MDAnalysis

GSOC2022 Proposal

Krishna Sharma

http://mdanalysis.org/

Content

Personal details

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About me

I am a 2nd year undergraduate at G L Bajaj institute of technology and management Greater Noida, India.when I was exploring all the tech world then I got my interest in data science.I am a fast learner and always want to do something good for society. I love to play badminton ,Football and Chess.

Experience

I have Selected for google secret developer challenge(FOOBAR) and completed all 5 levels. I have also done a project of machine learning with python which is face mask detection with use of tensorflow, opencv, sklearn model. I am very keen on working in Python and Data science. Doing the Python for MDAnalysis type hinting project greatly intrigues me and will definitely enable me to make a significant impact to the community by increasing the functionality of the MDanalysis more

understandable for users. I wish to keep contributing to the MDAnalysis projects and one day see it being used as best to analyze trajectories from molecular dynamics(MD) simulations in many popular formats. This is my first time participating in GSoC.

Why me

I am enthusiastic about machine learning and data science spending days learning this amazing technology and models, Also I have perseverance towards work. MDAnalysis is object oriented python library which is used for analyzing trajectories from molecular dynamics which uses machine learning and deep learning for analyzing trajectory. so, I am very excited about this project.

Proposed Project

Introduction:

MDAnalysis is developed and maintained as a freely available, open-source project by a global community of scientists. MDAnalysis is very useful in analyzing trajectories from molecular dynamics.

MDAnalysis has classes like AtomGroup,Universe which are used for simulation. It is a big library so we need to make it easy for the user to understand the functions of MDAnalysis more deeply and for this we need to do Type Hinting.

Synopsis

The Goal of this project is Type hinting of code or project code so that anyone can understand it more easily and properly. If they want to contribute something new then anyone can contribute to it easily.

Type hinting is a very useful way to make code easier to understand and contributors will connect more with the code easily.

Technical breakdown of project

- Read more about MDAnalysis and make understanding with MDAnalysis.
- Type hinting code of project.
- Consult with a mentor and enhance my project.
- Submission of project.

Deliverables/Tasks

I want to work on this project to improve my skill and give something good to society.

Things to be ensured while completing the project:-

- Set up type analysis in the continuous integration pipeline.
- Design a best-in-class annotation scheme that is informative,easy to use, and catch the most errors.
- Annotate as much of the code as possible.
- Document the type system for MDAnalysis contributors and for downstream users.

Tentative Timeline

Community Bonding (May 20 to June 12)

- This period will mostly be utilized for bonding with the community and learning more about MDAnalysis,and Type hinting.
- Discussing milestones about Type hinting in detail.
- Read more research papers about MDAnalysis.

- Do some Type hinting on project code to showcase my work to mentor and get feedback.

June 13 - June 26 (2 Week)
- Implementing Type hinting.
- Research more about MDAnalysis.
- Writing documentation about MDAnalysis.

June 27 - July 3(2 week)
- Learn more about MDAnalysis.
- Implementing Type hinting.
- Writing documentation about MDAnalysis.

July 11 - July 24 (2 week)
- Writing documentation and code enhancement.

Evaluation 1 (July 25 -July 29)
- Project Submission.

Availability

GSoC will be my only commitment for the upcoming summer.

During the community bonding period, my offline semester will be going on. During this time, I will try to squeeze out as much time as possible from my weekends for the project. This semester, I have relatively light courses so I can manage both of them simultaneously.

Towards the starting of the evaluation period, from July 10 to July 25, I will be having my end semester exams, so it might not be possible for me to work on GSoC during that time, but I will compensate for that by putting in extra hours during the Type Hinting phase.

Apart from that, I will be working full time on GSoC for about 30 hours a week and sincerely work on my project delivering the deliverables.

My vision

What are your long-term plans, if you have figured those out yet? Where do you hope to see yourself in 10 years?

I am really passionate about data science and machine learning. I want to work in the lambda AI or kaggle community at Google. I also want to work in the Tensorflow community.

My vision about MDAnalysis

In the next four to five years I would love to see MDAnalysis as the best tool for molecular dynamics. The MDAnalysis will provide lots of useful commands for users to analyze trajectories easily . I would like to stick to the MDAnalysis and let it achieve my vision.