HiLDe
Lattice Dynamics with python

Florian Knoop

hilde

Project ID: 8260678

Star 3 | Fork 1 | Clone

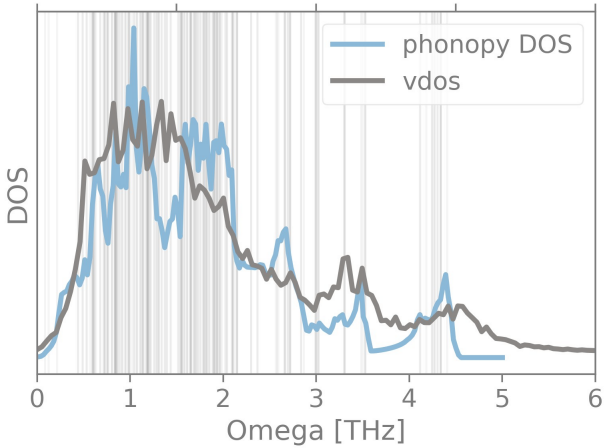
ISC License | **1,550** Commits | **8** Branches | **3** Tags | **21.3 MB** Files

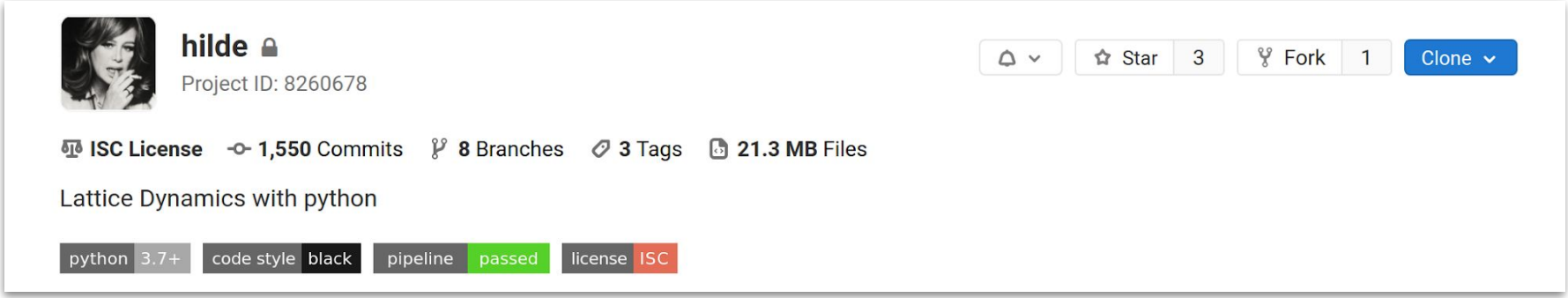
Lattice Dynamics with python

python 3.7+ | code style black | pipeline passed | license ISC

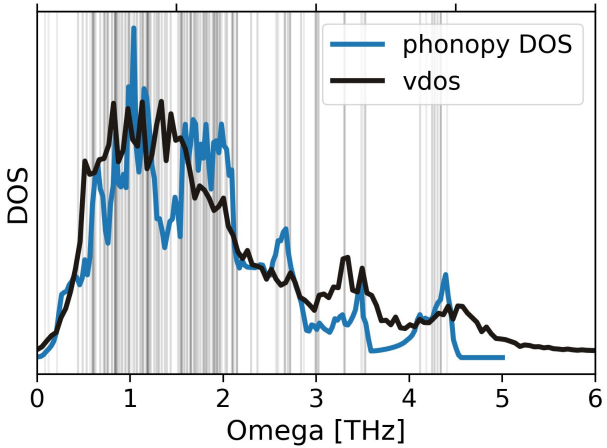
gitlab.com/flokno/hilde

- **H**aber **I**nstitute **L**attice **D**ynamics **E**nvironment
  - python package for **lattice dynamics investigations with FHIaims**
  - built on top of **ase**
- Current Features
  - **phonopy** calculations ➔ Handson 2019
  - **MD + heat flux** simulations
  - **toolset** for preparing, and analyzing data
  - high throughput functionality via ***fireworks***
    - ➢ Tom





