ecalj Install

1. Install fortran compilars and some tools

We need following tools to generate fortran binaries. ecalj made from source codes at `ecalj/SRC/main/*.f90` and `ecalj/SRC/subroutines/*.f90`.

- git (Tto download the ecalj. It is convenient to upgrade your code)
- Fortran compiler (we can choose gfortran, ifort, or nvfortran)
- Math library (blas, lapack, fft). We can usually use intel-mkl.
- MPI library (open mpi works for ubuntu24)
- cmake, make, bash, gnuplot

We can use apt to install them when ubuntu. Similar in other systems, or your system already have.

I use following versions for thinkpad T14: ubuntu 24.04
openmpi-bin/noble,now 4.1.6-7ubuntu2 amd64
openmpi-common/noble,noble,now 4.1.6-7ubuntu2 all
cmake/noble,now 3.28.3-1build7 amd64
make/noble,now 4.3-4.1build2 amd64
gfortran/noble,now 4:13.2.0-7ubuntu1 amd64
intel-mkl/noble,now 2020.4.304-4 amd64

2. Install `python` and required tools using `mise`

> [!TIP]
> For the case the default version of Python is outdated (python >3.9 needed). We will prepare the latest Python in your ./local.
> The mise is a package management software. We can use anaconda instead. Or you can install tools at the following step 4.

PROF

1. Add the following settings to `~/.bashrc` for the automatic installation and activation of `mise`:

```
export PATH="$HOME/.local/bin:$PATH"
type mise > /dev/null 2>&1 || curl https://mise.run | sh
eval "$(~/.local/bin/mise activate bash)"
```

2. Update `~/.bashrc` to install `mise`:

```
source ~/.bashrc
```

3. Install `python` using `mise`:

```
mise use python@latest -g
```

4. Install the required `python` libraries:

```
pip install numpy pandas seekpath spglib pymatgen mp-api scipy plotly
```

3. Install and InstallTest

For ohtaka and kugui in ISSP, skip here and see here

We recommend you to check ecalj/InstAll at first. InstallAll writes files to your $HOME/bin.
Add $HOME/bin to your path. (The install directory is `BINDIR = os.path.join(HOME, 'bin')`. to `BINDIR = os.path.join(HOME, 'bin2')`, for example, to change install directory).

Run the following command at ecalj/

```
FC=ifort ./Installall [Options]
(We can use gfortran or nvfortran instead of ifort)
```

It performs compile and link followed by the install test at ecalj/SRC/TestInstall/. (testecalj.py is the script for test)
If succeeded, we see 'OK! All PASSED!' at the end of tests.
The compile and install test may take 5~10 minutes (usually laptop is faster).

Following options are valid
Options:

PROF

- `-np` [value]:
  default: 8
  specify the number of MPI parallelization in test calculation
- `--clean`
  default: none
  delete the cache files before compiling
- `--gpu`
  default: none
  compile the GPU and GPU-MP version

- Qiitaでの解説(https://qiita.com/takaokotani/items/9bdf5f1551000771dc48)