GPU acceleration of CVODES for stiff integration of chemical kinetics

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Introduction

For numerical analysis of reaction flow, such as combustion, a strong integration of a highly stiffed chemical reaction system is required.

However, since the system grows proportionally to the number of chemical species, significant computational costs are incurred and an increase in computational speed is essential to address this.

The methods used for accelerating calculations include parallel processing using multiple processors of the central processing unit (CPU), and parallel operation using the graphics processing unit (GPU).

Goal: acceleration of CVODES for the numerical integration of chemical kinetics on GPU.

Background Information

CANTERA: a suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and/or transport process. The 0-D reactor needed for combustion response was implemented and operated through this tool.

CUDA: CUDA is a technology developed by GPU manufacturer nvidia, which stands for Computing Unified Device Architecture. GPU acceleration is implemented in other areas other than graphics through it.

MAGMA: linear algebra library based on GPU architecture. It provides several routines optimized for GPU and depend on CUDA.

CVODES: a solver which is part of SUNDIALS (Suite of Nonlinear and Differential/Algebraic equation Solvers) library and widely used as a stiff ODE interpreter.

Method

The mechanism is classified in three based on size: small, medium, large.

Used sundials-magma which is modified version of sundials for GPU-based LU factorization which is most computational part in numerical analysis.

Result is averaged total 3 trials and rounded at top of the decimal place for medium and large, and at second of the decimal for small system.

Result and Condlusion

	Small	Medium	Large
n_species/ n_rxns	53/325	2192/13927	7173/47157
	Running time (s)		
GPU	1.8	40.3	373
CPU (1 thread)	0.1	1630	63564
	Relative speed		
GPU	1	1	1
CPU (1 thread)	17.86	0.024	0.0059

On small size of system CPU based computation is much faster than GPU.

For medium and large system, GPU is extremely faster than CPU 1 thread.

It was concluded that GPU should be used when size of system is large and CPU should be used on the other situation.

Discussion

Comparing multi-thread CPU and GPU is needed because single threading method is really inefficient and multithreading is frequently used nowadays. But using mkl(math kernel library, intel)is not possible because for compiling and building all, gnu compiler is used, not intel, in this research. For better and abundant result, editing sundials-magma source code based on OpenMP parallel programming is required.

References

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