job.sh

```
#!/bin/bash
#SBATCH -A stf006
#SBATCH -J DFT-FE
#SBATCH -t 01:00:00
#SBATCH -p batch
#SBATCH -N 100
#SBATCH --gpus-per-node 8
#SBATCH --ntasks-per-gpu 1
#SBATCH --gpu-bind closest

module load ums
module load ums031

export OMP_NUM_THREADS=1
n=$((SLURM_JOB_NUM_NODES*8))
srun -n $n -c 7 --gpu-bind closest \
        dftfe.real input.prm
```

/sw/frontier/ums/modulefiles/ums031/default.lua

```
load("PrgEnv-amd")
load("amd/5.7.0")
load("cray-mpich/8.1.27")
prepend_path("LD_LIBRARY_PATH",
"/opt/cray/pe/mpich/8.1.27/gtl/lib")

load("craype-accel-amd-gfx90a")
load("openblas/0.3.17")
load("cray-python/3.11.5")
unload("cray-libsci")
load("netlib-scalapack/2.2.0")
prepend_path("PATH", "/sw/frontier/ums/ums031/gcc-mixed-
12.2.0/bin")

setenv("VIRTUAL_ENV", "/sw/frontier/ums/ums031/gcc-mixed-
12.2.0")
setenv("MPICH_GPU_SUPPORT_ENABLED", "1")
setenv("HSA_FORCE_FINE_GRAIN_PCIE", "1")
```

parameters.prm

Parameters Types:
- Input Geometry
- Accuracy
- Convergence
- Output

```
subsection Geometry
  set NATOMS=16
  set NATOM TYPES=4
  set ATOMIC COORDINATES FILE = coordinates.inp
  set DOMAIN VECTORS FILE = domainVectors.inp
  subsection Optimization
    set ION FORCE=true
  end
end

subsection Finite element mesh parameters
  set POLYNOMIAL ORDER=5
  subsection Auto mesh generation parameters
    set MESH SIZE AROUND ATOM  = 0.4
    set ATOM BALL RADIUS = 1.3
  end
end
```

```
subsection Boundary conditions
  set PERIODIC1                 = false
  set PERIODIC2                 = false
  set PERIODIC3                 = false
end

subsection GPU
  set USE GPU=true
  set USE ELPA GPU KERNEL=true
end

subsection SCF parameters
  set MIXING HISTORY   = 20
  set MIXING PARAMETER = 0.2
  set MAXIMUM ITERATIONS          = 50
  set STARTING WFC= ATOMIC
  set TEMPERATURE                 = 500
  set TOLERANCE                   = 1e-5
  subsection Eigen-solver parameters
    set NUMBER OF KOHN-SHAM WAVEFUNCTIONS = 40
  end
end
```

geometry

Documenting Structure Preparation Step / some useful pymatgen commands
- git+https://code.ornl.gov/datatrails/LK99_structure @HEAD:result.yaml

```
result:
  POSCAR:                VASP file
  Pb_apatite.pdb:        PDB
  Pb_apatite.csv:        DFT-FE crd
  Pb_apatite_cell.csv: DFT-FE vec


 environment:
   - type: Python
     specs:
       - pymatgen
```

