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A Nonlinear Projection-Based Iteration Scheme with Cycles over Multiple Time Steps for Solving Thermal Radiative Transfer Problems

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International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering
August 16, 2023

LA-UR-23-28597

Radiative Transfer

- We are interested in nonlinear radiative transfer problems
- Radiative transfer effects account for majority of energy redistribution in materials at extremely high temperatures
  - Strength increases as a quartic function of temperature ($\propto T^4$)
  - Energy redistributed by emission, propagation, absorption of photon radiation
  - Important in fields like astrophysics, plasma physics, high-energy density physics
- The involved systems of equations are typically:
  - Multiphysical systems of partial differential equations
  - Characterized by strong nonlinear behavior and coupling between equations
  - Multi-scale behavior in space, time, energy
- The Boltzmann transport equation (BTE) is used to model radiative transfer component of problems

Iteration Methods

- We consider problems which are discretized implicitly in time (Backward-Euler)
- An iterative method must be invoked to obtain the solution at each time step
- We present a novel iterative scheme for these problems based on the multilevel quasidiffusion (MLQD) method
  - Nonlinear projection approach, nonlinear method of moments
  - The BTE is projected onto several low-order subspaces to derive an effective low-order transport (ELOT) problem for moments
  - The ELOT problem is coupled to multiphysics equations at their scale
  - A nested set of iteration cycles is used to obtain the solution at each discrete time in chronological order
- The basic idea is to eschew the notion of solving the problem at each time step separately
  - Time steps are aggregated into time ‘blocks’
  - Nested structure of MLQD iterations allows for reorganization of iteration levels
  - These collections of time steps can be solved together with overarching iterative cycles

Thermal Radiative Transfer

- Boltzmann transport equation (BTE):

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \boldsymbol{\Omega} \cdot \nabla I_g + \varkappa_g(T) I_g = \varkappa_g(T) B_g(T)$$

$$I_g|_{\boldsymbol{r} \in \partial \Gamma} = I_g^{\text{in}} \text{ for } \boldsymbol{\Omega} \cdot \boldsymbol{n}_\Gamma < 0, \quad I_g|_{t=0} = I_g^0,$$

- Material energy balance (MEB) equation:

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G} \left(\int_{4\pi} I_g d\Omega - 4\pi B_g(T) \right) \varkappa_g(T), \quad T|_{t=0} = T^0$$

- Temperature: $T(\boldsymbol{r}, t)$
- Specific radiation intensity: $I_g(\boldsymbol{r}, \boldsymbol{\Omega}, t)$

Multilevel Quasidiffusion Method for TRT

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\nabla I_g + \varkappa_g(T) I_g = \varkappa_g(T) B_g(T)$$

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\left(\int_{4\pi} I_g d\Omega - 4\pi B_g(T)\right)\varkappa_g(T)$$

Multilevel Quasidiffusion Method for TRT

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\nabla I_g + \varkappa_g(T)I_g = \varkappa_g(T)B_g(T)$$

$$\mathcal{P}^0_\Omega u = \int_{4\pi} u d\Omega,\ \mathcal{P}^1_\Omega u = \int_{4\pi} \Omega u d\Omega$$

$$\mathcal{P}^0_\Omega\left[\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\nabla I_g + \varkappa_g(T)I_g\right] = \mathcal{P}^0_\Omega\left[\varkappa_g(T)B_g(T)\right]$$

$$\mathcal{P}^1_\Omega\left[\frac{1}{c}\frac{\partial I_g}{\partial t} + \mathbf{\Omega}\cdot\nabla I_g + \varkappa_g(T)I_g\right] = \mathcal{P}^1_\Omega\left[\varkappa_g(T)B_g(T)\right]$$

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\left(\int_{4\pi} I_g d\Omega - 4\pi B_g(T)\right)\varkappa_g(T)$$

Multilevel Quasidiffusion Method for TRT

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \boldsymbol{\Omega}\cdot\nabla I_g + \varkappa_g(T) I_g = \varkappa_g(T) B_g(T)$$

$$E_g = \frac{1}{c}\int_{4\pi} I_g d\Omega, \ \boldsymbol{F}_g = \int_{4\pi} \Omega I_g d\Omega$$

$$\frac{\partial E_g}{\partial t} + \nabla\cdot\boldsymbol{F}_g + c\varkappa_g(T)E_g = 4\pi\varkappa_g(T)B_g(T)$$

$$\mathfrak{f}_g = \frac{\int_{4\pi}(\boldsymbol{\Omega}\otimes\boldsymbol{\Omega}) I_g d\Omega}{\int_{4\pi} I_g d\Omega}$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\nabla\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g = 0$$

