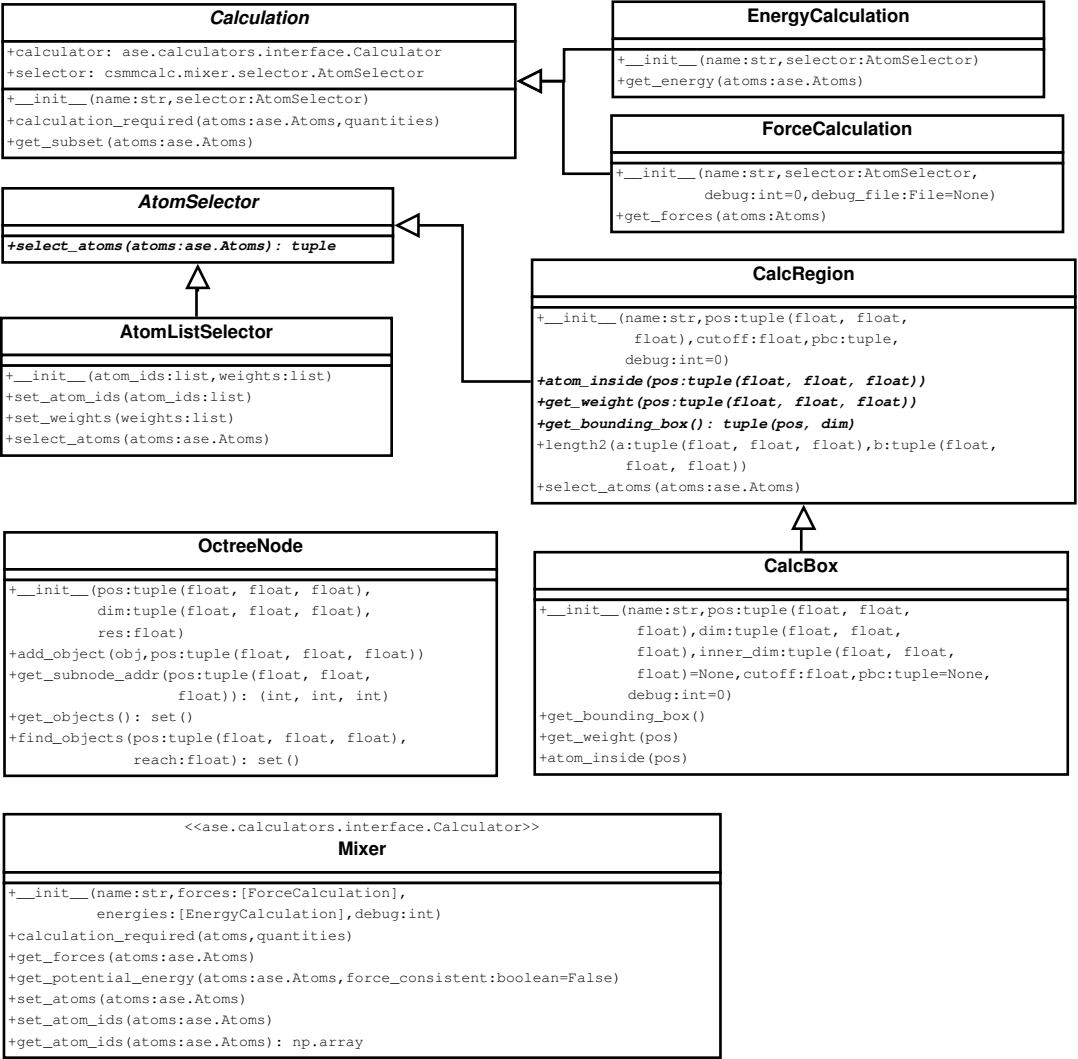
Calculation
+calculator: ase.calculators.interface.Calculator
+selector: csmmcalc.mixer.selector.AtomSelector
+__init__(name:str,selector:AtomSelector)
+calculation_required(atoms:ase.Atoms,quantities)
+get_subset(atoms:ase.Atoms)
EnergyCalculation
+__init__(name:str,selector:AtomSelector)
+get_energy(atoms:ase.Atoms)
ForceCalculation
+__init__(name:str,selector:AtomSelector,
debug:int=0,debug_file:File=None)
+get_forces(atoms:Atoms)
AtomSelector
+select_atoms(atoms:ase.Atoms): tuple
AtomListSelector
+__init__(atom_ids:list,weights:list)
+set_atom_ids(atom_ids:list)
+set_weights(weights:list)
+select_atoms(atoms:ase.Atoms)
CalcRegion
+__init__(name:str,pos:tuple(float, float,
float),cutoff:float,pbc:tuple,
debug:int=0)
+atom_inside(pos:tuple(float, float, float))
+get_weight(pos:tuple(float, float, float))
+get_bounding_box(): tuple(pos, dim)
+length2(a:tuple(float, float, float),b:tuple(float,
float, float))
+select_atoms(atoms:ase.Atoms)
OctreeNode
+__init__(pos:tuple(float, float, float),
dim:tuple(float, float, float),
res:float)
+add_object(obj,pos:tuple(float, float, float))
+get_subnode_addr(pos:tuple(float, float,
float)): (int, int, int)
+get_objects(): set()
+find_objects(pos:tuple(float, float, float),
reach:float): set()
CalcBox
+__init__(name:str,pos:tuple(float, float,
float),dim:tuple(float, float,
float),inner_dim:tuple(float, float,
float)=None,cutoff:float,pbc:tuple=None,
debug:int=0)
+get_bounding_box()
+get_weight(pos)
+atom_inside(pos)
<<ase.calculators.interface.Calculator>>
Mixer
+__init__(name:str,forces:[ForceCalculation],
energies:[EnergyCalculation],debug:int)
+calculation_required(atoms,quantities)
+get_forces(atoms:ase.Atoms)
+get_potential_energy(atoms:ase.Atoms,force_consistent:boolean=False)
+set_atoms(atoms:ase.Atoms)
+set_atom_ids(atoms:ase.Atoms)
+get_atom_ids(atoms:ase.Atoms): np.array