Ocean Wrapper Documentation v0.3.1

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1 Standard usage

Standard usage currently involves putting an atoms object into the Ocean calculator of decaf-espresso. Be sure that version 0.3.1 of `decaf-espresso` or newer is installed. Detailed installation instructions are provided at the GitHub repository.

One is attached here for demonstrative purposes: ./IrO2.traj

executing `calc.write_input()` will automatically write the files currently known to be necessary to the current working directory.

Files written include:

- `input.in`
- `run.sh`
- `photon1`
- `photon2`
- `photon3`
- `*.fill`
- `*.opts`
- `*.GGA.fhi`

Currently, only Oxygen `fill` and `opts` files are supported.

Pseudo potential files are taken from the defaults in decaf espresso: gbrv1.5pbe.

The `calc.write_input()` function also returns the `input.in` file content for quickly reading the written parameters.

```
from decaf import Ocean
from ase.io import read

atoms = read('IrO2.traj')

calc = Ocean(atoms)
inp = calc.write_input()

print(inp)
```

```
ppdir {../}
dft qe
control 0
ser_prefix {srun -n 1}
para_prefix {srun -n 192}

###################
dft.startingwfc {atomic+random}
dft.diagonalization {david}
dft_energy_range 50
nkpt {6 6 6}
ngkpt {6 6 6}
screen.nkpt {2 2 2}
screen.nbands 2000
ecut 120
core_offset .true.
metal .true.
occopt 3
degauss 0.004
fband 0.65
toldfe 1.7e-06
tolwfr 1.1e-16
nstep 600
mixing 0.1
mixing_ndim 20
etol 1.5e-07

###################
acell {1.8897261337300524 1.8897261337300524 1.8897261337300524}
```

```
rprim {
   4.50510 0.00000 0.00000
   0.00000 4.50510 0.00000
   0.00000 0.00000 3.15860
}

pp_list {
   08-O.GGA.fhi
   77-Ir.GGA.fhi
}

ntypat 2
znucl {8 77}

natoms 6
typat {2 2 1 1 1 1}

xred {
   0.50000 0.50000 0.50000
   0.00000 0.00000 0.00000
   0.19230 0.80770 0.50000
   0.80770 0.19230 0.50000
   0.30770 0.30770 0.00000
   0.69230 0.69230 0.00000
}

###################
opf.fill {
   8 O.fill
}
opf.fill {
   8 O.opts
}
diemac 30
nedges 1
edges {-8 1 0}
screen.shells {6.0}
cnbse.rad {6.0}
cnbse.broaden {0.3}
```

```
cnbse.niter 200
scfac 0.8
```

2 Adjusting parameters

Any parameter known to the wrapper can be adjusted. Currently supported parameters are listed in the output from the script above (Excluding the atomic parameters which are defined by the atoms object).

Also, the `nodes` argument is special and will adjust the `para_prefix {srun -n 192}` argument by the corresponding value multiplied by 32. `nodes` will also update in the `run.sh` file.

If a parameter which is not in the supported list is entered, a warning will be raised and the parameter will be ignored.

Notes:

- Perl lists, e.g. `{0.3}`, should be entered as a Python list, e.g. `[0.3]`
- Fortran boolians, e.g. `.true.` should be entered as Python boolians, e.g. `True`

```python
from decaf import Ocean
from ase.io import read

atoms = read('IrO2.traj')

parameters = {
    'nkpt': [5, 5, 5],
    'screen.nkpt': [1, 1, 1],
    'metal': False,
}

calc = Ocean(atoms, **parameters)
inp = calc.write_input()

print(inp)
```

```
ppdir {../}
dft qe
control 0
ser_prefix {srun -n 1}
para_prefix {srun -n 192}
```

```
##################
dft.startingwfc {atomic+random}
dft.diagonalization {david}
dft_energy_range 50
nkpt {5 5 5}
ngkpt {6 6 6}
screen.nkpt {1 1 1}
screen.nbands 2000
ecut 120
core_offset .true.
metal .false.
occopt 3
degauss 0.004
fband 0.65
toldfe 1.7e-06
tolwfr 1.1e-16
nstep 600
mixing 0.1
mixing_ndim 20
etol 1.5e-07

##################
acell {1.8897261337300524 1.8897261337300524 1.8897261337300524}

rprim {
   4.50510 0.00000 0.00000
   0.00000 4.50510 0.00000
   0.00000 0.00000 3.15860
}

pp_list {
   08-O.GGA.fhi
   77-Ir.GGA.fhi
}

ntypat 2
znucl {8 77}

natoms 6
```

```
typat {2 2 1 1 1 1}

xred {
   0.50000 0.50000 0.50000
   0.00000 0.00000 0.00000
   0.19230 0.80770 0.50000
   0.80770 0.19230 0.50000
   0.30770 0.30770 0.00000
   0.69230 0.69230 0.00000
}

###################
opf.fill {
   8 O.fill
}
opf.fill {
   8 O.opts
}
diemac 30
nedges 1
edges {-8 1 0}
screen.shells {6.0}
cnbse.rad {6.0}
cnbse.broaden {0.3}
cnbse.niter 200
scfac 0.8
```