Ojas Singh

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Research Interests

- Quantum Many Body Methods
- Time-Dependent Methods
- High Performance Computing
- Quantum Machine Learning
- Molecular Dynamics
- Ab-initio Methods

Research Experience

Time-Dependent Configuration Interaction (*Masters Thesis*)

Jan 2021 - Current

Dr. P. Balanarayan, IISER Mohali

I have developed a fast CI code for TDCI using BitArray and concurrent data structures in pure Rust. We have successfully leveraged Rust's rich type system to go beyond LLVM's optimizations, making our implementation extremely efficient. I am currently working on Time Propagation using the (t, t') method.

- Concurrent Programming / Compiler Optimizations
- Correlated Methods
- Sparse Matrix Algebra
- BitArray Manipulation

High-Performance Parallel Algorithm for Magnetic Tweezer for real-time monitoring of protein folding and unfolding

Feb 2021 - June 2021

Dr. S Rakshit, IISER Mohali

I have designed and developed a high-performance parallel python program for real-time Image Acquisition and Processing. We were able to analyze fast magnetic bead movement at the millisecond temporal resolution and nanometer spatial resolution. This implementation can process 3000+ frames per second which is three times faster than industry leading software.

- High-Performance Python Programming
- Image Acquisition / Analysis and Signal Processing

Spectral Clustering Based Fragmentation Approach for Ab-initio Quantum Calculation of large molecules

May 2019 - Dec 2020

Dr. P. Balanarayan, IISER Mohali

A Spectral-Clustering-based fragmentation scheme for estimating the electronic energy of a large molecule using ab-initio methods is devised. The method exploits salient properties of graphs to predict the best possible fragments and overlaps heuristically. In the tests performed, energy estimates obtained using this method show an excellent agreement with those obtained via the actual computation of the complete molecule. The accuracy of the results obtained deploying this method allows the quantum calculation of large molecules.

- Spectral Graph Partitioning Algorithm
- Python Programming Language
- Gaussian Software Package
- Scripting for Automated Computation

Non-linear Dynamics and Chaos Theory

April 2017 - May 2017

Prof. Sudeshna Sinha, IISER Mohali

Studied and analysed bifurcations in simple logistic maps, Lorenz systems and three dimensional chaos using C++ and Python.

Relevant Coursework

- Quantum chemistry
- Introduction to data science
- Differential equations for scientists
- Theory of computation
- Molecular spectroscopy
- Molecular dynamics simulations
- Numerical methods in chemistry
- Advanced optics and spectroscopy lab

Skills

- Multi-Processing Programming/ High Performance Python
- Spectroscopy
- Git/GitHub
- C++/Rust Programming Languages
- Linux/bash/Scripting/LaTeX
- Signal/Image Processing

Languages

- English
- Hindi

Education

2016 – 2021 **BS-MS dual degree** (Chemistry) Indian Institute of Science Education and Research Mohali

2016 **Intermediate** (12th) Brij Behari Sahai Inter College (BBS), Prayagraj (CBSE)

2014 **Matriculation** Swami Vivekanand Vidya Ashram, Prayagraj (CBSE)

Achievements

- **Kishore Vaigyanik Protsahan Yojna (KVPY Fellowship)**: Fellow since 2016 awarded to scholars pursuing pure science by the Department of Science and Technology, Government of India
- **Drishti Cryptex** cryptography CTF Winner in 2017,2018
- **Advitiya CS:GO** Tournament Winner in 2019
- **JEE Advanced** Secured All-India Rank Under 6000 in 2016
- **Project Euler** Level 2

Seminars and Conferences

- IBM Qiskit Global Summer School 2021
- RustCon 2020
- BMW Quantum Challenge 2021
- National Science Camp (VIJYOSHI) 2016

Co-curricular

- Volunteered and designed websites for IISERM Foundation Day and Insomnia (IISERM cultural and science fest).
- Earned the **Level B certificate** as an **NCC** (National Cadet Corps) cadet.
- Elected as co-convener (2017–2018) , Gaming Club, IISER Mohali.
- Built a Low Latency VPN for gaming and have 50+ active users.
- Coached a six-man team for eSports tactical shooter title.