Temporal Accuracy of the Solution of Nonequilibrium Radiation Diffusion Equations

Vincent A. Mousseau, Rick M. Rauenzahn

and Dana A. Knoll

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S.

Department of Energy at Los Alamos National Laboratory under Contract No. W-7405-ENG-36

Contact information

- Since many of the references in the paper are not yet published feel free to contact me for a PDF file of the paper that you are interested in.

vmss@lanl.gov

Outline

- Introduction
- Mathematical Model
- Solution Methods
- Test Problems
- Results
- Conclusions

LA-UR-05-3829

Introduction

- Traditional nonequilibrium radiation diffusion solution methods are linearized, operator split, and first order accurate in time.
- Research is continuing in developing higher order in time nonlinear solutions to the equations.
- Until the nonlinear solutions are available, second order in time linearized and operator split algorithms may be an improvement over the current solution methods.

Mathematical Model

(1) $$\frac{\partial E}{\partial t} - \nabla \cdot \left(D_r \nabla E \right) = \sigma_p c \rho \left(\frac{4\sigma_b T^4}{c} - E \right)$$

(2) $$\rho \frac{\partial E_m}{\partial t} - \nabla \cdot \left(D_m \nabla T \right) = -\sigma_p c \rho \left(\frac{4\sigma_b T^4}{c} - E \right)$$

(3) $$D_r = \frac{c}{3\rho\sigma_R + \frac{|\nabla E|}{E}}$$

(4) $$E_m = \frac{kT}{m_p} \left[\frac{3}{2}(1+\alpha) + \alpha\chi \right]$$

Solution Methods

- **NK2** - 2nd order, Newton-Krylov, no linearizations, no operator splitting
- **SR** - 2nd order, Strang-Rosenbrock, linearized and operator split
- **OS1** - 1st order, Olson Splitting, linearized and operator split
- **OS2** - 2nd order, Olson Splitting, linearized and operator split

2nd Order Olson Splitting

(1) $$\rho\frac{E_m^* - E_m^n}{\Delta t/2} - \frac{1}{2}\nabla\cdot\left(D_m^*\nabla T^*\right) - \frac{1}{2}\nabla\cdot\left(D_m^n\nabla T^n\right) = 0$$

(2) $$\rho\frac{E_m^{\sim} - E_m^*}{\Delta t} + \frac{1}{2}\sigma_p^{\sim}c\rho\left(\frac{4\sigma_b\left(T^{**}\right)^4_{lin}}{c} - E^{n+1}\right) + \frac{1}{2}\sigma_p^*c\rho\left(\frac{4\sigma_b\left(T^*\right)^4}{c} - E^n\right) = 0$$

(3) $$\frac{E^{n+1} - E^n}{\Delta t} - \frac{1}{2}\left\{\nabla\cdot\left(D_r^{n+1,**}\nabla E^{n+1}\right) + \sigma_p^{**}c\rho\left(\frac{4\sigma_b\left(T^{**}\right)^4_{lin}}{c} - E^{n+1}\right)\right\} - \frac{1}{2}\left\{\nabla\cdot\left(D_r^n\nabla E^n\right) + \sigma_p^n c\rho\left(\frac{4\sigma_b\left(T^n\right)^4}{c} - E^n\right)\right\} = 0$$

(4) $$\rho\frac{E_m^{n+1} - E_m^{**}}{\Delta t/2} - \frac{1}{2}\nabla\cdot\left(D_m^{n+1}\nabla T^{n+1}\right) - \frac{1}{2}\nabla\cdot\left(D_m^{**}\nabla T^{**}\right) = 0$$

Eight Test Problems

Nondimensional Const. c_v	Dimensional Const. c_v	Nondimesnional Simplified Saha	Dimensional Saha
2-D Blast	2-D Pipe	1-D Marshak	1-D Marshak
2-D Marshak		1-D Blast	2-D Blast
			2-D Marshak

Time step Control

$$\Delta t^{n+1} = \min\left\{1.05\Delta t^{n}, \eta_t \times \min_{i,j}\left[\tau_r^{n+1}(i,j), \tau_m^{n+1}(i,j)\right]\right\}$$

$$\tau_r^{n+1}(i,j) = \frac{1}{\left|\frac{1}{E_{i,j}^{n+1}}\frac{E_{i,j}^{n+1} - E_{i,j}^{n}}{\Delta t^{n}}\right|} \qquad \tau_m^{n+1}(i,j) = \frac{1}{\left|\frac{1}{T_{i,j}^{n+1}}\frac{T_{i,j}^{n+1} - T_{i,j}^{n}}{\Delta t^{n}}\right|}$$

