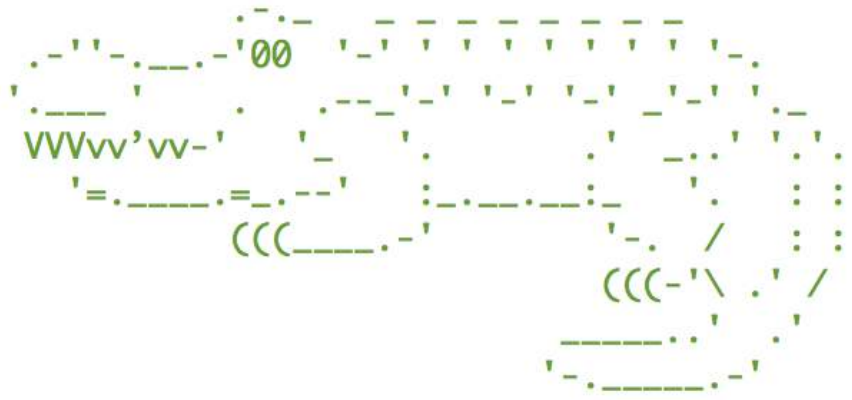
GAtor Genetic Algorithm for Molecular Crystal Structure Prediction



A User's Manual

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Contents

Chapter 1

Basic Installation and Tutorial

1.1 Introduction

Welcome to the GAtor genetic algorithm for molecular crystal structure prediction, which finds the most energetically stable crystal structures for (semi-)rigid molecules. GAtor uses principles from evolutionary theory such as survival of the fittest, crossover, and mutation that are implemented as operators acting on individual molecules and/or lattice vectors of the fittest crystal structures selected for mating. Energy evaluations and structural relaxations are performed using dispersion-inclusive density functional theory (DFT). For this purpose, GAtor currently interfaces with the all-electron numerical atom-centered orbital DFT code FHI-aims.

1.2 Installation Requirements for GAtor

GAtor is written is python and interfaces with the all-electron electronic structure theory code FHI-aims. GAtor can be downloaded from http://software.noamarom.com. To run GAtor the user will need to install:

- Python 2.7 http://www.python.org
- NumPy version $\geq$ 1.9 http://www.numpy.org
- Pymatgen version $\geq$ 4.4.0 http://www.pymatgen.org
- Sci-kit learn version $\geq$ 0.17.1 http://scikit-learn.org
- A build of FHI-aims (MPI and scalapack-supported, if possible).

Check that python and the dependent packages can be successfully imported:

```
$ python
» import numpy
» import sklearn
» import pymatgen
```

1.3 Structure of the Code

GAtor contains the main directories `/src`, `/tests` and `/tutorial`. The `/src` folder contains the master script `GAtor_master.py` along with core modules of the GA such as `/selection` and `/crossover`. The `/tutorial` folder provides an example GA run (see Section 1.4). The `/tests` folder contains different tests one should run when running a new molecule for the first time.

To run GAtor, one invokes the main script and inputs a user-defined configuration file `ui.conf` via `$ python gator/GAtor_master.py ui.conf`. For an explanation of the `ui.conf` file see Section 1.4.1.

1.4 Basic Tutorial

This section takes the user through the example calculation provided in `/tutorial`. This folder contains a `ui.conf` file, a sample initial pool, and sample FHI-aims control files `control.in.SPE.tier_1` and `control.in.FULL.tier_1`. The first control file is used just for single point energy evaluations, while the second is used for local optimization[1]. The energy cutoffs corresponding to each control file are detailed in Section 1.4.2.

1.4.1 The ui.conf file

The `ui.conf` is the only file the user needs to modify in order to use GAtor. It can be named anything as long as it ends with ".conf". A simple example for the molecule 3-4-cyclobutylfuran can be found in `/gator/tutorial/ui.conf`. The conf file contains the parameters that control all aspects of GAtor including parallelization options, paths to the user-input initial pool, options for interfacing with FHI-aims, and tuning parameters for GA tasks such as mutation probability and duplicate-check tolerances. For an explanation of the simple keywords shown in `/gator/example_calc/ui.conf` see Section 1.4.5. For a full catalog of all the possible keywords that can go into this file, see Section 2.

1.4.2 Basic ui.conf file settings

This section details the parameters you will see in the basic configuration file `ui.conf`. All parameters are grouped into main sections. This conf file runs GAtor for the molecule 3-4-cyclobutylfuran.

[1]To accelerate the DFT calculations for tutorial purposes, limitations are placed on the number self-consistent iterations and max relaxation steps in the control files. These control files should not be used for production purposes, as the calculations will not be fully converged.

`[GAtor_master]`

The GAtor_master section controls the main procedures of initial pool filling and running the GA.

- `fill_initial_pool = TRUE`
  - Fills the user-defined initial pool into the common pool of structures before running the rest of the GA tasks.
- `run_ga = TRUE`
  - Executes of the main GA procedure

`[modules]`

The modules section details the names of the individual GA modules used in the subfolders of /src/. Some of these modules (e.g. selection_module=tournament_selection) may be set to alternative options (e.g. selection_module=roulette_selection). For more information on alternative modules see Section 2.

`[initial_pool]`

- `user_structures_dir = initial_pool`
  - Path to the pre-prepared initial pool, as generated by *Genarris*. Structures are in a JSON format.
- `stored_energy_name = energy_tier1`
  - Stored energy name in initial pool json files (if other than "energy"). This should be at the same level of theory as the last control file listed in `control_in_filelist`.

