FLAME: a library for atomistic modeling environments

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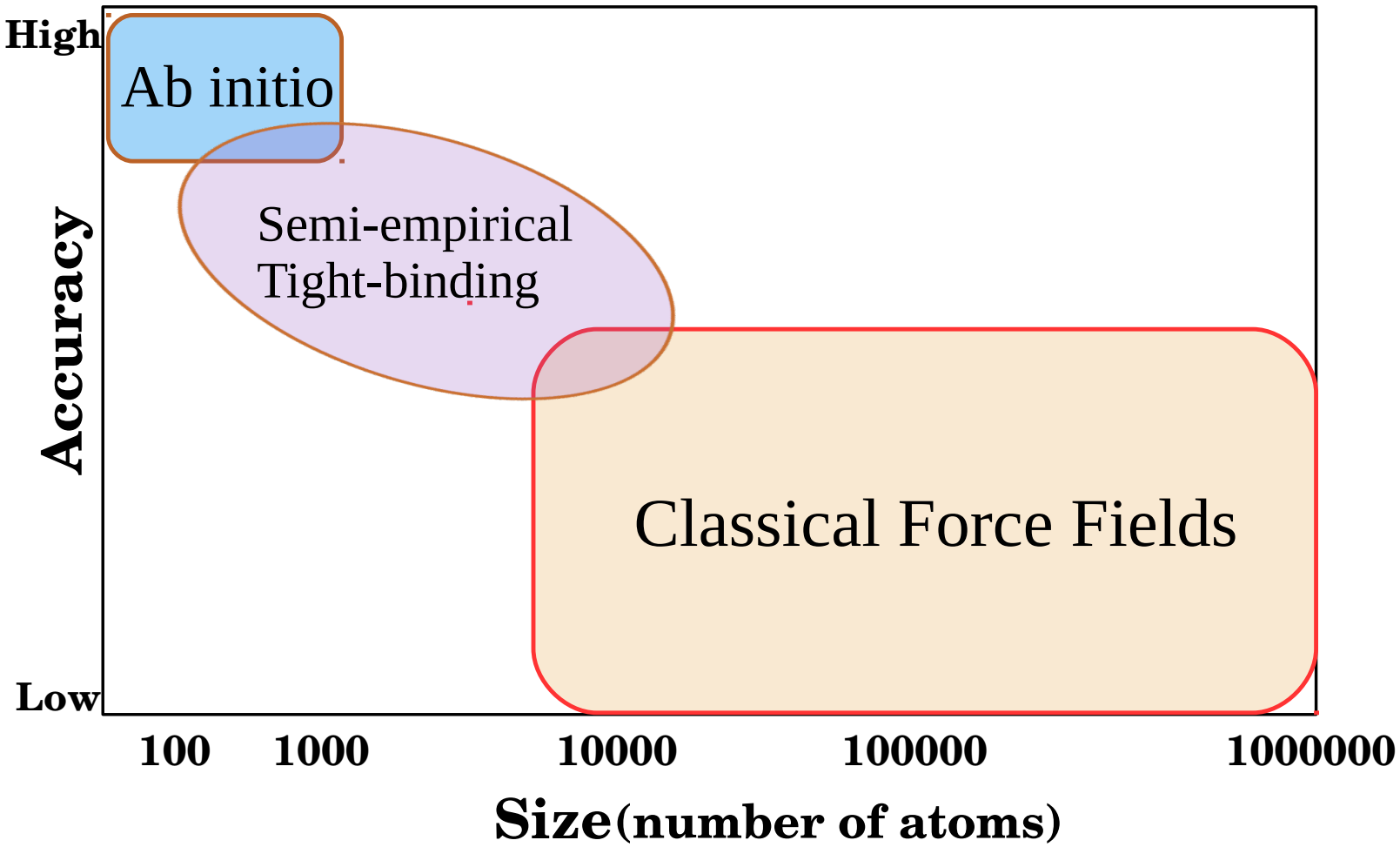
FLAME?


