Hackathon summary (DFT interface)

- Sent UnitCell, SuperCell, and Lattice classes to fortran routine dft__interface.F90
  - Would have computed a grid
    - SimpleCartGrid(nGridPts,3), …
  - Evaluated the density at a grid point
    - Density (nGridPts,nBfn)
  - Set necessary parameters for xc_fun lib and compute the V_{xc}
    - Vxc (UnitCell.nBfn,SuperCell.nBfn)

Evolved to programming this in C++

- There exists (G. K.) a routine that computes value of basis functions at a point
  - eval_basis_fn_on_grid

```
FORTINT nComp = 1;
FORTINT DerivOrder = 0;
FORTINT nMap;
FORTINT nGridPts = nGridPtCart;
uint TotNBfn = Solid.UnitCell.OrbBasis.nFn; //+ Solid.SuperCell.OrbBasis.nFn;
  xout << " TotNBfn " << TotNBfn << std::endl;
  FORTINT *pCentersOut[TotNBfn]; // used in gradient evaluation
  FORTINT *pMap[TotNBfn];
  double pOut[nGridPts * nComp * TotNBfn];
  FD(eval_basis_fn_on_grid)(&pOut[0],nComp,
            *pCentersOut, *pMap, nMap,
            Solid.UnitCell.OrbBasis, SimpleCartGrid, nGridPts,
            DerivOrder, ic);
```

```
FD(eval_basis_fn_on_grid)(&pOut[0],nComp,
            *pCentersOut, *pMap, nMap,
            Solid.UnitCell.OrbBasis, SimpleCartGrid, nGridPts,
            DerivOrder, ic);
```

```
void FD(eval_basis_fn_on_grid)(double *pOut, FORTINT const &nCompSt,
   FORTINT *pCentersOut, FORTINT *pMap, FORTINT &nMap,
   FBasisSet const &Basis, double  (*pGridPt)[3], FORTINT const &nGridPt,
   FORTINT const &DerivOrder, FORTINT &iContext);
```

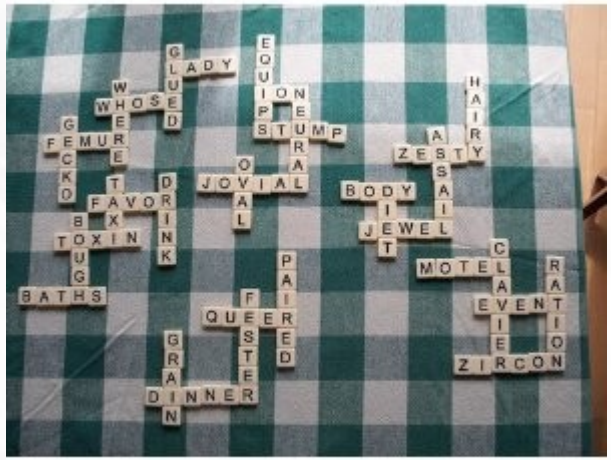
```
(*pOut)[0] = -0.282942
(*pOut)[1] = -0.278048
(*pOut)[2] = -0.272913
(*pOut)[3] = -0.267573
(*pOut)[4] = -0.262063
(*pOut)[5] = -0.256413
(*pOut)[6] = -0.250656
```

```
wheee!!
 Number of basis functions in unit cell:                    2
 Number of basis functions in supercell:                  128
 Number of unit cells in supercell:                 4                   4
4
 Size of matrices as expected
Segmentation fault
```

Next step: Obtain V_{xc}

- xc_fun is a C library that will compute exchange-correlation functionals

- Environment
  - Enjoyed the communal setting, though we typically get extremely focused
  - Analogous to the game Bananagram



- C++/Fortran interface is not ideal on Fortran users end
  - Solution: Learn C++