Contribution ID: **282**

Type: **not specified**

Algebraically-Stabilized Explicit Integration Of Extremely Stiff Reaction Kinetics Networks with GPU Acceleration

Systems of differential equations containing multiple, widely-separated timescales are termed “stiff”. It is commonly believed that specialized implicit methods must be used to solve such systems because stability limits on the timestep size make standard explicit integration impractical.
This talk will show that even extremely stiff sets of differential equations may be solved efficiently by explicit methods if limiting algebraic solutions are used to stabilize the numerical integration. Employing stringent tests with astrophysical thermonuclear networks, evidence is provided that these methods can deal with the stiffest networks with accuracy and integration timestepping comparable to that of standard implicit methods. Explicit algorithms can execute a timestep faster and scale more favorably with network size than implicit algorithms. Thus, these results suggest that algebraically-stabilized explicit methods might enable integration of much more complex reaction kinetics problems than have been feasible to this point for astrophysics and a variety of other disciplines. Recently we have implemented these new methods on Graphical Processing Unit (GPU) accelerators for large supercomputers such as Titan at ORNL, which permit many such networks to be integrated in parallel. Initial tests for the Type Ia supernova problem suggest that for realistic (hundreds of isotopes) thermonuclear networks these methods can integrate a single network 5-10 times faster than implicit methods, and can integrate of order 100 networks from different zones of the hydro simulation on a single GPU in the same length of time required to integrate a single such network using traditional implicit methods on a CPU. This implies that many problems in a variety of disciplines such as astrophysics, atmospheric and climate science, fission and fusion energy, and combustion chemistry that were previously thought not possible to solve with realistic kinetic networks may now be accessible to these new algorithms deployed on modern computational hardware.

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