LAMMPS ARTn

The LAMMPS implication of Activation Relaxation Technique nouveau.

Compiling

1. Put two files (min_artn.cpp min_artn.h) in the src directory.
2. Modify your Makefile.{machine} in LAMMPS to make sure that the MKL lib and include files can be linked. E.g. add the following lines in Makefile.{machine}

   ```
   PKG_INC = /opt/intel/compiler/composer_xe_2013_sp1.0.080/mkl/include
   PKG_HOM = /opt/intel/compiler/composer_xe_2013_sp1.0.080/mkl/lib/intel64
   PKG_LIB = -Wl,--start-group ${PKG_HOM}/libmkl_core.a ${PKG_HOM}/libmkl_sequential.a \
   ${PKG_HOM}/libmkl_intel_lp64.a -Wl,--end-group \
   /opt/intel/compiler/composer_xe_2013_sp1.0.080/compiler/lib/intel64/libiomp5.a \
   -lm -lpthread
   ```
3. Compile your LAMMPS codes.

Benchmark

After Compiling, you can run prepared tests on *./example* directory. One is Cu(110) surface diffusion events searching, and the other one is thermally activated events searching in $Cu_{64}Zr_{36}$ metallic glasses.

To launch a ARTn searching, two files are often needed.

- in.lammps: use the following command to activate ARTn process.

  ```
  min_style artn
  minimize etol fotl maxiter maxeval
  ```
- artn.control: Parameters that control ARTn simulation are defined in this file.

You can do the benchmark use the command that launch a LAMMPS simulation, like

```
mpirun -np 4 lmp -in in.lammps
```

Output files

1. **log.event**: is expected to record all the important thermo info of events. Meaning of each column

- Event: event index.

- del-E: activation energy, or called energy barrier.
- egv-sad: the lowest eigenvalue of saddle point
- nsadl: number of atoms that are displaced more than *atom_disp_thr*(defined in **artn.control**) in saddle point configuration choosing the initial configuration as the reference configuration.
- sad-dx: |x(sad) - x(minimum)|
- sad-dy: |y(sad) - y(minimum)|
- sad-dz: |z(sad) - z(minimum)|
- sad-dr: |r(sad) - r(minimum)|
- ref: id of reference configuration (initial minimum)
- sad: id of reference configuration
- min: id of new minimum configuration (final minimum)
- Center: id of center atom to do initial activation (perturbation)
- Eref: energy of reference configuration (initial minimum)
- Emin: energy of new minimum configuration (final minimum)
- nMove: number of atoms that are displaced more than *atom_disp_thr*(defined in **artn.control**) in final minimum configuration choose the initial configuration as the reference configuration.
- pxx: xx component of pressure in final minimum configuration (set flag_press to 1 to show the pressure info)
- pyy: yy component of pressure in final minimum configuration
- pxx: zz component of pressure in final minimum configuration
- pxy: xy component of pressure in final minimum configuration
- pxz: xz component of pressure in final minimum configuration
- pyz: yz component of pressure in final minimum configuration
- Efinal: Energy of final minimum configuration
- status: 1, accept the new minimum configuration as the initial minimum configuration to start new search. 0, reject. Used in Metropolis condition. Set tempertature to a positive float number to activate this feature. Negative temperature will alway reject the new minimum configuration and start new search from the same initial minimum configuration.
- dr: |r(final) - r(minimum)|

2. **log.artn** : is expected to record the detailed info of ARTn simulation process and give a brief summary on the successful attempt rate and number of force evaluation. Some important parameters:

- E-Eref: current potential energy.
- ftot: total force
- fpar: force component along the eigenvector of lowest eigenvalue of Hessian matrix.
- fperp: force component perpendicular to the eigenvector of lowest eigenvalue of Hessian matrix.
- eigen: lowest eigenvalue of Hessian matrix.
- evalf: number of force evaluation.
- h.h': previous eigenvector of lowest eigenvalue dot current eigenvector of lowest eigenvalue.

3. **sadl_press.dat**: Recording the pressure of all the saddle point in the order of xx, yy, zz, xy, xz, yz.
4. **min.lammpstrj**: configurations of all the minimums. Dump atom format. TIMESTEP: id of the configuration (also used in log.event).
5. **sad.lammpstrj**: configurations of all the saddle points. Dump atom format. TIMESTEP: id of the configuration (also used in log.event).

Parameters

All the parameters are defined in **artn.control**. Many parameters are self-explanatory. We review the others below.

Basic parameters (Standard ARTn process in the literature):

- group_4_activat: The LAMMPS group ID of the atoms that will be activated.
- cluster_radius: < 0, all atoms in the *group_4_activat* will be kicked in the initial pertubation in each ARTn loop; > 0, a cluster centers on a random atom in *group_4_activat* with a radius of cluster_radius will be kicked in each ARTn loop. $= 0$, a random atom in *group_4_activat* will be kicked in each ARTn loop.
- max_num_events: max number of events to be found.
- force_th_saddle: Force threshold for convergence at saddle point.
- flag_press: $= 1$, pressure of final minimum will be recorded in the **log.event**.
- flag_sadl_press: $= 1$, pressure of saddle point configuration will be recorded in the **sadl_press.dat**

Extended parameters (Customized ARTn process):

- events_per_atom: number of events that will be found on each atom. > 0, the max number of events will be the result of atom number in group_4_activat times events_per_atom
- flag_dump_direction: $= 1$, Define the initial kick direction from a dump file (name of this file is defined by fdump_direction).

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Reference

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2. R. Malek, et al., Phys. Rev. E 62, 7723-7728 (2000).
3. E. Cances, et al., J. Chem. Phys. 130, 114711 (2009).
4. N. Mousseau, el al., J. At., Mol., Opt. Phys. 2012, 1 (2012).