StructOpt
User Guide

Mehreen Ali

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1 Running a StructOpt job

There are two ways to run a StructOpt job.

1. By enterning parameter values
2. By uploading an input file

1.1 By entering parameter values

The below steps need to be followed in order to run a StructOpt job by entering the parameter values on the StructOpt web application.

1. Go to StructOpt's website by typing `http://128.104.200.99:5555/StructOpt` in the browser. The home page of the website will be displayed.
2. Click on **Primary parameters** tab on the left pane of the webpage. The primary parameters will be displayed on the right pane of the page.
3. The **Structure** parameter specifies the type of structure to be optimized. There are three options to choose for this parameter i.e. Cluster, Crystal and Defect. Select **Defect** structure.
4. The **Optimizer type** parameter specifies the type of optimizer to be used for optimization. There are three options to choose for this parameter i.e. Random, Simulated annealing (SA), Basin hopping (BH) and Genetic algorithm (GA). Select **Genetic algorithm (GA)** optimizer type.
5. The **Atom list** parameter allows you to set the number and type of atoms in a simulation. The details include Type of atom, No. of atom, Mass of atom and Chemical potential of atom. One row corresponds to one atom type. In order to add a row, click on the **Add row** button. In order to delete a row, click on **Delete row** button. In the first row, enter **C** as the Type of atom, **2** as No. of atom, **12** as Mass of atom and **-4.1224** as Chemical potential of atom. Add a new row by clicking on the Add row button and enter **Si** as the Type of atom, **3** as No. of atom, **28** as Mass of atom and **-4** as Chemical potential of atom.
6. The **Number of atoms** parameter denotes the number of atoms to be used in initiating a simulation. The value of this parameter is auto populated and is equal to the sum of the values in the **No. of atom** text box of the Atom list parameter.
7. The **Number of individuals** parameter specifies the number of individuals in a population. Enter **20** as the value for this parameter.
8. To enter the values for **Output parameters**, click on either the **Next** button on the bottom right of the center pane or on the Output parameters tab on the left pane of the webpage. The output parameters will be displayed on the right pane of the page.
9. The **Email address** parameter specifies the email address to which the notifications and StructOpt job output results will be mailed. Enter **mali24@wisc.edu** as the value for this parameter.
10. The **System name** parameter specifies the user-defined name for the StructOpt job run. Enter **System** as the value for this parameter.
11. The **File name** parameter specifies the name of output folder and file for optimizer data. Enter **Output** as the value for this parameter.
12. The **Genealogy** parameter is a flag indicating if a genealogy of the structures in a population should be written. Select **True** as the value for this parameter.
13. The **Output format** parameter specifies the format for outputting fitness data to files. Enter **formationenergy** as the value for this parameter.

14. The **All energy file output** parameter is a flag to determine whether to output all energy file for simulation. Select **True** as the value for this parameter.

15. The **Best individuals output** parameter is a flag to determine whether to output and track best structures. Select **True** as the value for this parameter.

16. The **Number of bests** parameter specifies the number of individuals to keep track of in best list. Enter **100** as the value for this parameter.

17. The **Write individual defect** parameter is a flag indicating if atoms in region 1 and 2 for defect calculation should be written. Select **False** as the value for this parameter.

18. The **Output vacancies** parameter is a flag indicating if vacancy atoms should be written to the structure output. Select **False** as the value for this parameter.

19. To enter the values for **Post processing parameters**, click on either the **Next** button on the bottom right of the center pane or on the Post processing parameters tab on the left pane of the webpage. The post processing parameters will be displayed on the right pane of the page.

20. The **Lattice concentration** parameter is a flag indicating if the concentration of lattice atoms versus defect atoms should be calculated. Select **True** as the value for this parameter.

21. The **Standard post-processing** parameter is a flag to determine whether to run basic post-processing analysis on optimization output. Select **False** as the value for this parameter.

22. The **Genealogy tree** parameter is a flag indicating whether or not to construct a full genealogy tree during prost-processing. Select **False** as the value for this parameter.

23. To enter the values for **General algorithm parameters**, click on either the **Next** button on the bottom right of the center pane or on the General algorithm parameters tab on the left pane of the webpage. The general algorithm parameters will be displayed on the right pane of the page.

24. The **Genealogy tree** parameter is a flag that indicates if the optimizer should load structures from a previously started simulation. Select **False** as the value for this parameter.

25. The **Number of restart atoms** parameter specifies the number of atoms included in region 1 and 2 for defect simulation for loading into a restarted simulation. Enter **0** as the value for this parameter.

26. The **Seed** parameter specifies the random number seed generator. Enter **0** as the value for this parameter.

27. The **Forcing control** parameter specifies the method for controlling realistic configurations. There are three options to choose for this parameter i.e. Concentration, Chemical potential and Energy bias. Select **Concentration** forcing control.

28. The **Parallel** parameter is a flag indicating whether a simulation should be conducted in parallel. Select **False** as the value for this parameter.

29. The **Debug** parameter specifies the method for debugging a section. There are nine options to choose for this parameter i.e. Main optimizer algorithm, Selection schemes, Mutation schemes, Crossover schemes, Fitness schemes, Energy evaluation algorithm, Find defects function, Setup calculator function and None. Select **None** debug method.

30. The **Algorithm type** parameter specifies the type of algorithm. There are four options to choose for this parameter i.e. $(\lambda + \mu), Island\_Method, (\lambda, \mu) and Island\_Method(\lambda, \mu)$. Select $(\lambda + \mu)$ algorithm type.

31. The **Finger printing** parameter is a flag determining whether fingerprint function for structures should be calculated. Select **False** as the value for this parameter.

32. The **Fixed region** parameter is a flag determining if region 3 should be fixed and forces set to zero for a Defect structure optimization. Select **False** as the value for this parameter.

33. The **Constrain position** parameter is a flag to constrain the area in which a defect can be located. Select **False** as the value for this parameter.

34. The **Rattle atoms** parameter is a flag indicating if atoms should undergo additional shaking before local minimization. Useful for systems with strong potentials. Select **False** as the value for this parameter.

1.2 By uploading an input file

2 StructOpt job tracking