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\Big(cE_g - 4\pi B_g(T)\Big)\varkappa_g(T)$$

Multilevel Quasidiffusion Method for TRT

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I_g + \varkappa_g(T)I_g = \varkappa_g(T)B_g(T)$$

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$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g = 0$$

$$\mathfrak{f}_g = \frac{\int_{4\pi}(\boldsymbol{\Omega}\otimes\boldsymbol{\Omega})I_g d\Omega}{\int_{4\pi} I_g d\Omega}$$

$$\mathcal{P}_G\left[\frac{\partial E_g}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{F}_g + c\varkappa_g(T)E_g\right] = \mathcal{P}_G\left[4\pi\varkappa_g(T)B_g(T)\right]$$

$$\mathcal{P}_G u_g = \sum_{g=1}^{G} u_g$$

$$\mathcal{P}_G\left[\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g\right] = 0$$

$$\frac{\partial \varepsilon(T)}{\partial t} = \sum_{g=1}^{G}\Big(cE_g - 4\pi B_g(T)\Big)\varkappa_g(T)$$

Multilevel Quasidiffusion Method for TRT

$$\frac{1}{c}\frac{\partial I_g}{\partial t} + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I_g + \varkappa_g(T) I_g = \varkappa_g(T) B_g(T)$$

$$\frac{\partial E_g}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{F}_g + c\varkappa_g(T)E_g = 4\pi\varkappa_g(T)B_g(T)$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}_g}{\partial t} + c\boldsymbol{\nabla}\cdot(\mathfrak{f}_g E_g) + \varkappa_g(T)\boldsymbol{F}_g = 0$$

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{F} + c\langle\varkappa\rangle_E E = c\langle\varkappa\rangle_B a_R T^4$$

$$\frac{1}{c}\frac{\partial \boldsymbol{F}}{\partial t} + c\boldsymbol{\nabla}\cdot(\langle\mathfrak{f}\rangle_E E) + \langle\varkappa\rangle_{|F|}\boldsymbol{F} + \bar{\boldsymbol{\eta}} E = 0$$

$$\frac{\partial \varepsilon(T)}{\partial t} = c\langle\varkappa\rangle_E E - c\langle\varkappa\rangle_B a_R T^4$$

$$E_g = \frac{1}{c}\int_{4\pi} I_g d\Omega, \ \boldsymbol{F}_g = \int_{4\pi} \Omega I_g d\Omega$$

$$\mathfrak{f}_g = \frac{\int_{4\pi}(\boldsymbol{\Omega}\otimes\boldsymbol{\Omega})I_g d\Omega}{\int_{4\pi} I_g d\Omega}$$

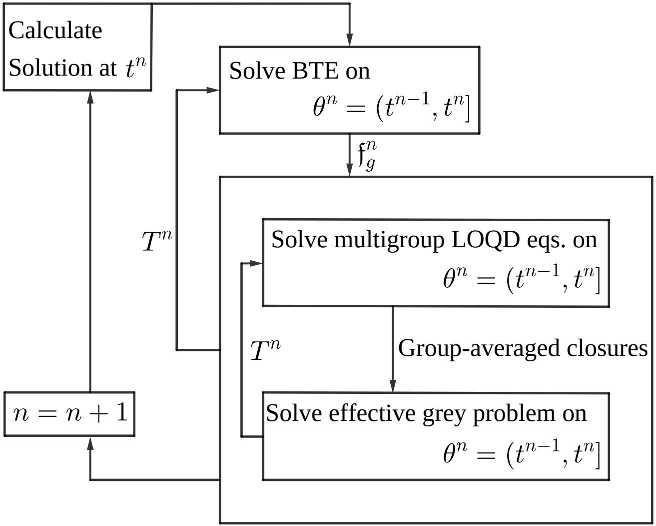
$$E = \sum_{g=1}^{G} E_g, \ \boldsymbol{F} = \sum_{g=1}^{G}\boldsymbol{F}_g$$