`[run_settings]`

This section controls general GA run settings.

- `num_molecules = 4`
  - This is the number of molecules in the unit cell to be run (must match number of molecules per unit cell in the initial pool). This must be specified by the user.
- `end_GA_structures_added = 5`
  - Setting which stops GAtor after a certain amount of children (in this case 5) have been added to the common pool. For more options for stopping/converging the GA refer to Section 2.
- `output_all_geometries = TRUE`

  - Prints the FHI-aims-style geometries of parents, children, and mutations to the main output `GAtor.out`. This setting is set to TRUE for easy visualization of the structures using Jmol (copy/paste) but may be uncommented for a less verbose output.

- `#skip_energy_evaluations = TRUE`
  - This parameter is uncommented by default, but may be used to skip FHI-aims energy evaluations of the generated structures (giving them an energy of 0 eV). This can be used to verify the structure selection and generation works (e.g. on a laptop) without having to run FHI-aims.

`[parallel_settings]`

- `parallelization_method = subprocess`
  - The parallelization setting of the GAtor replica(s) being run (not for FHI-aims). Subprocessing uses Python's Subprocess module (to run FHI-aims) and can be used on a laptop, or on a cluster (where the Python subprocess will run on the job scheduler nodes). See Chapter 2 for alternative options.

- `number_of_replicas = 1`
  - Number of GAtor replicas being run by user.

- `processes_per_replica = 1`
  - Number of parallel Python processes used per replica. This sets the number of python processes used for parallel GA tasks such as child generation. This make the child generation process faster but should be set with an awareness of the number of processes available on the given machine being used.

- `aims_processes_per_replica = 64`
  - Number of parallel processes used per replica to run FHI-aims for a given replica. For example, this is set to 64 if one is running 1 replica on 1 node of a cluster with 64 processes.

`[FHI-aims]`

- `execute_command = mpirun`
  - Command to run the FHI-aims binary. Since we will be using the scalable version of aims the command is `mpirun`.

- `path_to_aims_executable = aims.mpi.x`
  - Path to FHI-aims executable being used for energy evaluations and/or structural relaxations.

- `control_in_directory = control`
  - Name of the directory in the main calculations folder which can contain multiple FHI-aims control.in files (which can be named arbitrarily).
- `control_in_filelist = control.in.SPE.tier_1 control.in.FULL.tier_1`
  - Name of control file(s) in control directory being used within GAtor. The GA evaluates the control files in order, and the user can set energy cutoffs for each control file (see below). In the tutorial a dummy single-point energy and full relaxation control file are included for demonstrative purposes.
- `relative_energy_thresholds = 3 3`
  - Relative energy cutoffs (in eV) from the current global minimum structure for each control file specified in `control_in_filelist`. If a structure has a relative energy less than the minimum energy structure minus this cutoff, it is immediately rejected. For more energy cutoff options see Section 2.
- `save_failed_calc = TRUE`
  - If uncommented, saves aims calculations if they fail for some reason in `/tmp`
- `save_successful_calc = TRUE`
  - If uncommented, saves full aims calculations data for successful GA structures. Should be commented out if space is an issue.

`[selection]`

This section controls parameters related to the specific `selection_module` chosen.

- `tournament_size = 3`
  - For tournament selection, this controls the tournament size.

`[crossover]`

This section controls parameters related to the specific `crossover_module` chosen.

- `crossover_probability = 0.5`
  - This parameter controls the probability of crossover for a child structure. If set to 0.5 the child has a 50% chance of undergoing crossover, and a 50% chance of undergoing mutation. A separate parameter is not needed for mutation.

`[mutation]`

This section controls parameters related to the specific `mutation_module` chosen.

- `stand_dev_trans = 0.5`
  - Standard deviation (in Angstrom) of the random translation mutations applied.
- `stand_dev_rot = 30`
  - Standard deviation (in degrees) of the random rotation mutations applied.
- `stand_dev_strain = 0.3`
  - Standard deviation of the random strain mutations applied.

`[cell_check_settings]`

This section controls parameters related to the geometric constraints of generated crystal structures. Structures are rejected if they don't pass these constraints.

- `target_volume = 473`
  - The mean target_volume for generated structures
- `volume_upper_ratio = 1.4`
  - The upper ratio of target_volume accepted for generated structures.
- `volume_lower_ratio = .6`
  - The lower ratio of target_volume accepted for generated structures.

1.4.3 Filling the initial pool

An initial pool of structures, prepared by the user using the *Genarris* molecular crystal generation package is required to run GAtor. For more information on generating this initial pool see the *Genarris* user's manual. The path to this initial pool of structures is set in the ui.conf file in `[initial pool]/user_structures_dir`. To start, comment out `run_GA = TRUE` and comment `fill_initial_pool = TRUE`. This will just fill the initial pool without running the GA. Then run the master script

```
python ../src/GAtor_master.py ui.conf &
```

If the initial pool has properly been filled, one should see a nonempty file in `/tmp/num_IP_structs.dat` that contains the number of initial pool structures.

1.4.4 Running the GA

One the initial pool has been filled you may run the GA by uncommenting `run_GA = TRUE`. One can run the code in-shell (not recommended) by running again

```
python ../src/GAtor_master.py ui.conf &
```

Putting the `&` at the end of the script allows the code to run in the background and frees up your terminal. However, this may take quite a while to finish as FHI-aims calculations are being performed. Therefore, it is highly recommended to submit this command to a cluster. An example `submit_to_cluster.sh` is provided in the tutorial folder. Make sure the number of `aims_processes_per_replica` is set in accordance with the number of processes allocated on the cluster.

