THE GPU ACCELERATED ABSORPTION SIMULATION (GAAS) PLATFORM

CHARLIE SCOTT CALLAHAN, Mechanical Engineering, University of Colorado Boulder, Boulder, CO, USA; SEAN COBURN, GREGORY B RIEKER, Department of Mechanical Engineering, University of Colorado Boulder, Boulder, CO, USA.

We present the GPU Accelerated Absorption Simulation (GAAS). GAAS is an open-source software package for simulating broadband absorption spectra rapidly using Nvidia graphics processing units (GPUs). GAAS is intended to provide a fast alternative to HAPI [1], capable of simulating absorbance spectra given a pressure, temperature, and concentration. GAAS is written in C++ and C and comes with a python interface so that it can be easily integrated into existing codebases. GAAS supports Voigt lineshape profiles and primarily contains a python function to replace HAPI's absorptionCoefficientVoigt. GAAS uses spectroscopic data in HITRAN's "par" format in order to be compatible with existing codebases that use HAPI. The software realizes up to a 100x reduction in computation time by simulating each Voigt lineshape in the spectrum on its own GPU thread, achieving enough parallelization for full utilization of GPU resources for spectra containing a few thousand absorption lines.

[1] R.V. Kochanov, I.E. Gordon, L.S. Rothman, P. Wcisło, C. Hill, J.S. Wilzewski, HITRAN Application Programming Interface (HAPI): A comprehensive approach to working with spectroscopic data, Journal of Quantitative Spectroscopy and Radiative Transfer, Volume 177, 2016, Pages 15-30, ISSN 0022-4073