Short description for multi processor SPRKKR calculations

Currently version 5.4 of SPRKKR supports kkrscf and embscf calculations with MPI. MPI is currently not supported for kkrgen. A special binary of kkrscf is needed to perform parallel calculations. To use openmpi to compile this binary, edit the file make.inc and:

- supply information about basic linear algebra libraries, e.g.

```
LIB = -L/usr/local/intel/mkl/1x.insertversion/lib/em64t \
          -lmkl_intel_lp64 -lmkl_lapack -lmkl_sequential \
          -lguide -lpthread -lmkl_core
```

- supply information on openmpi includes, e.g.

```
INCLUDE = -I/usr/lib/openmpi/include
```

- set the fortran compiler to the openmpi compiler wrapper mpif90.openmpi

```
FC = mpif90.openmpi -c $(FFLAGS) $(INCLUDE)
LINK = mpif90.openmpi  $(FFLAGS) $(INCLUDE)
```

Then use

```
user@linux:/$  make scfmpi
```

to generate a binary called kkrscf5.4MPI. To run this binary, use

```
user@linux:/$  mpirun -np 4 kkrscf5.4MPI INPUT > OUTPUT
```

where in this example the number of used processors is set to 4. Please note that the < pipe symbol in front of the input which is needed in single processor calculations has to be omitted in multi processor calculations.

In scf calculations the energy loop is parallelized. To obtain optimal performance, consider using a number of energy points (variable NE = { } in the input file) which is a multiple of your available CPUs.