- **H**aber **I**nstitute **L**attice **D**ynamics **E**nvironment
  - python package for **lattice dynamics investigations with FHIaims**
  - built on top of **ase**
- Current Features
  - **phonopy** calculations ➔ Handson 2019
  - **MD + heat flux** simulations
  - **toolset** for preparing, and analyzing data
  - high throughput functionality via ***fireworks***
    - ➢ Tom



hilde: how to run an **MD**? Write **md.in**:

```
[geometry]
file:               geometry.in.supercell_120.300K

[control]
xc:                 pbesol
k_grid:             [2, 2, 2]
charge_mix_param:   0.3
sc_accuracy_rho:    5e-6

[basissets]
default:            light
```

hilde: how to run an **MD**? Write **md.in**:

```
[geometry]
file:               geometry.in.supercell_120.300K

[control]
xc:                 pbesol
k_grid:             [2, 2, 2]
charge_mix_param:   0.3
sc_accuracy_rho:    5e-6

[basissets]
default:            light

[md]
timestep:           5
maxsteps:           2000
driver:             Langevin
temperature:        300
friction:           0.02
compute_stresses:   10
```

hilde: how to run an **MD**? Run!

```
➢ hilde run md
```

hilde: how to run an **MD**? Run!

```
➢ hilde run md

[hilde.run]    run MD workflow with settings from md.in

[md]           driver: Langevin
[md]           settings:
[md]             type: molecular-dynamics
[md]             md-type: Langevin
[md]             timestep: 0.4911347394232032
[md]             temperature: 0.02585199101165164
[md]             friction: 0.02
[md]             fix-cm: True
```

hilde: how to run an **MD**? Run!

```
➢ hilde run md

[hilde.run]    run MD workflow with settings from md.in

[md]           driver: Langevin
[md]           settings:
[md]             type: molecular-dynamics
[md]             md-type: Langevin
[md]             timestep: 0.4911347394232032
[md]             temperature: 0.02585199101165164
[md]             friction: 0.02
[md]             fix-cm: True
[md]           Resume from step 2000 in
/home/knoop/working/projects/Talks_Presentations/coffee_talk_19-8/md/trajectory.son
[md]           Compute atomic stress every 10 steps
[watchdog]     seems we are not on a cluster, nothing to do for watchdog
[socketio]     Use SocketIO with port 12345
[md]           run already finished, please inspect
/home/knoop/working/projects/Talks_Presentations/coffee_talk_19-8/md
[md]           done.
```

hilde: how to run an **MD**? Run!

```
➢ hilde run md

[hilde.run]    run MD workflow with settings from md.in

[md]           driver: Langevin
[md]           settings:
[md]             type: molecular-dynamics
[md]             md-type: Langevin
[md]             timestep: 0.4911347394232032
[md]             temperature: 0.02585199101165164
[md]             friction: 0.02
[md]             fix-cm: True
[md]           Resume from step 2000 in
/home/knoop/working/projects/Talks_Presentations/coffee_talk_19-8/md/trajectory.son
[md]           Compute atomic stress every 10 steps
[watchdog]     seems we are not on a cluster, nothing to do for watchdog
[socketio]     Use SocketIO with port 12345
[md]           run already finished, please inspect
/home/knoop/working/projects/Talks_Presentations/coffee_talk_19-8/md
[md]           done.
```

➜ Output file: **trajectory.son**

hilde: read **trajectory.son**

```
{"MD": {
  "type": "molecular-dynamics",
  ...},
"calculator": {
  "calculator": "Aims",
  "calculator_parameters": {
    "xc": "pbesol",
    "k_grid": [2, 2, 2],
    ...}},
"atoms": {
  "cell":
    [[ 8.33141234000000e+00, -8.33141234000000e+00,  0.00000000000000e+00],
     [ 8.33141234000000e+00,  8.33141234000000e+00,  0.00000000000000e+00],
     [ 0.00000000000000e+00,  0.00000000000000e+00,  1.24971185100000e+01]],
  "positions":
    [[ 0.00000000000000e+00,  0.00000000000000e+00,  0.00000000000000e+00],
     [ 4.16570617000000e+00,  0.00000000000000e+00,  0.00000000000000e+00],
   ...}
===
...
```