Your GAtor replica is now running! The next step is to look at the different output files being produced.

1.4.5 Individual and Combined Replica Outputs

The output an individual replica is stored in, e.g.,

```
./tmp/replica_out/fa2f201fe6.out
```

This file records information from the genetic algorithm tasks from each iteration an individual replica and is reset when either a structure is rejected or successfully accepted. This file includes details from selection, crossover, mutation, comparison, and FHI-aims evaluation.

Since in the example ui.conf it was elected to output all FHI-aims geometries to the replica outputs in the configuration file, you may choose to visualize the geometries from the most recent parents, children, and mutations by copy/pasting their FHI-aims geometries from the replica output file into Jmol. The combined output from all successful iterations of all running replicas is stored in.

```
./GAtor.out
```

This combined output file is written to every time any replica starts and finishes an iteration. Feel free to inspect this file as GAtor runs.

1.4.6 GAtor time log

A time log that mainly entails information on the execution of FHI-aims energy evaluations for all replicas is stored in,

```
./GAtor.log
```

The user can refer to this file for inquiring when the latest FHI-aims evaluation for their replica has started and stopped as well as any errors that may have passed (hopefully not...).

1.4.7 Temp Directories for FHI-aims evaluations

The currently-running FHI-aims calculation folders are located in the directory, e.g.

```
./tmp/fa2f201fe6
```

If you change into this directory you will find the control.in, geometry.in, and aims.out files for the currently-running FHI-aims calculation for your replica, as well as a JSON file which includes properties of the currently running structure. The user can inspect aims.out if they wish to know exactly where an FHI-aims evaluation is at.

1.4.8 Structures directory

The database of the entire common pool of the genetic algorithm is located in the the directory, e.g.,

```
./structures/S:6_C:16_N:8/0
```

Each subfolder in this directory corresponds to one structure in the pool, and they are named according to random-indices (if they are an initial pool structure their original name is used). FHI-aims geometries as well as JSON files (which store the structure's geometry and properties) are stored in these files. Feel free to inspect any of these directories.

1.4.9 Energy Hierarchy

An energy hierachy, which ranks structures from the database by their energy is updated in,

```
./tmp/energy_hierarchy_S:6_C:16_N:8_0.dat
```

If you inspect this file, you will see it includes key information from each structure in the collection including their energy ranking, the size of the pool when they were added (initial pool structures have a value of 0, and GA structures indicate the size of the collection when the structure was added), which replica they came from, their structure index, their energy, their unit cell volume and parameters, and their spacegroup. Additionally, for GA-added structures, information about the mutation procedures performed to generate the structure, as well as the indices of the structure's parents, are included. This file is often the simplest one to look at to see if new structures have been added, and where they fall energy-wise in the collection.

1.4.10 Duplicates

An essential part of any genetic algorithm is the identification of duplicate structures as they are inevitably generated in random crossover processes. The database of structures that are deemed as duplicates (and not included in the common pool) are found in,

```
./structures/S:6_C:16_N:8/duplicates
```

Within the GA, GAtor uses *pymatgen's* `StructureMatcher` class to identify duplicate structures within a user-defined energy window. For more information on changing these duplicate tolerances from their default values, see the user manual.

Chapter 2

Full Configuration File Parameters

The configuration file ui.conf (or [user_defined_label].conf) is the only file the user has to modify to control all parameters used in GAtor. Listed below are all the possible parameters for ui.conf, listed under their respective section headings.

`[GAtor_master]`

- `fill_initial_pool =` (optional; Boolean)
  - If present, fills the user-defined initial pool into the common pool of structures before running the GA. The user should omit this keyword if the pool has already been filled and there are just desiring adding another replica to write to the common pool.
- `run_ga =` (optional; Boolean)
  - If present, enables execution of the main GA procedure. See the `parallel_settings` section for details on spawning additional replicas of GAtor.

`[run_settings]`

- `num_molecules =` (required; integer)
  - Number of molecules per unit cell for the current search (must match number of molecules in initial pool structures).
- `orthogonalize_unit_cell =` (optional yet recommended; Boolean, set to TRUE or omit)
  - If `TRUE` will orthogonalize all structures in the initial pool whose lattice vector angles are less than 60 degrees or greater than 120 degrees.
- `end_GA_structures_added =` (optional; integer)

  - A simple way to end the GA by stopping after this many structures have been added by the GA.

- `end_GA_structures_total =` (optional; integer)
  - A simple way to end the GA by stopping after this many structures total structures are in the common pool. This includes the structures added by the GA and the structures in the initial pool.
- `followed_top_structures =` (optional, must be used with `max_iterations_no_change`; integer)
  - Track the top number of structures (as ranked by their energy) to see if they have changed in `max_iterations_no_change`. This is a way of determining convergence.
- `max_iterations_no_change =` (optional, must be used with `followed_top_structures;` integer)
  - If `followed_top_structures` hasn't changed in `max_iterations_no_change`, then stop the GA.
- `verbose=` (optional; Boolean, set to TRUE or omit)
  - If `TRUE`, include for detailed information printed to outputs.
- `output_all_geometries =` (optional; Boolean, set to TRUE or omit)
  - Set to `TRUE` to enable replica output of FHI-aims style geometry whenever a new trial structure is generated or altered.
- `failed_generation_attempts =` (optional; default = 1000)
  - Number of attempts allowed for the structure generation scheme to fail (e.g., failed cell check) before an error is raised.