Effective group-averaged closures:

$$\langle\varkappa\rangle_E, \ \langle\varkappa\rangle_B, \ \langle\mathfrak{f}\rangle_E, \ \langle\varkappa\rangle_{|F|}, \ \bar{\boldsymbol{\eta}}$$

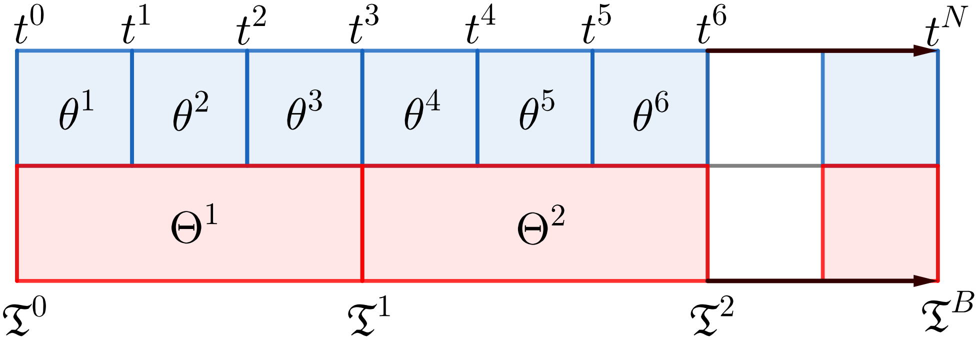
Standard Iterative Scheme

- Discretize all equations with implicit Backward-Euler time integrator
- Divide temporal domain into N intervals $\theta^n = (t^{n-1}, t^n]$
- Times: $\{t^n \mid 0 = t^0 < \cdots < t^N = t^{\text{end}}\}$



Amalgamation of Time Steps

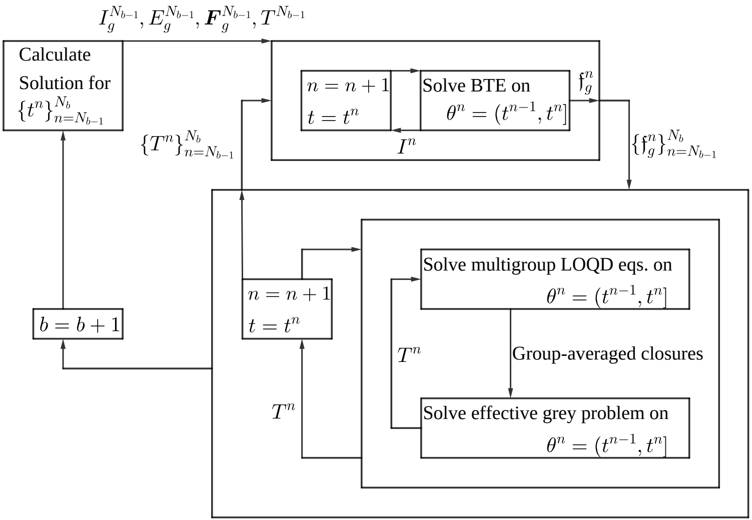
- Define B time blocks of time interval collections: $\Theta^b = \cup_{n=N_{b-1}+1}^{N_b} \theta^n$
- $0 = N_0 < \cdots < N_B = N$
- Idea: iterate on solution over blocks Θ^b with subgrid of the original time intervals
- Block lengths are $\Delta\mathfrak{T}_b$



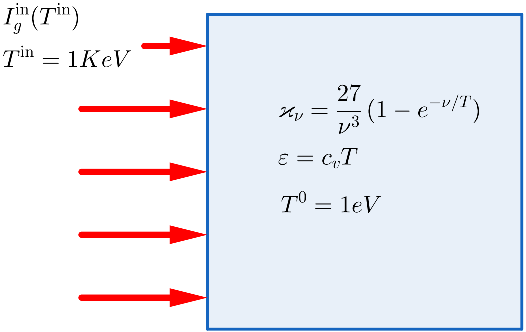
Basic Idea

- Consider the block Θ^b, with $\mathfrak{T}^{b-1} = t^{N_{b-1}}$, $\mathfrak{T}^b = t^{N_b}$
- Given an initial condition $I_g^{N_{b-1}}$ and material temperatures $\{T^n\}_{n=N_{b-1}}^{N_b}$, the BTE can be solved at all times $\{t^n\}_{n=N_{b-1}+1}^{N_b}$
- Given initial conditions $E_g^{N_{b-1}}$, $\boldsymbol{F}_g^{N_{b-1}}$, $T^{N_{b-1}}$ and Eddington tensor data $\{\mathfrak{f}_g^n\}_{n=N_{b-1}}^{N_b}$, the system of moment equations and the MEB can be solved at all times $\{t^n\}_{n=N_{b-1}+1}^{N_b}$
- The BTE and low-order system can be iterated with one another between entire blocks, communicating closures and temperatures on multiple time steps between cycles