github.com/flokno/son

pypi.org/project/son

hilde: read **trajectory.son**

```
{<<metadata json block>>}
===
{"atoms": {
  "info": {
    "nsteps": 0,
    "dt":  4.91134739423203e-01,
    "aims_uuid": "D985353A-F8FD-4635-A939-E129A7E6E146"},
  "positions":
    [[ 0.00000000000000e+00,  0.00000000000000e+00,  0.00000000000000e+00],
     [ 4.16570617000000e+00,  0.00000000000000e+00,  0.00000000000000e+00], …}
---
...
```

hilde: read **trajectory.son**

```
{<<metadata json block>>}
===
{<<structure  0 data>>}
---
{<<structure  1 data>>}
---
{<<structure  2 data>>}
---
{<<structure  3 data>>}
---
{"atoms": {
  "info": {
    "nsteps": 4,
    "dt":  4.91134739423203e-01,
    "aims_uuid": "D985353A-F8FD-4635-A939-E129A7E6E146"},
  "positions":
    [[ 1.62463733205010e-04,  7.52668360843155e-04, -4.84513363592926e-05],
     [ 4.16666097188355e+00, -4.45877229739784e-04, -3.12871862455504e-04], …}
---
...
```

hilde: extract data from trajectory.son

```
➢ hilde output md trajectory.son
```

trajectory.nc : netCDF (hdf5) file containing an **xarray.Dataset**

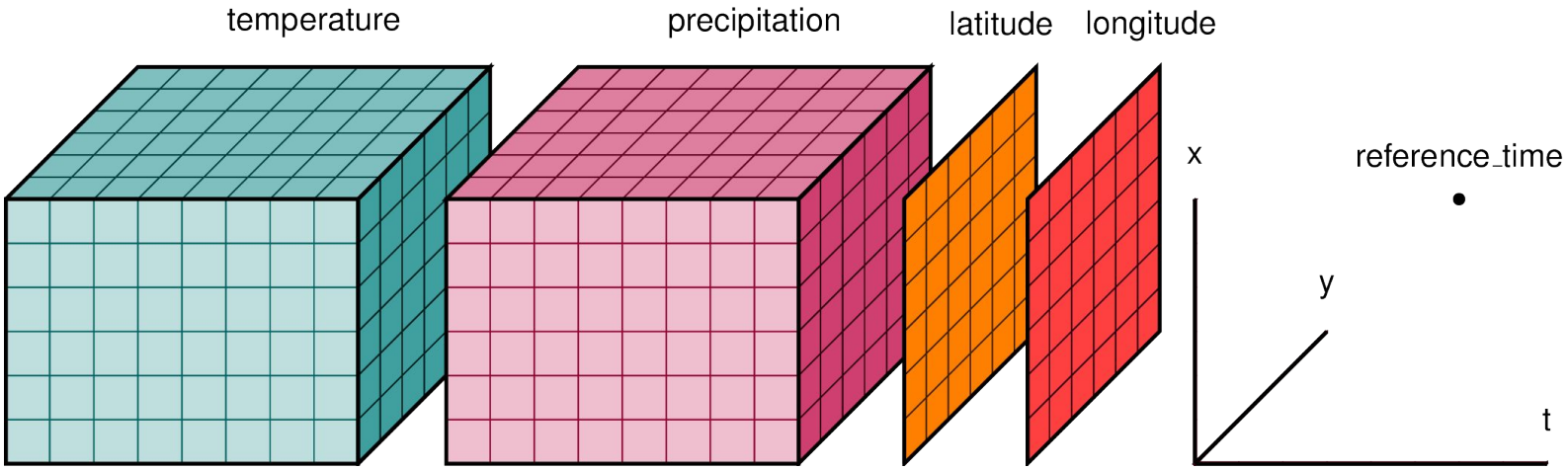
hilde: extract data from trajectory.son

```
➢ hilde output md trajectory.son

Extract Trajectory dataset from trajectory.son
[trajectory]   Parse trajectory
[son] read file:  trajectory.son
[son] process:    |||||||||||||||||||||||||||||||||||||||  2002/2002
.. create atoms:  |||||||||||||||||||||||||||||||||||||||  2001/2001
[trajectory]   .. done in 1.639s
[trajectory]   Get positions from trajectory
[trajectory]   .. time elapsed: 0.038s
[trajectory]   Get velocities from trajectory
[trajectory]   .. time elapsed: 0.009s
[trajectory]   Get pressure from trajectory
[trajectory]   .. time elapsed: 0.308s

Trajectory dataset written to trajectory.nc
```