High
Low
Accuracy
Ab initio
Semi-empirical
Tight-binding
Classical Force Fields
100
1000
10000
100000
1000000
Size(number of atoms)

Functionalities and link other codes

- Implemented within FLAME
  - Local optimization (SD, CG, FIRE, BFGS, SQNM)
  - Global optimization
  - Molecular dynamics
  - Interatomic potentials based on machine learning
  - Electrostatic interactions
  - Transition state search
  - Similarity recognition of structures
  - Bader charge analysis
- Linked with other software packages (FLAME $\leftrightarrows$ other)
  - The BigDFT : Poisson's solver
  - LAMMPS: Molecular dynamics and other functionalities
  - Several other packages (VASP, SIESTA, ABINIT, QUANTUMESPRESSO, $\cdots$)

Programming languages and libraries

- Programming languages
  - Fortran: main language of the code
  - Python: a number of scripts
  - C/C++: a few potentials and several core routines
- Libraries
  - futile: a prequisite, included in the FLAME
  - libyaml: a prequisite for futile, included in the FLAME
  - autotools: a prequisite for installation, available on Linux repositories
  - spglib: optional, freely available on GitHub
  - BLAS/LAPACK: a prequisite, we suggest Intel MKL

YAML: input and output files

- *flame_in.yaml* is the main input file of FLAME, an example:

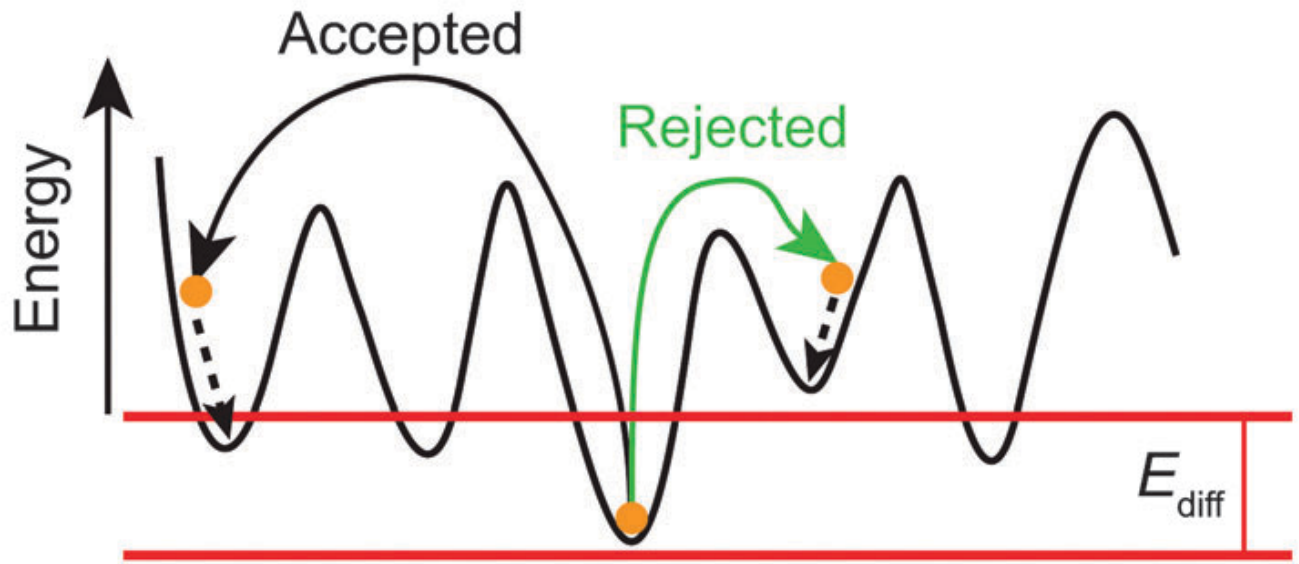
```
main:
    task: single_point
    types: Au

potential:
    potential: qsc

single_point:
    print_force: True
```

- *flame_log.yaml* is the main output file of FLAME.

