GPU ACCELERATED INTENSITIES: A NEW METHOD OF COMPUTING EINSTEIN-A COEFFICIENTS

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Abstract

The use of variational nuclear motion calculations to produce comprehensive molecular line lists is now becoming common. In order to produce high quality and complete line-lists in particular applicable to high temperatures requires large amounts of computational resources. The more accuracy required, the larger the problem and the more computational resources needed. The two main bottlenecks in the production of these line-lists are solving the eigenvalue problem and the computation of the Einstein-A coefficients. From the project's recently released line-lists, the number of transitions can reach up to 10 billion evaluated by the combination of millions of eigenvalues and eigenvectors corresponding to individual energy states. For line-lists of this size, the evaluation of Einstein-A coefficients take up the vast majority of computational time compared to solving the eigenvalue problem. Recently, as part of the ExoMol [1] project, we have developed a new program called **G**PU **A**ccelerated **IN**tensities (GAIN) that utilises the highly parallel Graphics Processing Units (GPU) in order to accelerate the evaluation of the Einstein-A coefficients. Speed-ups of up to 70x can be achieved on a single GPU and can be further improved by utilising multiple GPUs. The GPU hardware, its limitations and how the problem was implemented to exploit parallelism will be discussed.

References

[1] J. Tennyson and S. N. Yurchenko. ExoMol: molecular line lists for exoplanet and other atmospheres. *MNRAS*, 425:21–33, 2012.