trajectory.nc : netCDF (hdf5) file containing an **xarray.Dataset**

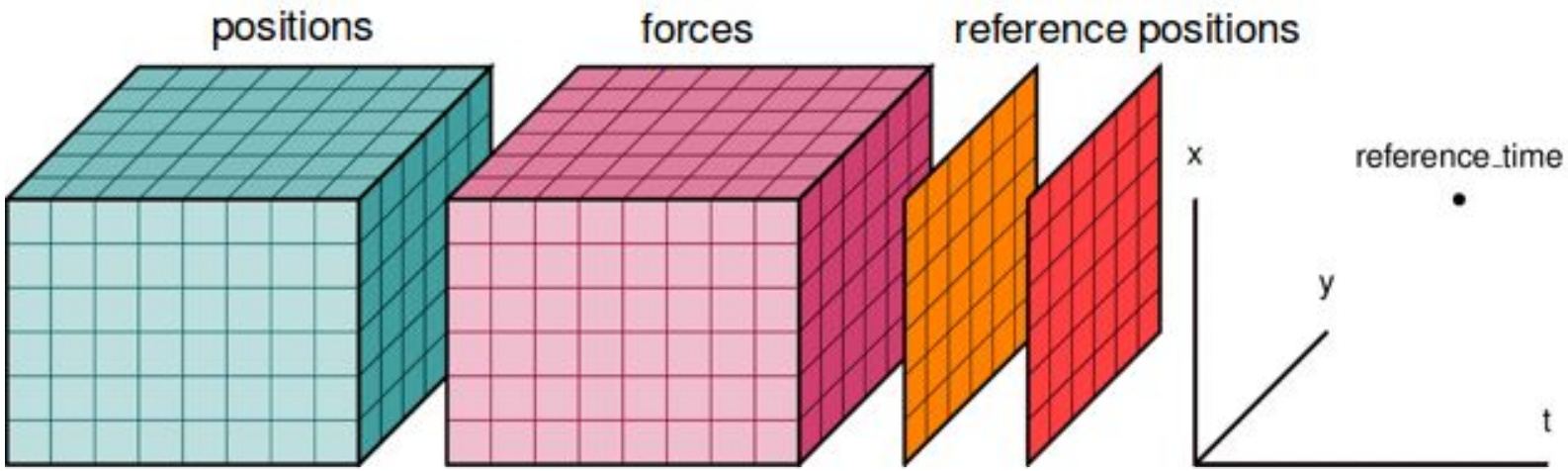
¿ xarray.Dataset ?

- Similar to pandas.DataFrame
  - for **multi-dimensional data** (former pandas.Panel)
- Philosopy: Data should be **bundled** and **labelled**
  - compare **.xyz files**
- xarray.pydata.org/en/stable/why-xarray.html



¿ xarray.Dataset ?

- Similar to pandas.DataFrame
  - for **multi-dimensional data** (former pandas.Panel)
- Philosopy: Data should be **bundled** and **labelled**
  - compare **.xyz files**
- xarray.pydata.org/en/stable/why-xarray.html