New Iterative Scheme



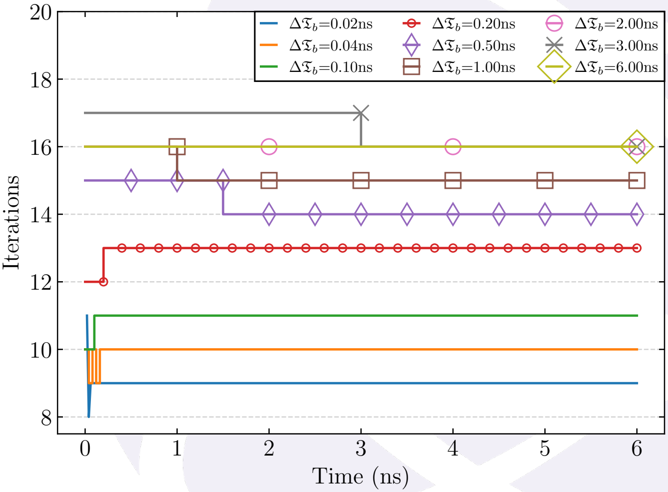
Fleck-Cummings Test Problem Description



- Specification:
  - 2D Cartesian domain 6×6 cm
  - Temporal interval $t \in [0, 6 \text{ ns}]$
- Discretization:
  - 20×20 spatial grid (0.3×0.3 cm cells)
  - 300 time steps of length 0.02 ns
  - 17 frequency groups
  - 144 discrete directions
  - All equations implicitly discretized in time (backward-Euler)
  - BTE discretized in space with simple corner balance
  - Low-order equations discretized with 2$^{\text{nd}}$ order finite volumes scheme

Number of Iterations per Time Block

- Iterations required over each time block to reach relative convergence criteria $\epsilon = 10^{-14}$
- Several block lengths tested, from each block being one time step to the entire temporal interval



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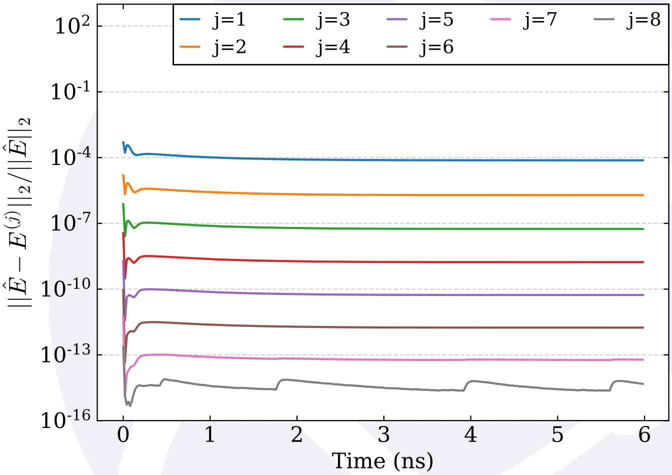
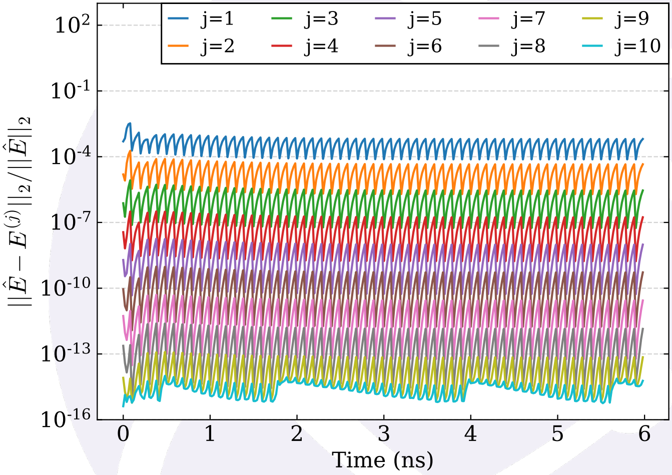
Errors in the Iterative Solution & Convergence

