Energy landscape exploration using BART

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Daubechies Wavelets in Electronic Structure Calculation: BigDFT Code Tutorial

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The central idea to ART is the activation, following the eigendirection corresponding to a negative eigenvalue, of a configuration from a local minimum to a nearby saddle point.

The basic algorithm can be divided into three steps:

1. Leaving the harmonic well
2. Converging to the saddle point
3. Relaxing to a new minimum

Input files

- bart.sh
- posinp.xyz (ascii)
- input.dft
- input.geopt
- psppar.*atom type*
- list_atoms.dat
- saddle.xyz (if EVENT_TYPE=GUESS_SADDLE)

bart.sh: general format

All parameters are reading as environment variable.

setenv in csh shells

export in sh and ksh shells

```
#/bin/csh
#---------------------------- ATOMS
setenv NATOMS                    8      # Number of atoms in the problem
setenv type1                     C
setenv type2                     H
#---------------------------- ART
setenv EVENT_TYPE GUESS_SADDLE # Either 'NEW', 'REFINE_SADDLE' when further converging a saddle point
# Or "REFINE_AND_RELAX", to refine at the saddle
# and check the final minimum
setenv ENERGY_CALC               BIG
setenv Temperature               -0.5   # Temperature in kcal/mol, if negative always reject the event
setenv Max_Number_Events         1000   # Maximum number of events
setenv Type_of_Events            local  # Activation: global, local, list_local, list
setenv Radius_Initial_Deformation  1.2  # Cutoff for local_coord (in angstroems)
setenv Central_Atom                     # Number of the atom around which the initial move takes place
setenv sym_break_dist            0.001  # Breaks the symmetry of the crystal by randomly displacing
                                        # all atoms by this distance
setenv Activation_MaxIter        300    # Maximum number of iteraction for reaching the saddle point
setenv Initial_Step_Size         0.05   # Size of initial displacement, in A
setenv Increment_Size            0.09   # Overall scale for the increment moves
setenv Force_Threshold_Perp_Rel  0.5    # Threshold for perpendicular relaxation
...
...
...
```

#------------------------ ATOMS

- NATOMS: Number of atoms in the problem
- type1: atom type 1 (obsolet)
- type#: atom type # (obsolet)

#_____ ART

- EVENT_TYPE:
  - NEW: simulation is started from scratch
  - REFINE_SADDLE: a previous rough evaluation of the saddle is refined
  - REFINE_AND_RELAX: same as before plus a relaxation
  - GUESS_SADDLE: the initial direction is given by the user

#_____ ART

- ENERGY_CALC:
  - BIG: for BigDFT
  - BSW: QM/MM (*in development*)
  - SWP: Stillinger-Weber potential

#_____ ART

- Temperature: (*real*) Fictive temperature (eV) for the acceptance ratio. If negative the event is rejected
- Max_Number_Events: (*integer*) number of trajectories between two minima in EVENT_TYPE = NEW
- Type_of_Events kind of initial perturbation
  - global: all atoms are perturbed
  - local: a central atom and its neighbours are perturbed
  - list: just the atoms in the list are perturbed
  - list_local: same as local but the central atom is randomly chosen from a list

#_____ ART

- Radius_Initial_Deformation:(*real*) define cutoff for the sphere of neighbours in Type_of_Events = local or list_local
- Central_Atom: (*integer*) central atom of deformation. If empty, it is randomly chosen
- sym_break_dist: (*real*) breaks the symmetry of the crystal by randomly displacing all atoms by this distance.
- Activation_MaxIter: (*integer*) maximum number of iteractions for reaching the saddle point
- Initial_Step_Size: (*real*) size of initial displacement in Å
- Increment_Size: (*real*) overall scale for the increment moves
- Force_Threshold_Perp_Rel: (*real*) threshold for perpendicular relaxation

#_____ HARMONIC WELL

- Basin_Factor: (*real*) factor multiplying Increment_Size for leaving the basin
- Max_Perp_Moves_Basin:(*integer*) maximum number of perpendicular steps leaving basin
- Min_Number_KSteps: (*integer*) min. number of ksteps before calling lanczos
- Eigenvalue_Threshold: (*real*) eigenvalue threshold for leaving basin
- Max_Iter_Basin: (*integer*) maximum number of iteraction for leaving the basin (kter)

#_____ LANCZOS

- gnrm: (*real*) convergence criterion for the wavefunction optimization for Lanczos Vectors. Reasonable values are in most cases between 2×10^{-5} and 1×10^{-5}
- calc_of_projection: (*logical*) it calculates the projection only at every two steps but after 4 steps above of an inflection in the eigenvalue, and if the last a1 ¿0.9d0.
- Lanczos_of_minimum: (*logical*) Calculation of the Hessian for each minimum
- Number_Lanczos_Vectors_A: (*integer*) number of vectors used in the lanczos recursion method for the harmonic well
- Number_Lanczos_Vectors_C: (*integer*) same as before but for the stage convergence
- delta_disp_Lanczos: (*real*) step of the numerical derivative of forces in lanczos (Å)

#_____ CONVERGENCE

- Max_Perp_Moves_Activ: (*integer*) maximum number of perpendicular steps during activation
- Exit_Force_Threshold: (*real*) threshold for convergence at saddle point
- Prefactor_Push_Over_Saddle: (*real*) fraction of displacement over the saddle
- Save_Conf_Int: (*logical*) save the configuration at every step?
- delta_threshold: (*real*) if E-Eref $<$ delta_thr .and. delr $<$ delr_thr kills the event. Test done in the convergence stage to see if the configuration is coming back to the original minimum.
- delr_threshold:

#_____ DIIS

- Use_DIIS: (*logical*) use DIIS for the final convergence to saddle
- Iterative: (*logical*) iterative use of Lanczos & DIIS
- Inflection: (*integer*) number of Lanczos steps after an inflection in the eigenvalue for calling DIIS
- Use_DIIS: (*logical*) use DIIS for the final convergence to saddle
- DIIS_Force_Threshold: (*real*) force threshold for call DIIS
- DIIS_Memory: (*integer*) number of vectors kepts in memory for the algorithm
- DIIS_Check_Eigenvector: (*logical*) check that the final state is indeed a saddle point
- DIIS_Step_size: (*real*) prefactor multiplying forces
- FACTOR_DIIS: (*real*) times Increment_Size, max allowed diis step size
- MAX_DIIS: (*integer*) max diis iterations per call

#_____ INPUT

- FILECOUNTER: (obsolet) file tracking the file (event) number - facultative
- REFCONFIG : reference minima for ENERGY_TYPE = REFINE_SADDLE or REFINE_AND_RELAX options

#------------------------ OUTPUT

- LOGFILE: name of file of general output for message
- EVENTSLIST: name of file. lists of events with success or failure
- Write_restart_file: (*logical*) it is useful only for ab-initio
- RESTART: name for the restart file
- Write_xyz: (*logical*) writes the configuration in .xyz format

Output files

- *.out: includes the BigDFT standard output information plus more detailed information about ART
- log.file.#: shows the evolution of the exploration for each event (minimum to minimum)
- min-event-.xyz: coordinates of the system at each minimum
- sad-event-.xyz: coordinates of the system at each saddle
- events.list:Includes the connection between minima. It states if the event was accepted. Useful for postprocessing.
- filecounter : obsolet
- p_*event_attempt_step_stage*.xyz: The coordinates of the system at each step if Write_xyz==.True.