Periodic Hartree-Fock: Hackaton 1 report

Progress (aka, what did I do):

- Implemented some 2e integral kernels [erf(r)/r, erfc(r)/r, r^{2n} exp(-w r^2)]

  (note: integrals and kernels are separated in AIC --- those kernels work in *all* routines)

- Implemented efficient 2e2c integral routines (mainly for overlap, kinetc, etc).

  (we now have the very fastest two-center integrals over contracted Gaussians for non-separable kernels)

Next steps:

- Improve integration of integral/orbital on grid routines with code.

  (in particular: screening ranges, super-cell translational symmetric orbitals on grid, interface examples)

- Tight binding band structure

  (requires $S^{-1/2}$, Fock matrix diagonalization, density matrix construction, symmetrized real-space vs k-space transformations [via Naoki], etc)

Next time:

- Would prefer having a day at the office.