- Relative error w.r.t. the numerical solution on the given grid in phase-space and time $(\hat{E},\ \hat{T})$
- Time block length: $\Delta\mathfrak{T}_b$
- Number of time steps in a time block: $\mathfrak{N}_b$
- shown: $\Delta\mathfrak{T}_b = 0.02$ ns (standard)



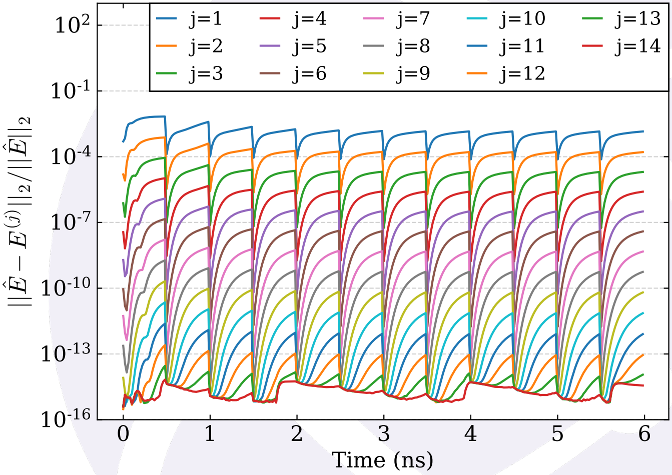
Errors in the Iterative Solution & Convergence

- Relative error w.r.t. the numerical solution on the given grid in phase-space and time $(\hat{E},\ \hat{T})$
- Time block length: $\Delta\mathfrak{T}_b$
- Number of time steps in a time block: $\mathfrak{N}_b$
- shown: $\Delta\mathfrak{T}_b = 0.10$ ns ($\mathfrak{N}_b = 5$)



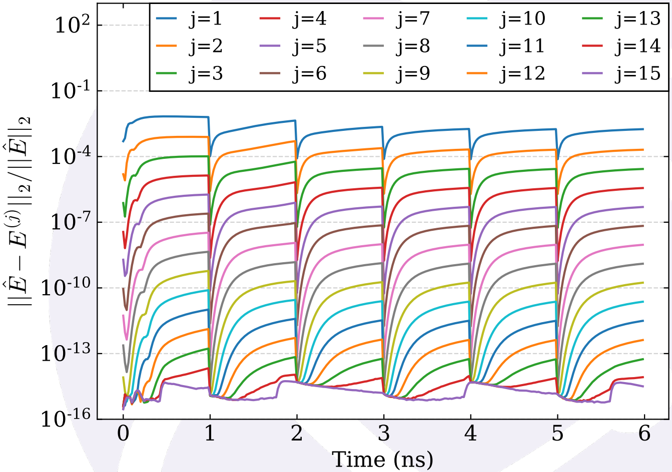
Errors in the Iterative Solution & Convergence

- Relative error w.r.t. the numerical solution on the given grid in phase-space and time $(\hat{E},\ \hat{T})$
- Time block length: $\Delta\mathfrak{T}_b$
- Number of time steps in a time block: $\mathfrak{N}_b$
- shown: $\Delta\mathfrak{T}_b = 0.50$ ns ($\mathfrak{N}_b = 25$)



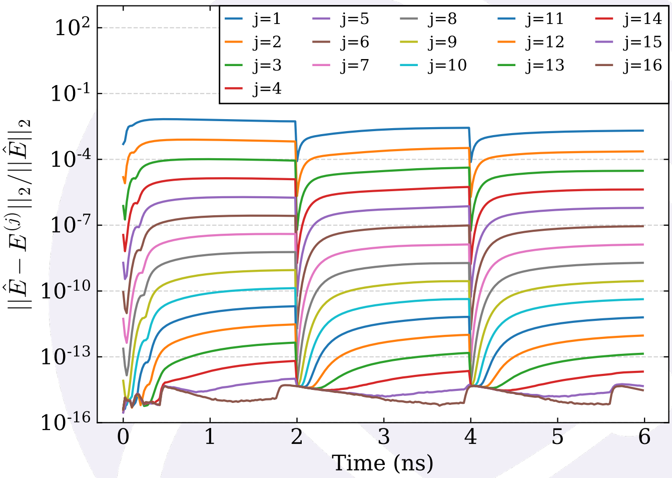
Errors in the Iterative Solution & Convergence