hilde: inspect trajectory dataset

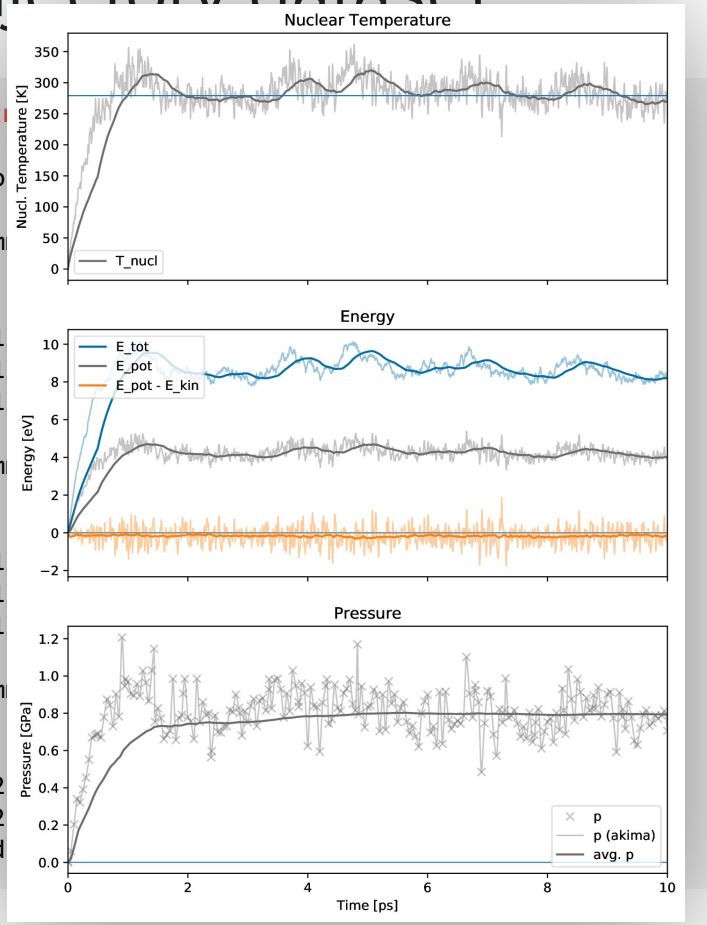
```
➢ hilde info netcdf trajectory.nc

<xarray.Dataset>
Dimensions:           (atom: 120, i: 3, j: 3, time: 2001)
Coordinates:
  * time              (time) float64 0.0 5.0 10.0 ... 9.99e+03 9.995e+03 1e+04
Dimensions without coordinates: atom, i, j
Data variables:
    positions         (time, atom, i) float64 ...
    velocities        (time, atom, i) float64 ...
    forces            (time, atom, i) float64 ...
    kinetic_energy    (time) float64 ...
    potential_energy  (time) float64 ...
    stress            (time, i, j) float64 ...
    pressure          (time) float64 ...
    temperature       (time) float64 ...
Attributes:
    System Name:                    BaHfO3
    natoms:                         120
    time unit:                      fs
    timestep:                       5.0
    nsteps:                         2000
    volume:                         1734.910767022666
    symbols:                        ['Ba', 'Ba', 'Ba', 'Ba', 'Ba', 'Ba', 'Ba'...
    masses:                         [137.327 137.327 137.327 137.327 137.327 ...
```

hilde: inspect trajectory dataset

```
➢ hilde info md trajectory.nc --plot

Dataset summary for trajectory.nc:

[info]         Summarize Temperature
Simulation time:            10.000 ps (2001 steps)
Temperature:                   279.270 +/-      40.4779 K
Temperature (1st 1/3):         261.954 +/-      59.1326 K
Temperature (2st 1/3):         294.874 +/-      21.3062 K
Temperature (3st 1/3):         280.982 +/-      20.5579 K

[info]         Summarize Potential Energy
Simulation time:            10.000 ps (2001 steps)
Pot. Energy:              -15676395.140 +/-       0.6166 eV
Pot. Energy (1st 1/3):    -15676395.381 +/-       0.9148 eV
Pot. Energy (2st 1/3):    -15676394.917 +/-       0.3248 eV
Pot. Energy (3st 1/3):    -15676395.121 +/-       0.3012 eV

[info]         Summarize Pressure
Simulation time:            10.000 ps (218 of 2001 steps)
Pressure:                     0.792685 +/-   0.164142 GPa
Pressure (last 1/2):          0.792882 +/-   0.105375 GPa
Pressure (last 1/2):          0.004949 +/-   0.000658 eV/AA**3
.. summary plotted to md_summary.pdf
```

hilde: inspect trajectory dataset

```
➢ hilde info md tr

Dataset summary fo

[info]          Sum
Simulation time:
Temperature:
Temperature (1st 1
Temperature (2st 1
Temperature (3st 1

[info]          Sum
Simulation time:
Pot. Energy:
Pot. Energy (1st 1
Pot. Energy (2st 1
Pot. Energy (3st 1

[info]          Sum
Simulation time:
Pressure:
Pressure (last 1/2
Pressure (last 1/2
.. summary plotted
```



Now what?