ART for DFT calculations (version 3.0) - Manual

This short manual provides the basis for using `ART with DFT`, a simulation package developed originally by Normand Mousseau and modified by Laurent Karim Béland and Eduardo Machado-Charry

To cite `ART with DFT`, please refer to:

R. Malek and N. Mousseau, *Dynamics of Lennard-Jones clusters: A characterization of the activation-relaxation technique*, Phys. Rev. E **62**, 7723–7728 (2000).

A paper that presents ART nouveau

and

Eduardo Machado-Charry, Laurent Karim Béland, Damien Caliste, Luigi Genovese, Normand Mousseau and Pascal Pochet, *Optimized energy landscape exploration using the ab initio based ART-nouveau*, J. Chem Phys. **135**, 034102, 11 pp., (2011).

That presents some of the most recent implementations coupled with BigDFT.

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Contact

Normand Mousseau
Departement of physics
Université de Montréal
normand.mousseau@umontreal.ca

Content

Introduction

`art_dft` is a package for efficiently finding local transition states without bias using the ART nouveau method ARTN[1]. It is written to be easily coupled to DFT methods. An example is provided for SIESTA but it can be applied to any code.

While this manual is relatively light. It is recommended to run the examples to better understand the code. Do not hesitate to contact the authors for help.

Installing and compiling

The latest version of the program is always available on Normand Mousseau's web site at : http://physique.umontreal.ca/~mousseau, under the tab : software

Once you obtain the file, unpack the tar-gzipped with

```
% tar xzvf art_dft.tgz
```

A listing will give : % ls Examples Manual README scripts source

To compile `art_dft`, you need a fortran compiler as well as access to `blas` and `lapack` libraries. These are generally available on most computers.

The code can be compiled with gfortran, g95, Intel fortran, etc. Various architectures are defined in the `*.arch` files found in the `source` directory. Modify the files to fit your need and indicate the right architecture file in the `Makefile`

If you are using Mac Os X with gfortran installed, modify the `Makefile` to SYS = MacIntel

Compile with % make

The executable is named : `artdft`

Using MPI

It is possible to compile artdft with MPI by simply adding the compilation option `-DMPI`. In this case, the ART nouveau part will only run on the master node, the other nodes being used by the DFT code with the appropriate submission shell commands.

Running the examples

Working examples are found in the `Examples` directory. They focus on running the code with an empirical potential (Stillinger-Weber) that is distributed with the code. To run DFT forcefields, see Coupling with DFT code.

Example 1

The first example shows how an ART nouveau simulation proceeds when searching for pathways. The Direction `Si_SW` containts only the submission script (`artdft.sh`) and an initial configuration (`refconfig`).

It is a 1000-atom box of amorphous silicon described with the Stillinger-Weber potential.

By running % ./artdft.sh

A new search is launched with a Metropolis temperature of 0.4 eV. (Note that to simply sample around a given minimum, to explore the local environment, one can set the temperature to ***negative*** values so that events are never accepted.)

Note also that the line output is rather verbose. You can ignore it as the information is also presented in a clearly way in the `logfile`.

An example of an output is given in `Si_SW_output` where a 10-event run was done .

```
% ls
artdft.sh   min1003     min1008     sad1002     sad1007
events.list min1003.xyz min1008.xyz sad1002.xyz sad1007.xyz
filecounter min1004     min1009     sad1003     sad1008
log.file.1  min1004.xyz min1009.xyz sad1003.xyz sad1008.xyz
min1000     min1005     min1010     sad1004     sad1009
min1000.xyz min1005.xyz min1010.xyz sad1004.xyz sad1009.xyz
min1001     min1006     refconfig   sad1005     sad1010
min1001.xyz min1006.xyz restart.dat sad1005.xyz sad1010.xyz
min1002     min1007     sad1001     sad1006
min1002.xyz min1007.xyz sad1001.xyz sad1006.xyz
```

The `log.file.1` contains the details of the events. This information is essential to understand how the convergence and search is taking place.

`events.list` provides the list of all events, as a series of initial minimum, saddle point and final minimum, indicating whether these events where accepted through Metropolis algorithm. In the example provide, two events out of 10 are accepted.

`filecounter` keeps track of the file number so that when a simulation is relaunched (as `NEW`), it continues where it stopped.

`restart.dat` contains all informations necessary to restart a simulation and the min and sad files are configuration files at energy minima and transition states.

Example 2

The directory `Example2`, for its part, contains an example of a test running a `REFINE_AND_RELAX` on an intermediate event.

You will find the appropriately modified `artdft.sh`, the starting configuration `ExcitedState` which corresponds to `REFCONFIG` and the output - a single saddle and minimum files.

Coupling with DFT code

To couple with DFT code, one needs to modify two files that have been setup for Siesta at the moment: `siesta_force.f90` and `siesta_min.f90`. This way, it is possible to simpy write down the configuration in the appropriate format, launch the ab initio code and read the configuration output to continue the ART simulation.

`siesta_force.f90` provides an interface to obtain ab initio force. Essentially, it receives the positions from the ART nouveau code, it write them in the appropriate format and launches siesta. Once the force has been calculated, it reads it and returns the information to ART nouveau.

The second file, `siesta_min.f90`, is used when one wishes to use the energy minimisation routine provided with the DFT package.

If you prefer to use ART nouveau's fire minimazation, simply modify the `min_converge`routine to call `min_converge_fire`.

Parameters

Parameters are defined by a `setenv` command, allowing greater flexibility in the shape of the parameter file.

The various examples provided with the code should help understand the minimum set of parameters to be used for each type of simulation.

They are described in details in the `artdft.sh` file.

Bibliography

1. R. Malek and N. Mousseau, *Dynamics of Lennard-Jones clusters: A characterization of the activation-relaxation technique*, Phys. Rev. E **62**, 7723–7728 (2000). ↩