The minima hopping method



S. Goedecker, J. Chem. Phys, 120, 9911 (2004)
M. Amsler, S. Goedecker, J. Chem. Phys, 133, 224104 (2010)

- *task: minhopp*
- *task: minhocao*

Input parameters for task minhopp

```
minhopp:
    nstep: 100
    nsoften: 20
    mdmin: 3
    etoler: 1.E-3
    nrandoff: 5
    eref: -44.325801
    npminx: 5000
    trajectory: True
    print_force: True
```

- nstep: number of Monte Carlo steps
- nsoft: number of softening steps (project out, velocity, high-f modes)
- mdmin: MD escape stops at the mdmin-th minimum along trajectory

NVT molecular dynamics: The Nose-Hoover thermostat

$$\dot{r}_i = \frac{p_i}{m_i}$$

$$\dot{p}_i = -\frac{\partial U(r)}{\partial r_i} - p_i \dot{\xi}$$

$$\ddot{\xi} = \frac{1}{Q}\left[\sum_{i=1}^{N} \frac{p_i^2}{m_i} - N_f k_B T\right]$$

- N_f: number of real degrees of freedom
- k_B: Boltzmann constant
- T: target temperature
- Q: fictitious mass

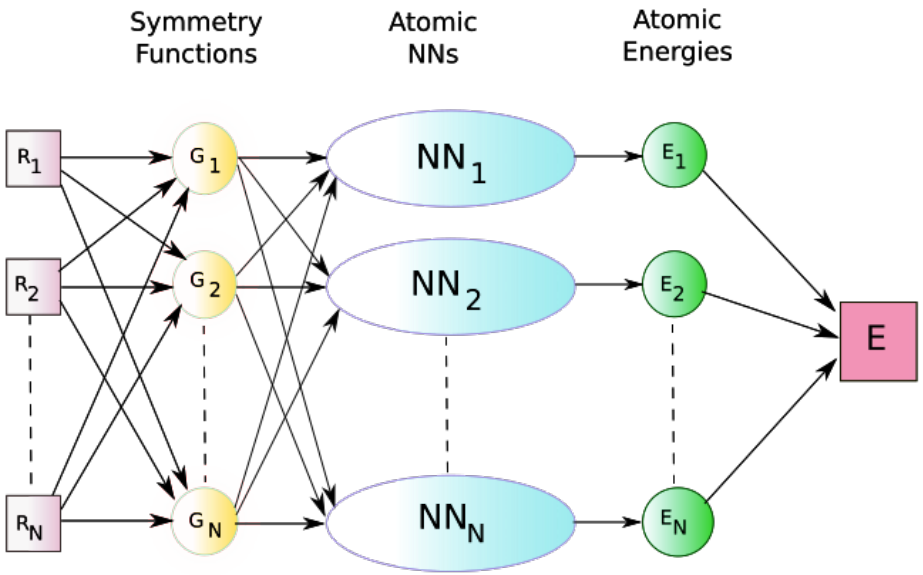
Input parameters for task dynamics

```
main:
    task: dynamics
    types: Na Cl

potential: INCOMPLETE

dynamics:
    md_method : nvt_nose
    #md_method : nvt_longev
    dt : 82                 # ~2 fs
    nmd : 10000
    temp : 300              # K
    init_temp : 300         # K
    ntherm : 2
    highest_freq : 10       # THz
```