`[parallel_settings]`

- `parallelization_method =` (optional; default = `serial`)
  - `serial` With this setting only one GA replica which reads and writes to the common pool is spawned. If this setting is used no additional keywords need to be specified in `[parallel_settings]`. If desired, additional simple multiprocessing can be used within the single replica (for parallel python processes such as child creation) by setting `processes_per_replica`. Make sure to not oversubscribe processes of the master node (especially log-in nodes).
  - `subprocess` With this setting the user can spawn several replicas of the GA in the master node (or where GAtor is running) using Python subprocessing. This setting also requires `number_of_replicas` to be set.

- `mpirun` With this setting the user can spread several replicas of the GA across multiple computing cores or nodes using the *mpirun* command. This setting requires additionally setting at least one of the following: `number_of_replicas`, `processes_per_replica`, or `nodes_per_replica`. If only one of these options is specified, GAtor will automatically calculate the others based on the available resources. If more than one of these options is specified, GAtor will check compatibility of the parameters with the system and proceed. Below are a few common scenarios in a sample job which has been submitted to 20 nodes with each node having 20 processes per node.
  - The user specifies `number_of_replicas = 10`. GAtor will allocate 2 nodes and 40 processes total for each of the 10 replicas.
  - The user specifies `number_of_replicas = 40`. GAtor will allocate 10 processes for each of the 40 parallel replicas. This means 2 replicas will be running per node.
  - The user specifies `number_of_replicas = 3`. GAtor will allocate 7 nodes = 140 processes each for 2 replicas, and 6 nodes = 120 processes to 1 replica.
  - The user specifies `processes_per_replica = 10`. GAtor will spawn 40 replicas (with 2 replicas assigned to each node) with 10 processes per replica.
  - The user specifies `processes_per_replica = 30`. GAtor will spawn 10 replicas, each assigned 2 nodes, but each replica only being assigned 30 processes each (used e.g. for memory requirements). User has to specify `additional_arguments` in order for the 30 processes to be evenly distributed across the 2 nodes (e.g. `-rr` for round-robin).
  - The user specifies `processes_per_replica = 6`. GAtor will spawn 60 replicas, assign 3 replicas to each node, and allocate 6 processes to each replica.
  - The user specifies `nodes_per_replica = 4`. GAtor will spawn 5 replicas,and allocate 4 nodes (80 processes) to each replica.
  - The user specifies `processes_per_replica = 20` and `nodes_per_replica = 2`. GAtor will spawn 10 replicas, each allocated 2 nodes with 20 processes total. The user has to specify `additional_arguments` (e.g., -rr for round-robin) in order for the 20 processes to be evenly distributed across the 2 nodes.
  - The user specifies `number_of_replicas = 5` and `nodes_per_replica = 2`. GAtor will spawn 5 replicas, each allocated 2 nodes and 40 processes total.
  - The user specifies `number_of_replicas = 20` and `nodes_per_replica = 1` and `processes_per_replica = 15`. GAtor will spawn 20 replicas, each on 1 node with 15 processes.
- If ValueError is raised when using `mpirun` for a job submitted to, e.g., 20 nodes with 20 processes per node, it is possibly caused by scenarios similar to the following:
  - The user specified `number_of_replicas = 10` and `nodes_per_replica > 2`. GAtor will raise a ValueError for oversubscription of nodes.

    - The user specified `number_of_replicas = 10` and `processes_per_replica > 40`. GAtor will raise a ValueError for oversubscription of processes.
  - `srun` With this setting the user can spread several replicas of the GA across multiple computing cores or nodes using the *srun* command. The same parallelization procedure is used as with the setting `mpirun`. See the description for `mpirun` for parameters requirements and how nodes and processes are distributed to each replica.
  - `mira` Special implementation for ALCF's IBM BG/Q cluster Mira. Required additional parameter: `nodes_per_replica`. Additional Python instances of GAtor will be spawned through subprocess on the front-end nodes. The blocks and corners in the back-end nodes are automatically assigned to each replica. Each replica can be assigned more front-end processes by the
  - `processes_per_replica` parameter.
  - `cetus` Special implementation for ALCF's IBM BG/Q testing cluster Cetus. Required additional parameter: `nodes_per_replica`. See the setting `mira` for further details. Different from the `mira` setting in that by default, blocks of 128 nodes are created, instead of 512.

- `python_command` (optional; default: python)
  - The command used to call Python. This parameter can be set to call an alternative version of Python.

- `number_of_replicas`
  - Required in "subprocess" parallelization mode; optional in "mpirun" and "srun"; ignored in "mira" and "cetus"
  - Number of parallel replicas running the GA.

- `processes_per_replica` (optional)
  - Number of processes allocated to each replica.
  - In "subprocess", "mira" or "cetus" parallelization modes, defaults to 1.
  - In "mpirun" and "srun" modes, defaults to be calculated according to other specified parameters. (See description above about the `mpirun` mode).

- `processes_per_node` (optional)
  - A further constraint on the size of a multiprocessing pool of workers that each replica can spawn. Useful when replicas control more than 1 node to constrain the amount of workers spawned on the main node. The smaller between codeprocesses_per_replica and `processes_per_node` determines the size of the multiprocesses.pool.
  - Honored only in "mpirun" and "srun" parallelization modes.