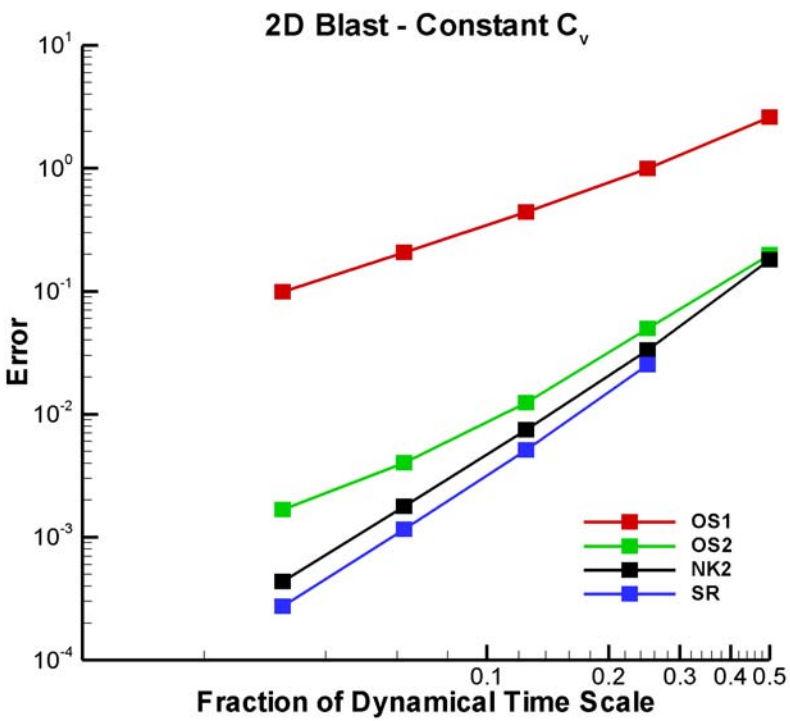
Accuracy

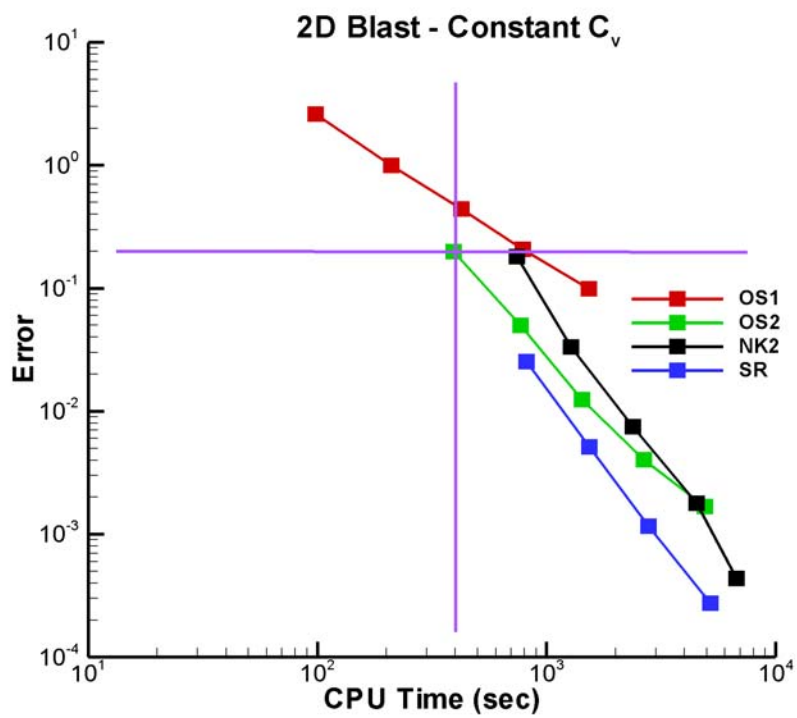
- Since it is difficult to obtain an analytical solution to the test problems, accuracy will be computed as an L2-norm of the difference between a “base” solution and the calculation. The “base” solution is computed at a time step 10 time smaller than the smallest data value.

$$Error = \sqrt{\sum_{i=1}^{nx}\sum_{j=1}^{ny}\left[T_r(i,j) - T_r^{base}(i,j)\right]^2}$$

