

Journal

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1 Spring 2007, March 28 to April 4

1.1 Week1 - Tasks Completed

This was the first week for me. I knew the basics of latex but haven't really used it lately. So I revised the basics for our task of writing the autobiography and the journal. Now I am ready to learn in detail about it.

I was planning to learn python since some time but could never get the opportunity to learn it. The research carried out Dr.Martin has given me the motivation to learn it.

I started learning python and find it quite simple since it is similar to the programming languages that i have worked with. I just started implementing some basic programs and hope that I can learn it quickly.

2 Week 2 - 04/03/07 to 04/10/07

This week my project assignment was to write some topic in math in latex. So I decided to write a report on the seminar that took place in the Mathematics department. The talk was given by Professor John Clark. The topic was Levitt Algebra. I enjoyed writing the assignment and also learnt a lot since the math involved was that of post-doctoral level involving rings etc.

3 Week 3 - 04/10/07 - 04/17/07

Last week, we were asked to read a paper on "Approximating a Wavefunction as an Unconstrained Sum of Slater Determinants" by Gregory Beylkin, Martin J. Mohlenkamp and Fernando Perez. This is a research paper that Dr.Mohlenkamp is currently working on. I read the paper and tried to understand the basic purpose of the research and the steps that are taken to achieve the goal. The paper deals with solving the wavefunction for the multiparticle

Schrodinger equation with fewer constraints. According to the paper, currently the procedures provide useful approximations at relatively low computational cost because of the limited computer capacity. But, when higher quality approximations are needed the current methods scale badly. So, the paper proposes the use of an integral formulation of the problem, a Green's function iteration and a fitting procedure based on the computational paradigm of separated representations. For this, the authors considered the time-independent, nonrelativistic, multiparticle Schrodinger equation and fix the nuclei according to the Born-Oppenheimer approximation.

The paper goes on to describe the machinery and algorithms tfor computing antisymmetric inner products involving the Hamiltonian operator.

I read the paper and understood the theory behind it, however i think i will get a better idea and completely understand it if i do some research on it and gain some more background knowledge.

4 Week 4 - 04/18/07 - 04/24/07

The task for this week was to write a program in python to add the first n numbers. This was a good way to be introduced to the python environment. It was easy to learn as this language is similar to some of the other common programming languages.

5 Week 5 - 04/25/07 - 05/01/07

This week, the exploratory members were asked to help the research members by preparing a plan to code the mathematical derivation they were proving in python. As of now the research team does not require any help so in the meantime I started learning the syntax and other details of the language and hopefully by the time research team requires us to code the derivation, we would be able to do it.

6 Week 6 - 05/01/07 - 05/08/07

This week, we were asked to plan out and start coding the determinant derivation in python. I started learning about the functions and commands that would be related and useful for the derivation. I am learning to create multidimensional lists which would be used for the code for the determinant derivation.

7 Week 7 - 05/09/07 - 05/16/07

This week we had to search for two journal papers in order to prepare for the presentation. I searched for the papers and found them. I also prepared the other functions in python.

8 Week 8 - 05/17/07 - 05/22/07

This week we had to prepare to present one of the two journal papers that we found last week. I prepared the power point presentation for the topic "Sparse grid spaces for the numerical solution of the electronic Schrodinger equation".The author is H.Yserentant.

9 Week 9 - 05/23/07 - 05/29/07

The exploratory members presented their papers. The presentation was good and we enjoyed it. I prepared the presentation for the research paper and though the paper was difficult to understand, I presented whatever I could understand. The presentation was a good way to learn the different ways one can present a paper. I learned a lot from the presentation.