Dr. J. D. Gorfinkiel
Dept. Of Physics and Astronomy
The Open University
Walton Hall
Milton Keynes MK7 6AA

+44(0)1908 858 205
J.Gorfinkiel@open.ac.uk

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Dear Sir/Madam,

I am writing to support Zdenek Mašin's request to attend the Autumn Academy.

Zdenek is in his third year of PhD, studying low energy electron collisions with diazines. He uses a well established method, the R-matrix method, and is significantly involved in developing its computational implementation, the UKRMol suite.

Zdenek joined the group at the OU as part of the uptake of PhD students under the UK-RAMP, the UK R-matrix Atomic and Molecular Physics HPC Code Development Project. This project is funded by the EPSRC as part of the High Performance Computing Software Development call; one of its declared aims is to train a cohort of people with expertise in HPC software development. To this end, groups at UCL, QUB and the OU have taken on PhD students who, in addition to their research in Molecular Physics, are contributing to the development of the UKRMol suite. We place significant effort in training our group members in software development: over the last couple of years, we have developed a culture of best practice, encouraging extensive use of version control tools, instituting coding standards, encouraging interaction between geographically distributed developers, etc..

Zdenek has shown himself to be a conscientious programmer. He has written a couple of programs that have enabled him, and our collaborators, to improve the quality of the scattering calculations that are being performed. However, these are programs designed to run on desktop computers, rather than on HPC platforms. Zdenek has taught himself the basics of parallel programming but we both acknowledge that in order for him to progress in this area, it is fundamental that he receives formal expert training.

As part of the work he will be performing in the next year, we expect he will be able to run calculations using much more sophisticated scattering models that it is currently possible. This will require him to make use of, and probably help debug, an MPI implementation of part of the UKRMol suite. In addition, Zdenek has started to explore the use of B-splines in electron-molecule scattering calculations. We hope he will be able to use of the programs he's started developing too. In any case, the move to using B-splines is fundamental for further developments under UK-RAMP and any experience he gains and software he develops will be of great use for the team.

Regards,

Dr. Jimena D. Gorfinkiel