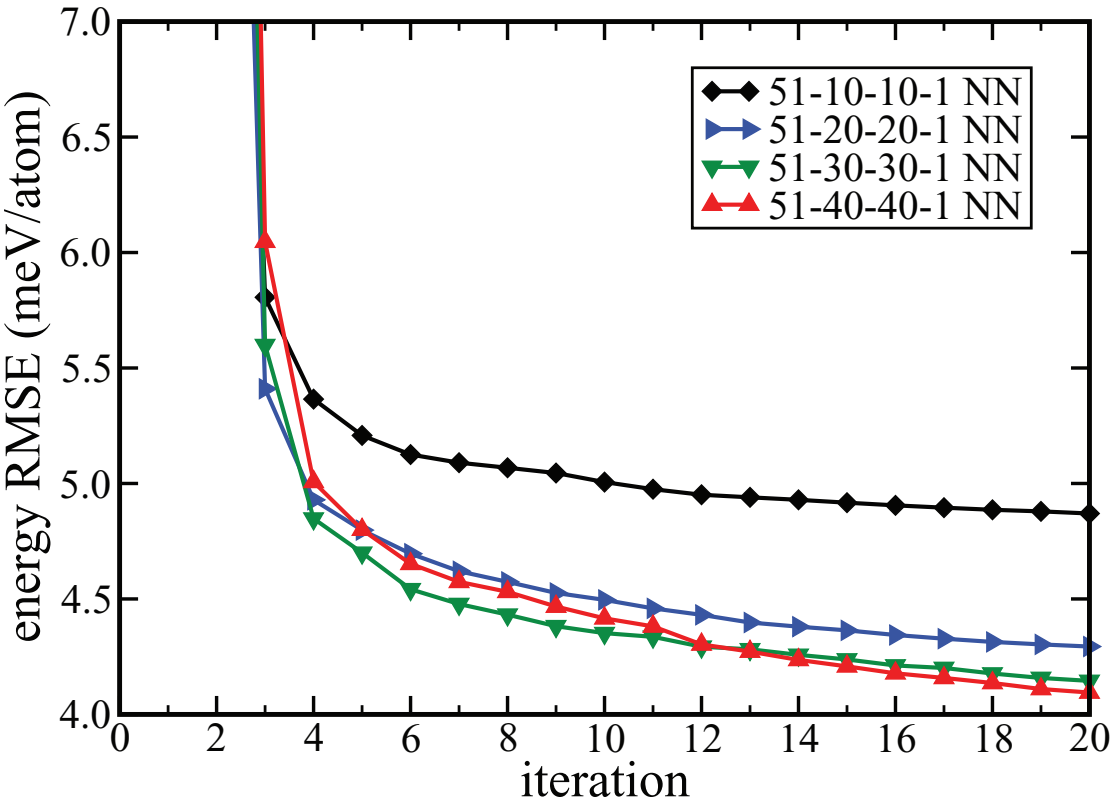
High-dimensional neural network potential



$$E = \sum_{i=1}^{N} E_i \quad \text{where} \quad E_i = f_1^3 \left(b_1^3 + \sum_{k=1}^{N_2} a_{k1}^{23} f_k^2 \left(b_k^2 + \sum_{j=1}^{N_1} a_{jk}^{12} f_j^1 \left(b_j^1 + \sum_{i=1}^{N_0} a_{ij}^{01} G_i \right) \right) \right).$$

J. Behler and M. Parrinello, Phys. Rev. Lett. **98** (2007) 146401.

Training Neural Network Potential



- penalty $= \frac{1}{2N}\sum_{i=1}^{N}(E_{i,NN} - E_{i,ref})^2$
- Data points are splitted into three sets, namely training, validation, and test.

input parameter task train

```
main:
    task : ann
    seed : 535424
    types : B
    verbosity : 1

ann:
    subtask : train
    optimizer : rivals
    approach : atombased
    nstep_ekf : 20
    nconf_rmse : 500
    ampl_rand : 0.05
    symfunc : only_calculate
    print_energy : True
```

Boundary conditions

There are four types of boundary conditions (BC) in FLAME

Key	periodic directions	open directions
free	zero	three
wire	one	two
slab	two	one
bulk	three	zero

Boundary condition must be given in the input file of structure.

