Journal of Computational Physics 231 (2012) 5266–5288

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Algebraic stabilization of explicit numerical integration for extremely stiff reaction networks

Mike Guidry *

Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA
Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA
Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

ARTICLE INFO

Article history:
Received 21 December 2011
Received in revised form 3 April 2012
Accepted 10 April 2012
Available online 28 April 2012

Keywords:
Ordinary differential equations
Reaction networks
Stiffness
Reactive flows
Nucleosynthesis
Combustion

ABSTRACT

In contrast to the prevailing view in the literature, it is shown that even extremely stiff sets of ordinary differential equations may be solved efficiently by explicit methods if limiting algebraic solutions are used to stabilize the numerical integration. The stabilizing algebra differs essentially for systems well-removed from equilibrium and those near equilibrium. Explicit asymptotic and quasi-steady-state methods that are appropriate when the system is only weakly equilibrated are examined first. These methods are then extended to the case of close approach to equilibrium through a new implementation of partial equilibrium approximations. Using stringent tests with astrophysical thermonuclear networks, evidence is provided that these methods can deal with the stiffest networks, even in the approach to equilibrium, with accuracy and integration timestepping comparable to that of implicit methods. Because explicit methods can execute a timestep faster and scale more favorably with network size than implicit algorithms, our results suggest that algebraically-stabilized explicit methods might enable integration of larger reaction networks coupled to fluid dynamics than has been feasible previously for a variety of disciplines.

1. Introduction

Problems from many disciplines require solving large coupled reaction networks. Representative examples include reaction networks in combustion chemistry [1], geochemical cycling of elements [2], and thermonuclear reaction networks in astrophysics [3,4]. The differential equations used to model these networks usually exhibit stiffness, which arises from multiple timescales in the problem that differ by many orders of magnitude [1,5–7]. Sufficiently complex physical systems often involve important processes operating on widely-separated timescales, so realistic problems tend to be at least moderately stiff. Some, such as astrophysical thermonuclear networks, are extremely stiff, with 10–20 orders of magnitude between the fastest and slowest timescales in the problem. Our concern here is with stiffness as a numerical issue, but we remark that stiffness can have important physical implications because complex processes often function as they do precisely because of the coupling of very slow and very fast scales within the same system.

Books on numerical and computational methods routinely state [1,6,7] that stiff systems cannot be integrated efficiently using explicit finite-difference methods because of stability issues: for an explicit algorithm, the maximum stable timestep is set by the fastest timescales, even if those timescales are peripheral to the main phenomena of interest. The standard

* Address: Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA.
E-mail address: guidry@utk.edu

0021-9991/$ - see front matter © 2012 Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.jcp.2012.04.026

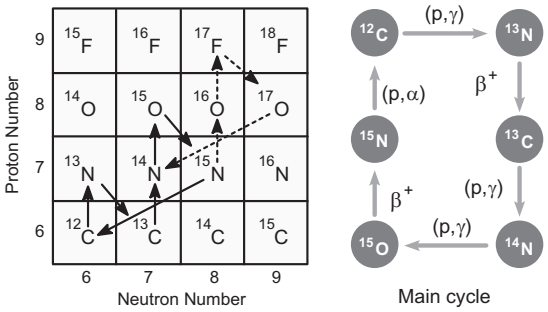

Fig. 1. The CNO (carbon–nitrogen–oxygen) cycle. On the left side the main branch of the cycle is illustrated with solid arrows and a side branch is illustrated with dashed arrows. On the right side, the main branch of the CNO cycle is illustrated in more detail.

resolution of the stiffness problem uses implicit integration, which is stable for stiff systems but entails substantial computational overhead because it requires the inversion of matrices at each integration step. Because of the matrix inversions, implicit algorithms tend to scale from quadratically to cubically with network size unless favorable matrix structure can be exploited. Thus, implicit methods can be expensive for large networks.

A simple but instructive example of stiffness is provided by the CNO cycle for conversion of hydrogen to helium, which powers main-sequence stars more massive than the Sun (Fig. 1). In the CNO cycle the fastest rates under characteristic stellar conditions are β-decays with half-lives $\sim$100 s, but to track the complete evolution of main-sequence hydrogen burning may require integration of the network for hydrogen burning over timescales as large as billions of years ($\sim 10^{16}$ s). If one tries to implement this integration using explicit forward differencing, the largest stable integration timestep will be set by the fastest rates and will be of order 10^2 s. Thus 10^{14} or more explicit integration steps could be required to integrate the CNO cycle to hydrogen depletion. Conversely, typical implicit integration schemes can take stable and accurate timesteps equal to 1–10% of the local time over most of the integration range, and would compute the above numerical integration in a few hundred implicit steps. By virtue of examples such as this, it is broadly accepted that explicit methods are not viable for stiff networks. To quote the authoritative reference *Numerical Recipes* [7], "For stiff problems we *must* use an implicit method if we want to avoid having tiny stepsizes."

Our main interest lies in simulations where the reaction network is one part of a broader problem. Let us take as representative astrophysical thermonuclear networks coupled to multidimensional hydrodynamics. The hydrodynamical evolution controls network conditions (temperature, density,...), and the network influences the hydrodynamics through energy production and modification of composition. Solution of large networks by the usual means is costly in this context and even ambitious simulations use only small networks, or replace the network entirely by parameterization. Then a more realistic network is used in a separate "post-processing" step, where fixed hydrodynamical profiles computed in the original simulation specify the variation of temperature and density with time. Such approximations are especially at issue for problems like Type Ia supernovae, which are 3D asymmetric explosions powered by a complex reaction network releasing energy greater than that of a large galaxy on a timescale of order 1 s.

Astrophysical reaction networks have been used to illustrate, but problems in various fields exhibit a similar complexity. For example, in astrochemical kinetics large chemical evolution networks must be modeled in dynamical environments such as contracting molecular clouds, or in combustion chemistry the burning networks are strongly coupled to dynamical simulations of the air and fuel mixture. Realistic networks in all such applications may be quite large. Modeling combustion of larger hydrocarbon molecules or soot formation can require hundreds to thousands of reacting species with up to 10,000 reactions [1], and realistic networks for supernova explosions imply hundreds to thousands of nuclear isotopes with tens of thousands of reaction couplings [3]. In all such cases current techniques do not permit the coupling of realistic reaction networks to the full dynamics and highly-schematic reaction networks are used in even the most realistic contemporary simulations.

2. Stiffness under equilibrium and non-equilibrium conditions

The pessimism engendered by the Introduction notwithstanding, it would be highly desirable to integrate large, complex networks by explicit means because explicit algorithms are simple and economical, and scale favorably with network size. In principle, this could be accomplished by identifying conditions under which some equations in the network have an approximate analytical solution and using that information to remove algebraically the stiffest components from the general numerical solution, thereby replacing the original network with an approximation that permits larger stable explicit-integration timesteps. To that end, the first task is to understand clearly the nature of the stiffness that we wish to remove from the equations.