

- Grid_class:

Generate the grid point from a set of non-orthogonal lattice vectors

```
grid_3d::grid_3d( FSolidModel& Solid );
```

- AO basis value generating

Using Gerald's basis function value generator

```
FD(eval_basis_fn_on_grid)( pOrbVal, nComp, pCenterIndices, pMap, nMap, *p_bas, GridPt, nGridPt, nDiffBf, ic );
```

TO DO:

Need a real one-body density matrix to test the charge density generating

Fourier transformation

- Solving the Poisson Equation in k space
- Transform electron density to k space, get the potential, then transform the potential back to real space
- Using FFTW
- Future: make the code parallelized
multi-thread FFTW
FFTW with MPI