Abstract

This work shows the potential in the use of graphics processing units (GPU) to speed up the calculation of radiative energy absorption by atmospheric gases. Gas absorption calculations are needed at millions of spectral lines (wavelengths) in order to have an accurate depiction of the Earth’s in-coming and out-coming radiative energies. The CUDA/GPU portion of the code obtains fast Voigt lineshapes at several spectral locations, whereas the JAVA portion of the code performs efficient random file access on the large HITRAN database to obtain molecular gas parameters. The first advantage of this programming model is the great speed up obtain by the introduction of parallel GPU algorithms, and the second advantage is the modular combination of the lower-level CUDA algorithms for the GPU calculations and the higher-level Java language for efficient input/output of files (I/O). The latter results in an accessible interface to the end-user that is not an expert in GPU programming.

Introduction

- Modeling radiative transfer in the atmosphere is an extremely challenging task
- Current needs:
  - Fast, accurate and robust PARALLEL models (GPU, MPI, Threads)
  - Sub-grid models for coupling with other phenomena (i.e. turbulence, convection, cloud physics)
  - Avoid computationally expensive codes (i.e. Monte Carlo)
- General computing in graphic processing (GPGPU) units is a powerful alternative
- Drawbacks:
  - Full speed up only for single precision (4 bytes)
  - GPU low memory and CPU/GPU communication are bottlenecks
  - Lack of documentation, validation and applications to radiative transfer

Mathematical Formulation

- Gas absorption is a extremely noisy function along the spectrum [1]
- Line-by-line (LBL) calculations using Voigt lineshapes are required for every single gas at every single state [2]
- Slow process as there is many gas species and thousands of millions of important wavenumbers

Summary & Conclusions

- A hybrid Java/CUDA model allows the modular combination of GPU and high-level I/O algorithms
- The model allows for code reusability with an accessible learning curve for the end user
- Errors due to GPU single precision are less than 0.3% in the case of atmospheric H2O and CO2 at sea level
- Maximum speed up of 18 for 50,000 tested wavenumbers, speed ups grow proportional to the number of wavenumbers
- Potential extension to entire spectrum and multiple gaseous species is a must!

CUDA GPU / JAVA IO Programming Model

GPU Parallel Model: Voigt Lineshape - Integral Function[2]

\[ \int \frac{J\left(\nu - \nu_j\right)}{\sqrt{2\pi} \sigma_x} e^{-\frac{\left(J\nu - \nu_j\right)^2}{2\sigma_x^2}} d\nu \]

where \( J \) is the line strength, \( \nu \) is the frequency, \( \nu_j \) is the frequency of the line center, \( \sigma_x \) is the line width, and \( e \) is the base of natural logarithms.

CUDA / JAVA flow diagram

GPgpu programming basis [3, 4]

- Cost, 8 per thread (fp32 floating point operations) is low
- A GPU has thousands of processors for lightweight tasks
- Parallel processes (threads) launch from CPU
- High CPU/GPU data transfer reduces efficiency
- Double-precision is needed for Jacobian-free calculations

Results and Speed up for Atmospheric H2O and CO2

Atmospheric Profile at 50 Altitudes

<table>
<thead>
<tr>
<th>U.S. Standard Atmosphere ’76</th>
<th>p (mbar), ( 1 \times 10^5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000</td>
<td>1700</td>
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<td>5000</td>
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</tr>
<tr>
<td>6000</td>
<td>1300</td>
</tr>
</tbody>
</table>

Gas Absorption Coefficient at \( z = 0 \) m

<table>
<thead>
<tr>
<th>Wavenumber (cm(^{-1}))</th>
<th>( \alpha ) (cm(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>10,000 wavenumbers</td>
<td>0.001</td>
</tr>
<tr>
<td>50,000 wavenumbers</td>
<td>0.002</td>
</tr>
<tr>
<td>100,000 wavenumbers</td>
<td>0.003</td>
</tr>
</tbody>
</table>

Gas Absorption Relative Error on GPU

<table>
<thead>
<tr>
<th>Wavenumber (cm(^{-1}))</th>
<th>Relative Error (%)</th>
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</thead>
<tbody>
<tr>
<td>10,000 wavenumbers</td>
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References


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