Dear Sir or Madam,

My PhD project is set in the field of computational quantum physics, namely in the theory of electron-molecule collisions. The target molecules I am looking at are related to the single-ring molecule pyrimidine, which also serves as a model molecule for the bases of DNA.

Our group (UK-RAMP) has been using the "UK R-mol" computational suite. These sets of codes, parts of which are a few decades old, are now undergoing a major rewrite, whose goal is to update the code to the modern standards of high performance computing. The aim is to make use of the computing power of the large computer clusters available at present, while improving on the abilities of the code itself. With some parts of the suite (e.g. diagonalization of large sparse matrices) are already being parallelized by other developers in the team, we are also looking at other parts of it, which may benefit from parallelization, being made more effective or completely rewritten.

Being in the second year of my PhD I have started a development of a completely new core of our codes, which deals with calculation of a large number of integrals needed for evaluation of matrix elements of the Hamiltonian. This new set of codes based on B-splines will overcome some of the limitations of the current computational suite and allow me to run calculations describing collisions of electrons with more complex molecules and for a wider range of energies of the incoming electron as well, which will result in a considerable improvement on the abilities of the code, from which a future research in this field will benefit greatly. I have some basic experience with parallelization, but I need to improve on my knowledge of it and practical abilities in using it effectively. I would also benefit from training in more general HPC skills. The new codes will be applied to calculations on the molecules that I have been studying and a future development will then be continued within the UK-RAMP project.

The Programme of the Autumn Academy covers perfectly the areas of HPC, which I need to master as a part of my PhD. As a result of attending I expect to bring new ideas into our group as to how to make our code more effective, better coded and what might be the promising directions for its development in the future. Because HPC itself has become increasingly interesting for me, I have started considering it a major focus of my career after finishing my PhD. Therefore I expect to benefit greatly from the Autumn School. Thank you very much for considering my application!

Yours sincerely,

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