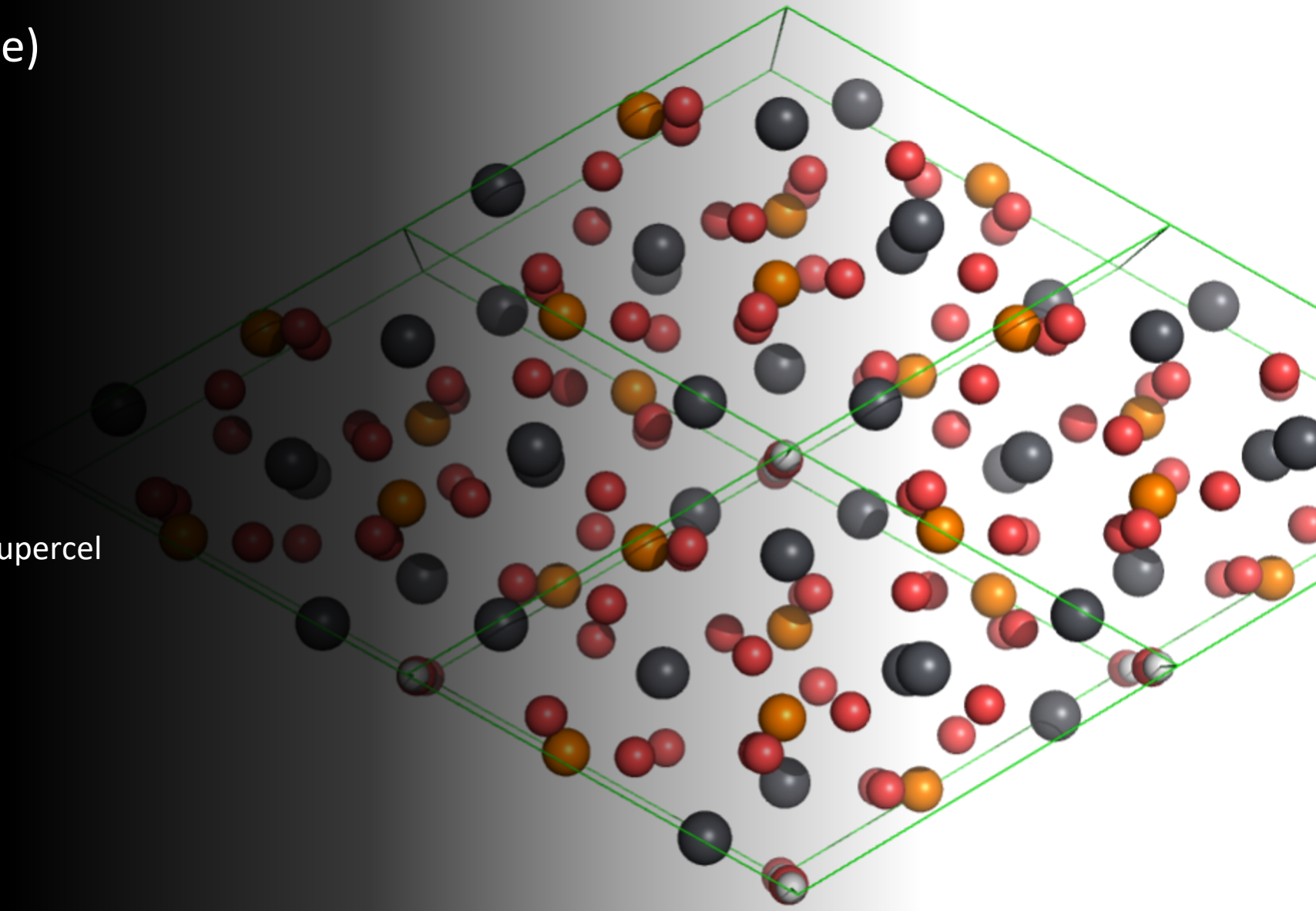
```
script: |
    #!/usr/bin/env python3
    from pymatgen.io.cif import CifParser
    from pymatgen.core import SymmOp

    parser = CifParser("9012631.cif")
    ls = parser.parse_structures()
    assert len(ls) == 1
    structure = ls[0]
    o1 = structure.sites[-2]
    o2 = structure.sites[-1]
    zlen = structure.lattice.c
    structure.insert(len(structure), "H", [o1.a, o1.b, o1.c+0.98/zlen])
    structure.insert(len(structure), "H", [o2.a, o2.b, o2.c+0.98/zlen])

    structure.to('POSCAR')
```

Starting structure (lead apatite)

- pymol Pb_apatite.pdb
- set sphere_scale=0.3
- # render PBC images using https://pymolwiki.org/index.php/Supercell