  - Defaults to the value obtained through mpirun a Python test code on a node.

- `allocated_nodes` (optional)
  - Nodes allocated for this replica. While additional replicas are spawned, this value is set internally to allocate nodes to each replica.
  - Honored only in "mpirun" and "srun" parallelization mode
  - Defaults to the returned value of the function, *parallel_run.get_all_hosts()*.

- `replica_name` (optional; default: "master"):
  - Name of the currently running process.
  - A random replica name is assigned while internally spawning replicas, or when the main GA processes begin with this parameter still being the default "master" (to avoid conflict of names).

- `im_not_master_replica` (optional; Boolean):
  - If present and set to TRUE, suppresses all initialization information printed to time log.

    Here are a few parameters specifically set for the implementation on system using the `srun` command. Note that overcommitting memory resources will lead to job unable to run. To successfully run on system with srun, make sure to allocate the necessary general resources in the submission file.

- `srun_max_runtime`:
  - Maximum run time in seconds before the master process kills the job

- `srun_gator_memory` (optional; default = 2048):
  - Memory (in MB) devoted to the GAtor python processes spwaned in a different node.

- `srun_memory_per_core` (optional; default = 1024):
  - Memory per core (in MB) devoted to additional srun processes (e.g., for FHI-aims calculations).

- `srun_command_file` (optional; default = ./srun_calls.info)
  - The path to the file where each replica sends an `srun` call's command to be picked up by the master thread that spawned all the replicas. This is necessary because `srun` does not allow nested calls.

- `srun_submitted_file` (optional; default = ./srun_submitted.info):
  - The path to the file where the internal job id of srun calls that are picked up by master process and executed is recorded

- `srun_completed_file` (optional; default = ./srun_completed.info)
  - The path where completed commands are sent to notify replicas to pick up results.
- `srun_gres_name` (optional; default = "craynetwork"):
  - Name to the generic resource to that serves as the first field in the argument `-gres` for an srun command. Make sure to configure such resources in the original submission file.
    Here are a few parameters specifically set for the implementation on IBM's BG/Q system with the runjob command:
- `bgq_block_size` (optional):
  - Number of nodes per booted block
  - Defaults to 512 for `mira` mode, 128 for `cetus` mode.
- `runjob_processes_per_node` (optional; default: 16):
  - Number of processes per node. Should be set to the number of cores per node.
- `runjob_block` (optional):
  - For internal distribution of nodes only. The block that is assigned to the replica.
- `runjob_corner` (optional):
  - For internal distribution of nodes only. The corner that is assigned to the replica.
- `runjob_shape` (optional):
  - For internal distribution of nodes only. The shape of the corner that is assigned to the replica.

`[bundled_run_settings]`

- `parallelization_method` (required)
  - Parallelization method to spawn additional replicas.
  - Currently only supporting `mira` and `cetus`
  - `mira` Achieves node distribution for bundled run on ALCF's IBM BG/Q cluster Mira. Required additional parameters for each run: `number_of_blocks`, `nodes_per_replica`
- `run_names` (required)
  - Names of each one of the bundled runs. Given as a list of strings delimited by space. Each run must have a section in the configuration file bearing the same section name, where the additional parameters are stored.

- `bgq_block_size` (optional):
  - Number of nodes per booted block on Mira or Cetus.
  - Defaults to 512 for `mira` mode, 128 for `cetus` mode.
- `runjob_processes_per_node` (optional; default: 16):
  - Number of processes per node. Should be set to the number of cores per node.

Here are the additional parameters that should be included in the section for each of the bundled runs:

`[sample_bundled_run_section]`

- `working_directory` (required)
  - Working directory for this run.
- `config_file_path` (required)
  - Path to the configuration file for this run.
- `number_of_blocks`
  - Number of blocks for this run.
  - Required for `mira` and `cetus` mode.
- `nodes_per_replica`
  - Nodes per replica for this run.
  - With the `mira` and `cetus` mode, this value should divide the block size.

`[FHI-aims]`

- `path_to_aims_executable =` (required; /path/to/aims.x)
  - Path to FHi-aims executable being used for energy evaluations and/or structural relaxations.
- `execute_command =` (required; `mpirun`, `srun`, `runjob`, or `shell`).
  - Command to run the FHI-aims binary. The shell command should be used when calling a serial version of aims via /path/to/aims.x control.in. Note that if `execute_command = shell`, then `additional_arguments` will not be appended to the execute command.
- `additional_arguments=` (optional; not valid if `execute_command = shell`)

  - A Python-evaluable list of strings to append as additional arguments used in the subprocess.Popen call of the FHi-aims binary. For example, set this to ["-rr"] to enable round-robin spawning method in mpirun. Or set this to ["–envs","OMP_NUM_THREADS=4"] to allow the runjob command to alter the environmental variable, OMP_NUM_THREADS. Note that the nodes and processes information are automatically included in the argument list via keywords set in `parallel_settings`.

