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GPU-ACCELERATED INTERSTELLAR CHEMISTRY WITH WIND: A GENERAL ORDINARY DIFFERENTIAL EQUATION SOLVER

Alexander Gurvich, Northwestern University
2018–2019 Graduate Fellow

EXECUTIVE SUMMARY

Radiative cooling owing to interstellar chemistry is an important component of modern cosmological simulations, but the fully time-dependent calculation is often too computationally expensive to include for large-volume and high-resolution simulations. To address this limitation, the PI created WIND, a general GPU-accelerated ODE (ordinary differential equation) solver that supports systems that are coupled and stiff. After a naïve first implementation, we have seen a speedup by a factor of three for our problem. In addition, we have identified a number of bottlenecks whose mitigation can improve the code substantially, with the goal of making WIND a public code that is applicable to a wide variety of problems.

RESEARCH CHALLENGE

Many simulations of radiative cooling approximate the processes of interstellar chemistry by assuming that the gas in the simulation is in chemical equilibrium; however, comparisons with time-dependent interstellar chemistry in the FIRE simulations show that there is a significant difference. Including time-dependent chemistry results in more accurate cooling processes during the course of the simulation also enhances the predictive power and applicability of the simulation to interpreting real-life observations. Nevertheless, it is computationally expensive—taking up to 98% of the computational cost of the simulation when enabled, which has restricted the volume and resolution of the simulations we have been able to run.

METHODS & CODES

We developed WIND, a brand-new GPU-accelerated code, to address the challenge of simulating radiative cooling so that we can apply our time-dependent chemistry model in a new regime of simulation. WIND is a general ODE solver and can be applied to any system of ODEs, either coupled or independent. WIND also includes two numerical methods for integrating ODEs, one of which is an "implicit method" that allows WIND to efficiently solve stiff systems of ODEs (ones that involve many very different timescales). We have implemented these algorithms for both GPUs in CUDA and for CPUs in C, allowing users to take advantage of GPUs when they are available but switch to the CPU version if they are not.

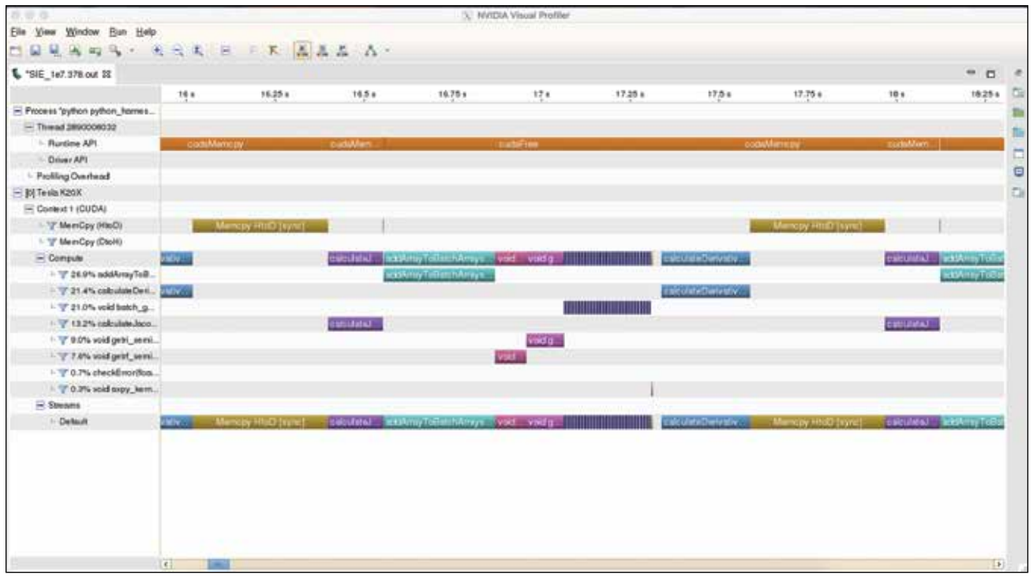

Figure 1: An example profiling session in NVidia's visual profiling program NVVP. Time is along the horizontal axis and different CUDA kernels called in WIND are represented in rows. Colored blocks represent time spent by the GPU accelerator within each CUDA kernel. Visual profiling can quickly identify severe bottlenecks and algorithmic inefficiencies. In this session, memory communication (top row) is shown to be a major limiting factor.

RESULTS & IMPACT

We have preliminarily found that our new ODE solver is three times faster on GPUs than when run on CPUs, with increasing speed as the system of equations is made larger. Additionally, there are at least three concrete targets for improving this result where naïve first-attempt implementations were used. Future work will be focused on these hotspots to improve the speed of WIND so that it can be made public and applicable to a wide variety of problems.

WHY BLUE WATERS

Blue Waters gave me access to GPUs when I had none; the XK nodes on Blue Waters were absolutely critical to the development and testing of WIND.

Alexander Gurvich is a third-year Ph.D. candidate in astronomy and astrophysics at Northwestern University. There, he works under the direction of Claude–André Faucher–Giguère. He hopes to graduate in 2023.