Electrostatic interaction

- Hartree energy of superposition of atomic Gaussian charges in bulk BC
- Solving Poisson's equation for slab BC
- Point particle charges in slab BC
- Electrostatic interactions of charged particles confined by parallel metallic plates
- Electrostatic interactions of charged particles confined by dielectric materials
- For other types of BCS and continuous charge densities, FLAME uses the BigDFT PSolver.
- Ewald-type techniques can be used for (almost) all types of electrostatic interactions.

Calculation of Hartree energy in CENT

- For free boundary conditions:
  - Direct approach
  - Gradient-based iterative methods
- Fully periodic systems
  - Iterative methods using Fourier summation for smaller systems

$$E_L(\mathbf{r}) = \frac{2\pi}{V} \sum_{\mathbf{k}\neq 0}{}' \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{q_i q_j}{\mathbf{k}^2} e^{i\mathbf{k}.(\mathbf{r}_i - \mathbf{r}_j)} e^{-(\alpha_i^2+\alpha_j^2)\mathbf{k}^2/4}$$

$$= \frac{2\pi}{V} \sum_{\mathbf{k}\neq 0}{}' \frac{1}{\mathbf{k}^2} \left\{ \left| \sum_{i=1}^{N} q_i cos(\mathbf{k}.\mathbf{r}_i) e^{-\alpha_i^2\mathbf{k}^2/4} \right|^2 + \left| \sum_{i=1}^{N} q_i sin(\mathbf{k}.\mathbf{r}_i) e^{-\alpha_i^2\mathbf{k}^2/4} \right|^2 \right\},$$

  - BigDFT Poisson's solver
- Surface boundary conditions
  - The P^{3}D method, S. A. Ghasemi et al, J. Chem. Phys. **127**, 224102 (2007).
  - BigDFT Poisson's solver

$\mathcal{O}(N)$ scaling with respect to number of atoms if

- appropriate Poisson's solver is used,
- effective preconditioner is implemented for CEP.

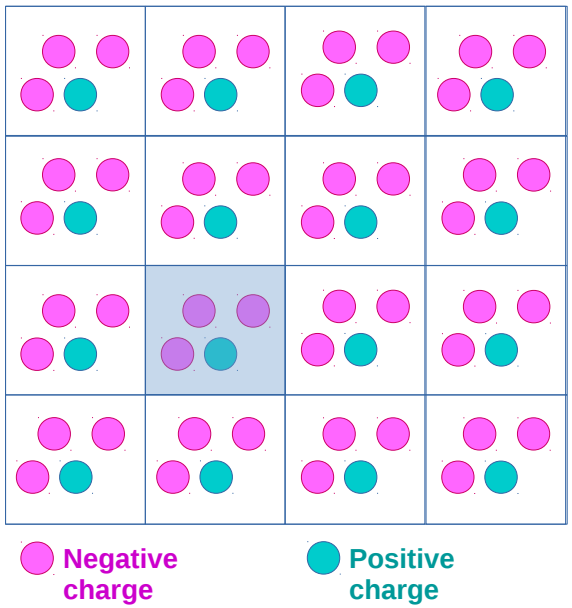
Calculation of Hartree energy and Ewald summation

$$E = \frac{1}{2} \sum_{\mathbf{n}}^{\prime} \sum_{i,j=1}^{N} \frac{q_i q_j}{|\mathbf{r}_{ij} + \mathbf{n}|}$$

$$E = \frac{1}{2} \sum_{\mathbf{n}}^{\prime} \sum_{i,j=1}^{N} \left[\frac{q_i q_j}{|\mathbf{r}_{ij} + \mathbf{n}|} - \iint \frac{\rho_i(\mathbf{r}) \rho_j(\mathbf{r}' + \mathbf{n})}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' \right]$$