- `control_in_directory =` (required; control_directory_name)
  - Folder name in current directory that holds the control.in files used within GAtor.
- `control_in_filelist =` (required; control.in.1 control.in2 ...)
  - Folder name in current directory that holds the control.in files used within GAtor for successive steps of the FHI-aims cascade. These can be named arbitrarily in the `control_in_directory`. e.g. perform single point calculations with control.in.1 and full relaxations with control.in.2.
- `monitor_execution =` (optional; Boolean)
  - If present, enables monitoring of the FHI-aims binary call spawned through Python's subprocess.Popen module. The monitoring involves: (1) Confirmation of successful job launch, and (2) prevention of job being hung. A job is given 10 attempts to launch before being determined as failed.
- `absolute_thresholds=` (optional; energy1 energy2 ...)
  - List of highest total energies (in eV) allowed for a structure to to be deemed as acceptable for each level of `control_in_filelist`. Must match length of `control_in_filelist`. For example, if one does not want to allow into the common pool structures with a single point energy higher than -45,000 eV or a fully-relaxed energy higher than -45,575 eV, then `absolute_thresholds= -45000 -45575`.
- `relative_energy_thresholds=` (optional; rel_energy1 rel_energy2 ...)
  - Energy (in eV) allowed for a structure to to be deemed as acceptable for each level of `control_in_filelist`, relative to the current running global minimum. Must match length of `control_in_filelist`. For example, if one does not want to allow into the common pool structures with a single point energy 5 eV higher than minimum energy in the pool or a fully-relaxed energy higher than 3 eV than the minimum energy in the pool, then `relative_thresholds= 5 3`.
- `double_store_last_energy` (optional; Boolean)

  - Enables additional storing of the energy obtained from the last tier of the FHI-aims cascade to the key `[run_settings]/property_to_optimize`. For example, this parameter can be used if the final tier of FHI-aims is first stored as "energy_tier_1_full_relax" but should be further used for fitness evaluation of the structure when the property being optimized is simply named “energy".

- `absolute_success` (optional; Boolean)
  - If set to `TRUE`, requires "Have a nice day" to appear in the FHI-aims output file in order for a job to be determined as successful.

- `save_failed_calc` (optional; Boolean)
  - If set to `TRUE`, entire failed FHi-aims calculation folders will be saved to (./failed_calc).

- `save_successful_calc` (optional; Boolean)
  - If set to `TRUE`, entire successful FHI-aims calculation folders will be saved to (./successful_calc). By default, only necessary information such as a structures energy and geometry are saved from FHI-aims' outputs before the output files are discarded.

- `update_poll_interval =` (required if `monitor_execution = TRUE`; time)
  - Length of time in seconds to sleep between two checks on the FHI-aims output file. An FHI-aims job must output something within the time period of `update_poll_interval` * `update_poll_times`; otherwise, the job is determined to be hung. Must match the length of `control_in_filelist`.

- `update_poll_times =` (required if `monitor_execution = TRUE`; integer)
  - Number of times the FHI-aims output file is polled without new updates before determining that the FHI-aims job has hung. Must match the length of `control_in_filelist`.

`[initial_pool]`

- `user_structures_dir =` (required; /path/to/user_defined_initial_pool)
  - Path to the user-defined initial pool, as generated by *Genarris*.

- `duplicate_check =` (optional; Boolean)
  - If present, will perform a duplicate check on the initial pool of structures by 1) computing cosine similarity between the RDF vectors of pairs structures in the initial pool. If these vectors are determined as similar as defined by `RDF_sym_tol` then 2) pymatgen's structure_matcher function is called.

- `vector_cosdiff_threshold =` (used when `duplicate_check = TRUE` and `vector_for_comparison` is set; default = 0.001)
  - This parameter sets the tolerance for determining if two `vector_for_comparison` vectors from pairs of structures in the initial pool are similar using cosine similarity. If similiar, structure's will further be checked for duplication with pymatgen's structure comparer. If not set by user, only pymatgen's structure comparer will be used, but this takes more time depending on the size of the initial pool.
- `vector_for_comparison =` (string; used when `vector_cosdiff_threshold` is set)
  - Name of vector in initial pool jsons (e.g. a distance, RDF, or fingerprint function) to be compared as a preliminary measure to determine if two structures are similar.
- `scale_vol =` (used when `duplicate_check = TRUE`; Boolean)
  - This option determines whether or not to scale the cell volume of two structures when using pymatgen's structure_matcher. If not set as `TRUE` by user, the volume is not scaled by default.
- `ltol =` (used when `duplicate_check = TRUE`; default = 0.2)
  - This parameter determines the fractional length tolerance of lattice vectors allowed between two duplicate structures using pymatgen's structure_matcher. If not set by user the default value is used.
- `stol =` (used when `duplicate_check = TRUE`; default = 0.3)
  - This option determines the site tolerance allowed between two duplicate structures using pymatgen's structure_matcher. It is defined as the fraction of the average free length per atom. If not set by user the default value is used.
- `angle_tol =` (used when `duplicate_check = TRUE`; default = 3 (degrees))
  - This parameter determines the lattice vector angle tolerance allowed between two duplicate structures using pymatgen's structure_matcher. If not set by user the default value is used.

`[cell_checks]`

- `full_atomic_distance_check` (optional; default= 0.211672 Angstrom)
  - Enforces a minimum distance between all pairs of atoms in the system. The default value 0.211672 Å is the equivalent of 0.4 bohr, which is the minimum distance enforced by FHI-aims.

- `interatomic_distance_check =` (optional; default= 1 Angstrom) If present, enforces a minimum distance for atom pairs from different molecules. This value should usually be set larger than full_atomic_distance_check to enforce a larger distance between atoms from different molecules.

- `COM_distance_check =` (optional) If present, enables the COM distance check, which enforces minimum distance between the center of mass of different molecules.

