Ojas Singh

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Research Interests

- High Performance Computing
- Quantum Many Body Methods
- Quantum Chemistry
- Machine learning
- Molecular Dynamics
- Bio Physics

Research Experience

Time-Dependent Configuration Interaction (*Masters Thesis*)

Jan 2021 - Current

Dr. P. Balanarayan, IISER Mohali

Developed fast CI code for TDCI using BitArray and concurrent data structures in pure Rust, which is the fastest implementation of CI code till date. Currently working on dynamics using the (t, t′) method.

- Second Quantizations
- Compiler Optimizations
- Sparse Matrix Algebra
- Concurrent Programming
- BitArray Manipulation
- Quantum Dynamics

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
- Protien Folding / Unfolding
- Image Acquisition / analysis (FFT)
- Single Molecule Study / Magnetic Tweezer

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 at abinitio level of theory is devised. The method exploits few properties of Graphs to predict the best possible fragments and overlaps heuristically. In the tests performed, energy estimates obtained from this method show an excellent agreement with those obtained from 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 Program
- Scripting for Automated calculation

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 dynamics simulations
- Molecular spectroscopy
- Numerical methods in chemistry
- Advanced optics and spectroscopy lab

Skills

- Multi-Processing Programming/ High Performance Python
- Git/GitHub
- Data Structures and algorithms
- C++/Rust Programming Languages
- Linux/bash/Scripting/LaTeX
- OpenCV/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)**: Fellow since 2016 (SX-1511066)
- **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.

Referees

- Available on request