
MCSMRFF Documentation

Release 0.0.1

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A LAMMPS fix for parameterizing Tersoff potentials. Optional Coulombic and Lennard-Jones contributions are available for the range outside the Tersoff cutoffs.

Getting started

1. Download [LAMMPS](<http://lammps.sandia.gov/download.html>) ([older versions here](<http://lammps.sandia.gov/tars/>)). Some versions will not work - the 7 Dec 2015 is the one we've tested the most, so use that one.
2. Open a terminal in the src directory in your lammps folder
3. In your LAMMPS src directory run *make yes-manybody*
4. If you don't have an SSH key, generate one like this:

```
ssh-keygen -t rsa -b 4096 -C "your_email@example.com" #Creates an ssh key, using your GitHub
e-mail as a label
```

When prompted to "Enter a file in which to save the key," press Enter If asked to Overwrite, enter 'y' At the prompt, type a secure passphrase Retype your secure passphrase

5. Adding a new SSH key to your GitHub account

```
gedit ~/.ssh/id_rsa.pub
```

In the top right corner of any GitHub page in your browser, click on your profile photo, then click 'Settings' In the user settings sidebar, click 'SSH keys' Click 'New SSH key' In the "Title" field, add a descriptive label for the new key Copy and Paste the contents from the 'id_rsa.pub' file into the "Key" field Click 'Add SSH key'

6. Load your keys into your SSH agent

```
eval "$(ssh-agent -s)"
```

```
ssh-add
```

Enter passphrase

7. Test your SSH connection

```
ssh -T git@github.com
```

You should see the message "Hi 'username'! You've successfully authenticated, but GitHub does not provide shell access."

8. Clone repository wherever

```
git clone git@github.com:hherbol/Grad-MCSMRFF.git
```

9. Copy over contents of Grad-MCSMRFF/LAMMPS to your lammps src folder. Note, this overwrites the min.h and pair_tersoff.h files.

10. Make using the new Makefile.mcsmrff

```
make mcsmrff -j 4
```

11. You're done! Now you can use lammps with the `imp_mcsmrff` file in your lammps/src directory.

To parameterize a force field

1. Build example structures for your system in Avogadro (including any OPLS bonds)
2. Optimize with orca (e.g. Opt B97-D3 def2-TZVP)
3. Analyze at higher level (e.g. SP RI-B2PLYP D3BJ def2-TZVP)
4. Great a training set directory that houses directories for each orca result. Each directory must include the .out, .engrad and system.cml file for that system

5. Run `python gradient_tersoff.py RUN_NAME`. The output parameters will start to appear in `lammps/RUN_NAME_best.tersoff`.
6. ...

INDICES AND TABLES

- `genindex`
- `modindex`
- `search`