- `specific_radius_proportion =` (optional)

  - A closeness check for potential structures where each atom is assigned a specific radius (by default, their van der Waals radii). In this check, two atoms from different molecules need to be at least a certain proportion (specified by this parameter, which is often shortened as s_r) of the sum of their specific radii apart. E.g. the van der Waals radius of carbon is 1.70 Å, nitrogen's is 1.55 Å; thus if sr=0.75, then any pair of intermolecular C-N contact must be at least (1.70+1.55)*0.75=2.44 Å apart.

- `target_volume = None` (optional) If present, enables volume checks on generated structures. Enforces the volume of a newly generated structure to be within target_volume*volume_lower_ratio - target_volume*volume_upper_ratio.:wq

- `volume_upper_ratio = 1.2` (optional) The upper ratio that defines the lower bound of the volume of a newly generated structure when times by the target_volume.

- `volume_lower_ratio = 0.8` The lower ratio that defines the lower bound of the volume of a newly generated structure when times by the target_volume.

`[selection]`

- `percent_best_structs_to_select` (optional; default = 100)

  - The user may set this parameter if they wish to bias selection to only a certain percentage of top fitness structures.

- `fitness_function =` (optional; default = `standard`)

  - If the user wishes fitness to be calculated on a linear scale, the default value of `standard` is used, and the user doesn't need to explicitly specify this parameter. However, if the user wishes for fitness to be scaled in an exponential fashion, they may choose to set this paramater to `exponential`.

- `fitness_reversal_probability =` (optional; default = 0.0)

  - The user may set this parameter to be between 0.0 and 1.0 to allow a probability of the fitness function being reversed when selecting parents. This may create better diversity in the pools to allow an occasional unfit structure to be selected.

- `pre_relaxation_comparison` (optional; defaults: `ltol = 0.2`, `stol = 0.4`, `angle_tol = 3`)

  - Determines if a structure is too similar to an existing structure in the collection before passing it on to relaxation.(See `[initial_pool]` or pymatgen's structure comparer for definitions of these parameters).
  - User may also set `scale_vol = TRUE` if they wish to scale the structure's before comparison. By default this keyword is omitted and structures are not scaled.
  - It is recommended to to set `stol` larger than in the `post_relaxation_comparison` section since in this section you are most likely comparing un-relaxed structures to relaxed one.

- `post_relaxation_comparison` (optional; defaults: `ltol = 0.2`, `stol = 0.3`, `angle_tol = 3`)
  - Determines if a structure is too similar to an existing structure in the collection after it has been relaxed (See `[initial_pool]` or pymatgen's structure comparer for definitions of these parameters).
  - User may also set `scale_vol = TRUE` if they wish to scale the structure's before comparison. By default this keyword is omitted and structures are not scaled.
  - It is recommended to to set `stol` smaller than in the `pre_relaxation_comparison` section since in this section you are most likely comparing newly relaxed structures to relaxed structures in the common pool.

`[mutation]`

- `mutation_probability =` (required)
  - This parameter sets the probability of performing mutation on structures which have been crossed over. IF set to, e.g., 0.3, the structure has a 30% chance of undergoing mutation. Can be set $0.0 \leq$ mutation_probability ≤ 1.0.
- `double_mutate_prob =` (optional)
  - A user may set this parameter to allow double mutations on crossover structures. If set, the probability of a structure undergoing double mutation is `double_mutate_prob` * `mutation_probability`
- `stand_dev_trans =` (optional; default = 0.3 A)
  - Sets the standard deviation of the random translation mutations to the COM of the molecules in the cell. The translations are randomly picked from a gaussian distribution of this with.
- `stand_dev_rot =` (optional; default = 5 degrees)
  - Sets the standard deviation of random rotation mutations to the COM of the molecules in the cell (euler angles).

- `stand_dev_strain =` (optional; default = 0.25) This parameter sets the standard deviation of mutations which involve strain (using a generic strain tensor) on the lattice of the child structure. It's a proportional parameter so, e.g., (default $stand\_dev\_strain = 0.25$ so e.g. $Ax_{strain} = Ax + (0.25 * Ax\ )$).
- `enable_symmetry` (optional; Boolean)
  - If set to `TRUE`, allows mutation to preserve the highest level of symmetry in the pre-mutation structure.

`[symmetric_crossover]`

The term, "seed molecules," means the symmetrically independent molecules within a structure. The symmetric crossover module takes the 1st selected structure as standard and conducts crossover that blends/swaps certain features of the 1st structure with/by that of the 2nd.

- `swap_sym_prob` (optional; default = 0.50)
  - The probability of the symmetry operation of the 2nd structure to be applied to the 1st. In this case, the seed molecules of the 1st structure become those closest, in terms of absolute COM coordinates, to the seed molecules of the 2nd structure.
- `swap_sym_tol` (optional; default = 0.01)
  - Tolerance for determining whether the 2nd structure's symmetry operations are compatible with the 1st structure's lattice vectors.
- `blend_lat_prob` (optional; default = 0.50)
  - The probability for the lattice vectors to be blended during crossover. If without blending, the vectors will be taken straight from the 1st selected structure.
- `blend_lat_tol` (optional; default = 0.01)
  - Tolerance for determining whether the blended lattices are compatible with the symmetry operations.
- `blend_lat_cent` (optional; default = 0.50)
  - The center of the Gaussian sampling for the blending parameter, b. Let L_1 be the lattice matrix of the first structure, L_2 be that for the second. Then the blended lattice matrix will be $b \cdot L_2 + (1 - b) \cdot L_1$. Therefore, $b = 0$ takes the unchanged lattice of first structure. $b = 1$ takes the unchanged lattice of second structure.
- `blend_lat_std` (optional; default = 0.25)
  - The standard deviation for the Gaussian sampling of the blending parameter.