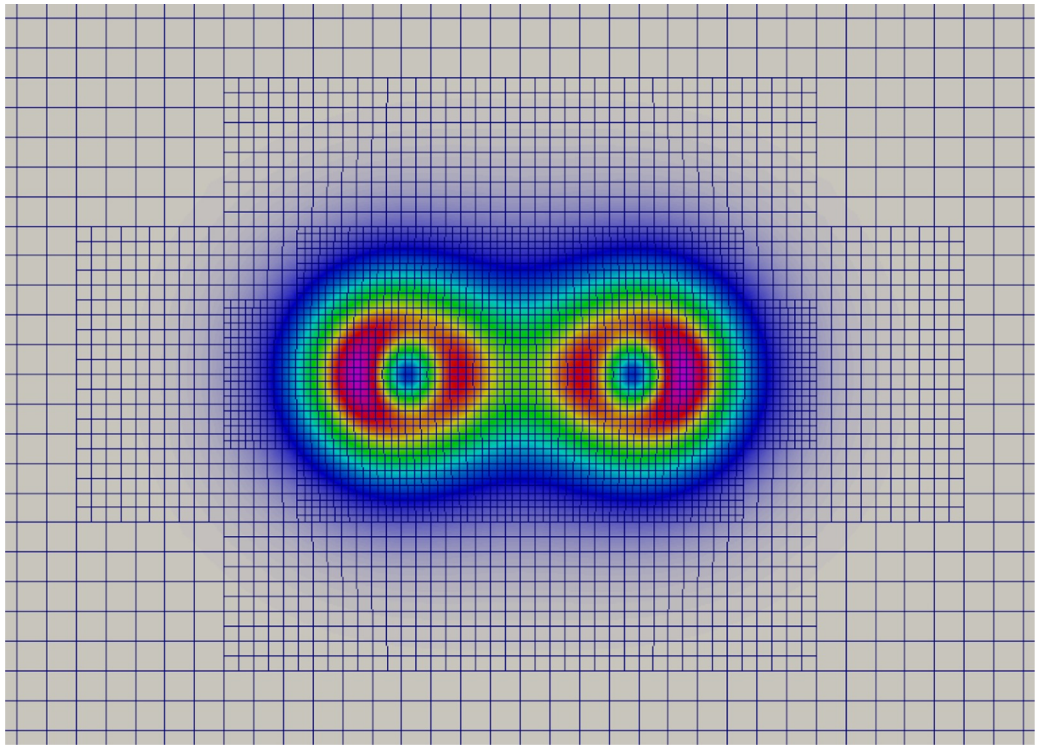
accuracy

POLYNOMIAL ORDER
- 7 for soft pseudopotentials (<20 Ha)
- 6 for hard pseudopotentials
- 5 for all-electrons

MESH SIZE AROUND ATOM

~ inverse of plane-wave cutoff (smaller for high accuracy)
- order 7 <-> 1.5 to 2.5 Bohr
- order 6 <-> 0.5 to 1.5 Bohr
- all-electron <-> 0.5 Bohr

ATOM BALL RADIUS
- 0 = conservative heuristic (good for periodic, pseudopot.)
- pseudopotentials <-> use 3 to 6 Bohr
- all-electron <-> 1.0 - 2.5 Bohr



See: https://github.com/dftfeDevelopers/dftfe-benchmarks/blob/master/accuracyBenchmarks
https://github.com/dftfeDevelopers/dftfe/raw/manual/manual-current-release.pdf (page 18)

convergence

MIXING METHOD
- ANDERSON
- ANDERSON WITH KERKER
- BROYDEN

MIXING HISTORY
- default to 50 steps - OK for metallic systems
- really only need 8-15 steps for systems with a band gap

MIXING PARAMETER
- default 0.2 (keep 80% of old electron density)

KERKER MIXING PARAMETER
- default 0.05, represents k_TF^2

MAXIMUM ITERATIONS – default 200
TOLERANCE – L^2 norm of electron density update (default 1e-5)
STARTING WFC – ATOMIC or RANDOM

output

Sambit Das, 2021
https://github.com/dftfeDevelopers/dftfe-benchmarks/tree/master/accuracyBenchmarks/BCCMo

README.md

Description of the example

This example demonstrates a ground-state calculation with fully periodic boundary conditions on BCC Mo 4x4x4 supercell with a mono-vacancy, containing 127 Mo atoms (1778 electrons) ONCV pseudopotential from sg15 database, PBE exchange correlation, and Fermi-Dirac smearing temperature of 500 K are used.

Studies performed

- i. Ground-state calculation using DFT-FE at a FE discretization commensurate with chemical accuracy (~1e-4 Ha/atom in energy, ~1e-4 Ha/Bohr in ionic forces and ~1e-6 Ha/Bohr^3 in cell stresses). The reference ground-state energy, ionic forces, and cell streses are computed using QUANTUM ESPRESSO (QE) at a high plane-wave cutoff of 50 Ha.

Discussion on the input parameters and the results

- Since it a homogeneous metallic system, we use Keker preconditioner implemented in DFT-FE, via the ANDERSON_WITH_KERKER choice for the MIXING METHOD. We also use a MIXING PARAMETER value of 0.7, which is higher than the default value of 0.2.

