
John, N Shadid
**The Split Personality of Operator Splitting Methods:
Diffusion/Reaction Systems***

Computational Science Department
PO Box 5800 MS 1111
Sandia National Laboratories
Albuquerque
NM 87185
jnshadi@sandia.gov
David, L Ropp

In this talk we present numerical experiments of time integration methods applied to coupled time dependent nonlinear systems of reaction-diffusion equations. Our main interest is in evaluating the relative accuracy and asymptotic order of accuracy of the methods on problems which exhibit an approximate balance between the competing component time scales. Nearly balanced systems can produce a significant coupling of the physical mechanisms and introduce a slow dynamical time scale of interest. These problems provide a challenging test for this evaluation and tend to reveal subtle differences between the various methods. The methods we consider include first- and second-order fully implicit, and operator-splitting techniques. The test problems include a prototype propagating nonlinear reaction-diffusion wave, a non-equilibrium radiation-diffusion system, and a Brusselator chemical dynamics system. In this evaluation we demonstrate a “split-personality” for the operator-splitting methods that we consider, in that, while they often have very good accuracy, they are not always robust.

*This work was partially supported by the ASCI program and the DOE Office of Science MICS program at Sandia National Laboratory under contract DE-AC04-94AL85000.