# Nonadiabatic Molecular Dynamics



# Application Dependencies

The application is written as a set of scripts that use **QMWorks** to call the quantum packages and **Noodles** to schedule some number crunching python functions from the **NAC** package.




The **HDF5** is used to communicate Numerical arrays between schedule functions.