$$+ \frac{1}{2} \sum_{\mathbf{n}} \sum_{i,j=1}^{N} \iint \frac{\rho_i(\mathbf{r}) \rho_j(\mathbf{r}' + \mathbf{n})}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'$$

$$- \frac{1}{2} \sum_{i=1}^{N} \iint \frac{\rho_i(\mathbf{r}) \rho_i(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'$$



$$E = \frac{1}{2} \sum_{\mathbf{n}}^{\prime} \sum_{i,j=1}^{N} \frac{q_i q_j \ \operatorname{erfc}\left[\frac{|\mathbf{r}_{ij}+\mathbf{n}|}{\alpha\sqrt{2}}\right]}{|\mathbf{r}_{ij} + \mathbf{n}|} + \frac{1}{2} \sum_{\mathbf{n}} \sum_{i,j=1}^{N} \iint \frac{\rho_i(\mathbf{r}) \rho_j(\mathbf{r}' + \mathbf{n})}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' - \frac{1}{\alpha\sqrt{2\pi}} \sum_{i=1}^{N} q_i^2$$

P. P. Ewald, Ann. Phys, **369**, 253 (1921).

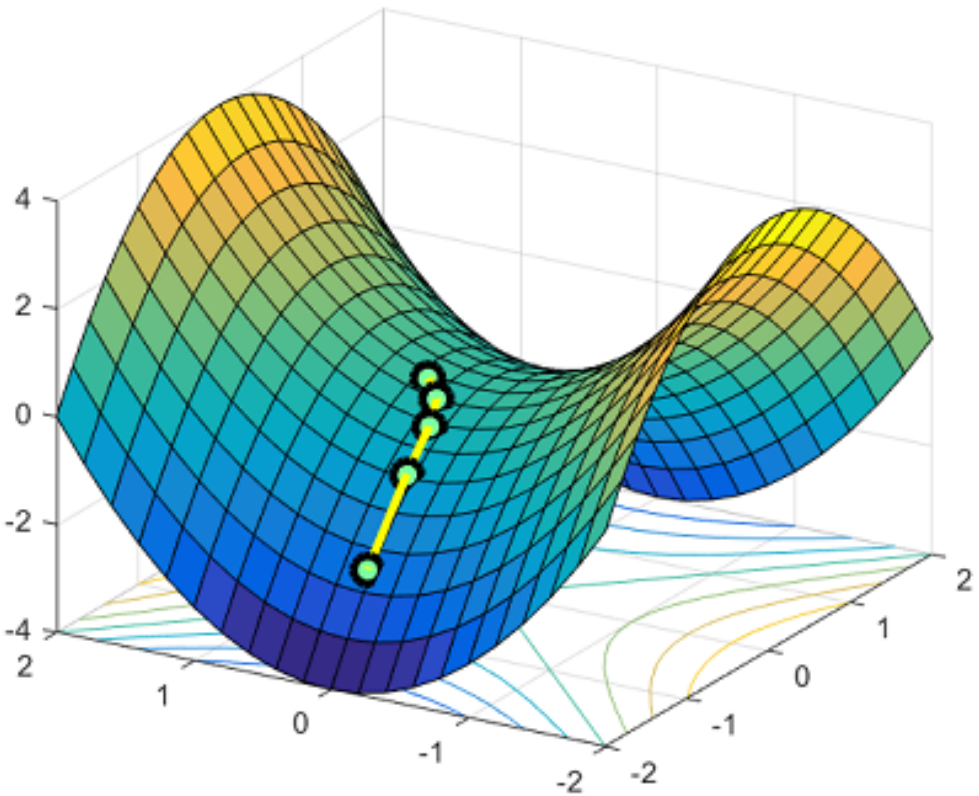
Input parameters for task minhopp

```
potential:
  potential: forcefield
  component_ff: coulomb
  ewald:
    psolver: p3d
    cell_ortho: True
    ecut: 10.0
    ecutz: 12.0
    alpha: 2.0
    rcut: 15.0
    rgcut: 6.0
    nsp: 10000
    ewald: True
```

- psolver: the method for the solver of the Poisson equation.
- ecut: cutoff energy that determines number of grid points.
- cell_ortho: a key for efficiency

Transition state

A transition state is a saddle point on potential energy surface, i.e. the second derivative (Hessian matrix) of the station point has at least one negative eigenvalue.