- `blend_lat_ext` (optional; Boolean)
  - If set to TRUE, then the blending parameter can be smaller than 0 or greater than 1.
- `blend_mol_COM_prob` (optional; default = 0.50)
  - The probability for the COM of the molecules to be blended during a crossover. During the blending process, each "seed molecule" in the 1st structure will be paired up with a closest neighbor in the 2nd structure, in terms of absolute COM coordinates. If without blending, the absolute COM coordinates will be taken from the 1st selected structure.
- `blend_mol_COM_cent` (optional; default = 0.50)
  - The center of the Gaussian sampling for the blending parameter, b. Let c_1 be the COM of the seed molecule. Let c_2 be the COM of the paired molecule. Then the COM of the seed molecule will be moved to $b \cdot c_2 + (1 - b) \cdot c_1$. Thus, $b = 0$ takes the unchanged COM positions of the seed molecule in the first structure. $b = 1$ takes that of the second structure. If there are multiple seed molecules, b is generated seperately for each blending.
- `blend_mol_COM_std` (optional; default = 0.25)
  - The standard deviation for the Gaussian sampling of the blending parameter.
- `blend_mol_COM_ext` (optional; Boolean)
  - If set to TRUE, then the blending parameter can be smaller than 0 or greater than 1.
- `swap_mol_geo_prob` (optional; default = 0.50)
  - The probability for the molecule geometry of the 2nd structure to be swapped into the 1st. The final orientation will be selected from 20 random orientations that have the least coordinate residual from the original geometry in the 1st structure.
- `swap_mol_geo_tol` (optional; default = 3.0)
  - The tolerance on coordinate residual in determining whether two molecule conformations are the same. If yes, then the geometry will not be swapped. If all pairs of molecules are the same, then this operation will be ruled invalid.
- `swap_mol_geo_orient_attempts` (optiona; default = 100)
  - Number of attempts to randomly orient the swapped geometry. The final orientation is selected to be the orientation that has the least coordinate difference with the original molecule.

- `blend_mol_orien_prob` (optional; default = 0.50)
  - The probability for the orientation of the molecules to be blended during a crossover. During the blending process, each "seed molecule" in the 1st structure will be paired up with a closest neighbor in the 2nd structure, in terms of absolute COM coordinates.
  - If the paired up molecule has different geometry than the seed molecule (see parameter `blend_mol_orien_tol`), then blind blending will be pursued. a number of random rotations (`blend_mol_orien_orient_attempts`) will be applied and the new orientation with the minimum average coordinate difference from the two original molecules will be selected. The average is weighted by the blending parameter b (the coordinate difference from the paired molecule gets weighted as b, while that from the seed molecule gets $1 - b$).
  - The blind blending has a probability specified by `blend_mol_orien_ref_prob` to allow exploration of reflection after applying random rotations. If the exploration is pursued, half of the random rotations will be followed by a mirror reflection across z axis.
  - If the paired up molecule has the same geometry as the seed molecule, then the blending will be based on the calculated mapping information from one to the other. The mapping information gives whether or not a mirror reflection is involved, and a rotation in terms of an axis and an angle in degrees. If the mapping does not involve a mirror reflection, then a portion (b) of the rotation will be applied to the seed molecule as the final rotation.
  - If the mapping involves a mirror reflection, then a mirror reflection is applied with a probability given by `blend_mol_orien_ref_prob` . If the mirror reflection is not applied, then blind blending will be pursued. If it is applied, first the orientation of the reflected molecule that has the smallest coordinate differences from the original will be found (with `blend_mol_orien_orient_attempt` random rotation attempts). Then the mapping information will be recalculated. A portion (b) of the rotation will be applied to the reflected and readjusted molecule geometry as the final orientation. Note that it is likely for the mapping calculation to yield a larger tolerance and thus consider the molecules to be different after reflection is applied. In that case, blind blending will be pursued.
- `blend_mol_orien_cent` (optional; default = 0.50)
  - The center of the Gaussian sampling for the blending parameter, b. See description above for parameter `blend_mol_orien_prob` for how b is used.
- `blend_mol_orien_std` (optional; default = 0.25)
  - The standard deviation for the Gaussian sampling of the blending parameter, b.
- `blend_mol_orien_ext` (optional; Boolean)

  - If set to TRUE, then the blending parameter b can be smaller than 0 or greater than 1.

- `blend_mol_orien_tol` (optional; default = 3.0)
  - The coordinate difference tolerance in determining whether the seed molecule has the same geometry as the paired molecule. See description above for parameter `blend_mol_orien_prob` for how this affects the procedure.

- `blend_mol_orien_ref_prob` (optional; default = 0.5)
  - The probability for mirror reflection to be allowed in the final orientation. See description above for parameter `blend_mol_orien_prob` for the usage of this parameter.

- `blend_mol_orien_orient_attempts` (optional; default = 100)
  - The number of attempts to randomly orient a molecule. See description above for parameter `blend_mol_orien_prob` for the usage of this parameter.

- `allow_no_crossover` (optional; Boolean)
  - If set to TRUE, then a crossover attempt that did not invoke any of the above listed operations will be allowed. Otherwise, a `while` loop will be used until 1 attempt uses any of the operations above.