Study1---ground-state calculation results

- The run successfully converged in 19 SCF iterations.
- POLYNOMIAL ORDER=7 and MESH SIZE AROUND ATOM=2.0 are found to be sufficient to obtain chemical accuracy as shown below. Total degrees of freedom are 614125 (4835 per atom).
- DFT-FE Energy per atom comparison with QE reference: 8.2e-5 Ha/atom. In particular we compared the "Total energy per atom" printed from DFT-FE output and "(Total energy+TS)/totalNumberAtoms" from QE, since QE's Total energy is the free energy.
- DFT-FE Ionic forces comparison with QE reference: 5.1e-5 Ha/Bohr (max absolute error among all atoms and force components).
- DFT-FE Cell stress comparison with QE reference: 2.6e-6 Ha/Bohr^3 (max absolute error among all stress components)

See: https://github.com/dftfeDevelopers/dftfe/raw/manual/manual-current-release.pdf (page 37)

output

```
================================================
================================================

        Welcome to the Open Source program DFT-FE version     1.0

....

************************Begin Self-Consistent-Field Iteration: 18 *************
ANDERSON_WITH_KERKER mixing, L2 norm of electron-density difference: 1.109052973188105046e-04
Fermi Energy computed: 7.295526075656315612e-01
************************Self-Consistent-Field Iteration: 18 complete**********
Wall time for the above scf iteration: 3.090505490299999991e+01 seconds
Number of Chebyshev filtered subspace iterations: 1

************************Begin Self-Consistent-Field Iteration: 19 ***********
ANDERSON_WITH_KERKER mixing, L2 norm of electron-density difference: 2.964283665712466595e-05
Fermi Energy computed: 7.295525484985341258e-01
************************Self-Consistent-Field Iteration: 19 complete**********
Wall time for the above scf iteration: 3.470953350799999981e+01 seconds
Number of Chebyshev filtered subspace iterations: 1

SCF iterations converged to the specified tolerance after: 19 iterations.
Printing KS eigen values (spin split if this is a spin polarized calculation ) and
fractional occupancies for kPoint 0

0 : -1.513729054128706508e+00      1.000000000000000000e+00
1 : -1.511030179866667433e+00      1.000000000000000000e+00
2 : -1.511030171506868580e+00      1.000000000000000000e+00
3 : -1.511024426169628843e+00      1.000000000000000000e+00
```

```
Energy computations (Hartree)
------------------------------------------------------
Band energy                    :  -3.2289438869100269e+02
Exchange energy                :  -9.1002082914268078e+02
Correlation energy             :  -8.4046241694575798e+01
Total energy                   :  -8.7098294793297136e+03
Total energy per atom          :  -6.8581334482911132e+01
------------------------------------------------------
Total entropic energy: 4.601991873393219013e-04
Total free energy: -8.709829939528901377e+03
Total scf solve, wall time: 802.776s.
```

```
+-----------------------------------------+-----------+------------+
| Total wallclock time elapsed since start  | 9.756e+02s |            |
|                                           |            |            |
| Section                       | no. calls |  wall time | % of total |
+-------------------------------+-----------+------------+------------+
| Atomic system initialization  |         1 | 1.550e-01s | 0.000e+00% |
| Cell stress computation       |         1 | 1.151e+02s |  1.18e+01% |
| Init local PSP                |         1 | 4.616e-01s | 0.000e+00% |
| Ion force computation         |         1 | 8.836e+00s |  9.06e-01% |
| KSDFT problem initialization  |         1 | 2.503e+01s |  2.57e+00% |
| Nuclear self-potential solve  |         1 | 2.152e+01s |  2.21e+00% |
| Total scf solve               |         1 | 8.028e+02s |  8.23e+01% |
+-------------------------------+-----------+------------+------------+

================================================
DFT-FE Program ends. Elapsed wall time since start of the program:
9.757485980801284313e+02 seconds.
```

Key Points

- dftfe.real and dftfe.cplx available on Frontier using ums031 module.
  - See https://docs.olcf.ornl.gov/software/UMS/index.html for more info on UMS/install/etc.
- Example calculations are present on github
- Always add **USE GPU = true** parameter!
- Pay careful attention to accuracy and convergence settings.
- Many types of outputs can be written, but not everything. You can write your own analysis based on the electron density quadrature grid though.