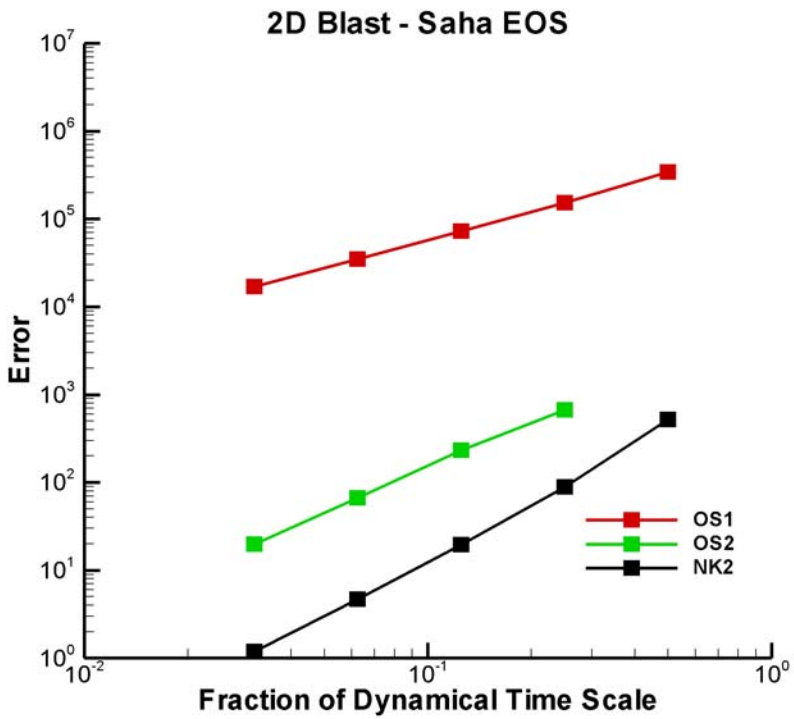
$$T_r = \left[\frac{cE}{4\sigma_b}\right]^{\frac{1}{4}}$$

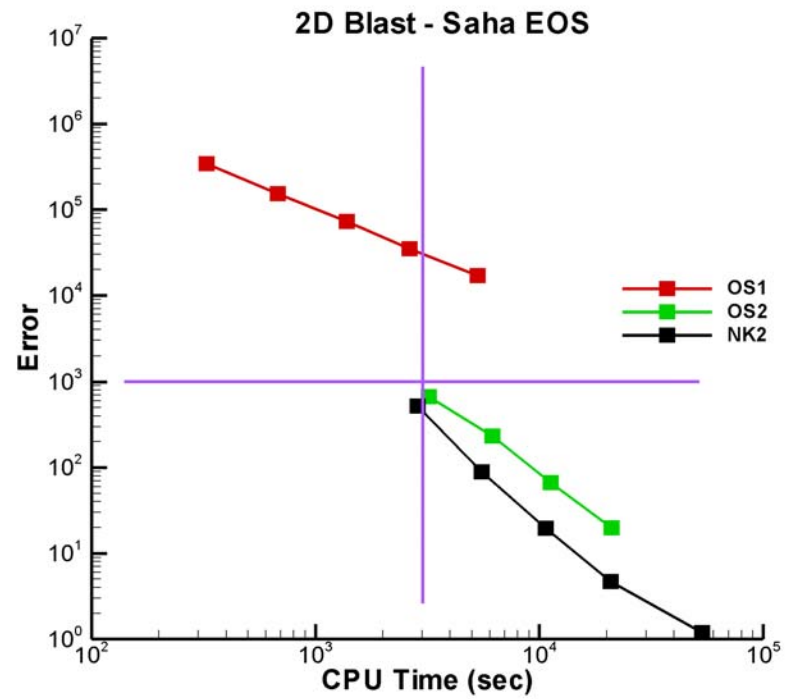
Results for the Nondimesnional, Const. c_v 2-D Blast Problem





Results for the dimensional, Saha ionization, 2-D Blast Problem





Conclusions

- 2nd order, operator split and linearized solutions can be constructed for nonequlibrium radiation diffusion equations.
- The 2nd order methods are more efficacious than the traditional 1st order methods for small error.
- The 2nd order split and linearized methods have problems with robustness so they should be used with caution.
- The 2nd order nonlinear methods are accurate, robust, and efficacious, but they may be difficult to implement.