- Relative error w.r.t. the numerical solution on the given grid in phase-space and time $(\hat{E},\ \hat{T})$
- Time block length: $\Delta\mathfrak{T}_b$
- Number of time steps in a time block: $\mathfrak{N}_b$
- shown: $\Delta\mathfrak{T}_b = 1.00$ ns ($\mathfrak{N}_b = 50$)



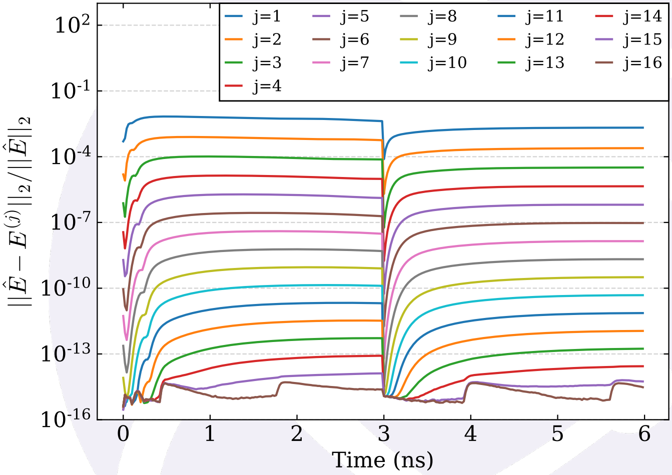
Errors in the Iterative Solution & Convergence

- Relative error w.r.t. the numerical solution on the given grid in phase-space and time $(\hat{E},\ \hat{T})$
- Time block length: $\Delta\mathfrak{T}_b$
- Number of time steps in a time block: $\mathfrak{N}_b$
- shown: $\Delta\mathfrak{T}_b = 2.00$ ns ($\mathfrak{N}_b = 100$)



Errors in the Iterative Solution & Convergence

- Relative error w.r.t. the numerical solution on the given grid in phase-space and time $(\hat{E},\ \hat{T})$
- Time block length: $\Delta\mathfrak{T}_b$
- Number of time steps in a time block: $\mathfrak{N}_b$
- shown: $\Delta\mathfrak{T}_b = 3.00$ ns ($\mathfrak{N}_b = 150$)



Estimated Spectral Radii of Iterations

- Let $\hat{E}$, $\hat{T}$ be the the numerical solution on the given grid in phase-space and time
- $E^{(j)}$, $T^{(j)}$ are the j^{th} iterate's solution
- Errors are calculated in the norm $\|\cdot\|_2^t$, which is the 2-norm over space and time for the temporal interval of a given time block.
- Spectral radii values are averaged over all time blocks and iterations
- $\rho_E^{(j)} = \|\hat{E} - E^{(j)}\|_2^t / \|\hat{E} - E^{(j+1)}\|_2^t$
- $\rho_T^{(j)} = \|\hat{T} - T^{(j)}\|_2^t / \|\hat{T} - T^{(j+1)}\|_2^t$

$\Delta\mathfrak{T}_b$ (ns)	$\mathfrak{N}_b$	ρ_E	ρ_T
0.02	1	0.042	0.035
0.04	2	0.068	0.049
0.10	5	0.067	0.058
0.20	10	0.128	0.100
0.50	25	0.158	0.136
1.00	50	0.171	0.154
2.00	100	0.194	0.178
3.00	150	0.177	0.167
6.00	300	0.159	0.156

Discussion

- A new iterative scheme is presented for TRT problems with cycles over collections of time steps (time blocks)
  - Iterations converge rapidly
  - The scheme is stable even for cycles over the entire temporal range of a problem
  - Can be interpreted as a diagonally-implicit Runge-Kutta method (see paper)
- The scheme introduces possibility for parallel-in-time calculations
  - Could solve high-order and low-order problems in parallel to one another
  - Frequency of communication between processors and sizing of time blocks remain open questions in this regard

Acknowledgments

Los Alamos Report LA-UR-23-28597. This research project was funded by the Department of Defense, Defense Threat Reduction Agency, grant number HDTRA1-18-1-0042. This work was supported by the U.S. Department of Energy through the Los Alamos National Laboratory. Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of U.S. Department of Energy (Contract No. 89233218CNA000001). The content of the information does not necessarily reflect the position or the policy of the federal government, and no official endorsement should be inferred.

Questions?