Input parameters for task

```
main:
    task: saddle_1s
    two_level_geopt: True
    seed: 3
    types: Si

potential:
    potential: ltb

saddle_1s:
    ampl: 6.E-1
    dimsep: 1.E-3
    list_random_displace: 1 57

saddle_1s_opt: INCOMPLETE
geopt: INCOMPLETE
geopt_prec: INCOMPLETE
```

Similarly recognition

Identifying similarity of structures have two major application:

- Structural similarity and classification of molecules and solids
- Construction of reference data points for machine learning

Environment descriptors:

- Translation and rotation invariance
- Invariance of permutation of two atoms of the same type

Link with the BigDFT PSolver

A new installation of FLAME is required. At the configure must include:
–with-bps BDIR=/home/ghasemi/build/bigdft/bigdft_lp

- No extra extra input file at the run time, i.e. you do not need to know how to run the BigDFT code.
- The BigDFT PSolver is the most advanced library for the solution of Poisson's equation for atomistic problems:
  - MPI parallelization, but FLAME ···
  - OpenMP parallelization, but FLAME ···
  - GPU accelerated, but FLAME ···

Link with the LAMMPS code

A new installation of FLAME is required. At the configure must include: **–with-lammps LAMMPS_ROOT=/home/ghasemi/tests/lammps-flame/lammps-16Mar18**

- You must be familiar with LAMMPS, and its input file is required.
- FLAME can be built with both BigDFT PSolver and LAMMPS enabled.

Environment descriptors/symmetry functions/fingerprints

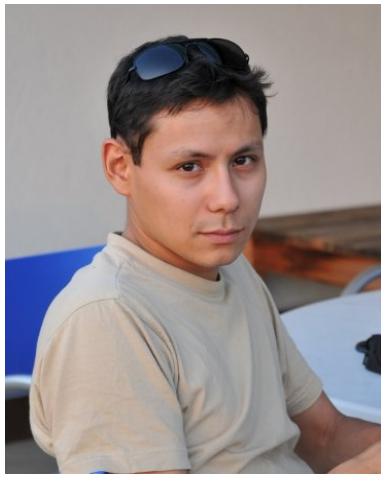
- Atom-centered symmetry functions
- Smooth overlap of atomic positions (SOAP)
- Overlap matrix formed by atom centered Gaussian basis set
- A number of other descriptors

Summary

- **src/input_variables_definition.yaml**

FLAME

- An open source package, available at: https://github.com/flame-code/FLAME
- Website under construction: www.flame-code.org
- Several functionalities such global optimization, molecular dynamics, electrostatic calculations, ...
- Interfaced to a number of atomistic software packages such as VASP, GULP, etc. to use their energy/forces/stress values.
- Interfaced to LAMMPS to use its functionalities where the potential is provided by FLAME.



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Thank you for your attention!

FLAME has been used in several studies so far:

- Samare Rostami et al, J. Chem. Phys. **149**, 124106 (2018).
- Roohollah Hafizi et al, J. Chem. Phys. **147**, 234306 (2017).
- Asnaashari Eivari et al, Chem. Mater. **29**, 8555 (2017).
- Robabe Rasoulkhani et al, Phys. Rev. B **96**, 064108 (2017).
- Somayeh Faraji et al, Phys. Rev. B **95**, 104105 (2017).
- Samare Rostami et al, J. Chem. Phys. **145**, 124118 (2016).
- S. Alireza Ghasemi et al, Phys. Rev. B **92**, 045131 (2015).