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Title: High-Order Thermal Radiative Transfer

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High-Order Thermal Radiative Transfer

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Los Alamos National Laboratory

14 September 2017



Slide 1

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Research objectives

- Assess the sensitivity of the linearized thermal radiation transport (TRT) equations to finite element order on unstructured meshes.
- Investigate the sensitivity of the nonlinear TRT equations due to evaluating the opacities and heat capacity at nodal temperatures in 2-D using high-order finite elements.

Background

- Linear transport spatially converges with $O(h^{p+1})$ on unstructured meshes.
 - More degrees of freedom in fewer mesh zones
 - Increased accuracy per CPU time
- Limited amount of research available on high-order methods for TRT (Maginot, 2016).
 - Linearized equations
 - 1-D

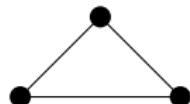
High-order finite elements

Approximate temperature as a polynomial expansion

$$T(\mathbf{x}) \approx \sum_j T_j b_j(\mathbf{x})$$

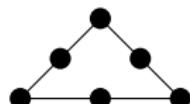
- Low-order (1st-order) basis functions assume flat (linear) shape:

$$b_j(\mathbf{x}) = ax + by + c$$



- High-order (2nd-order) basis function allow for solution curvature:

$$b_j(\mathbf{x}) = ax^2 + by^2 + cxy + dx + ey + f$$



Thermal radiation transport

The nonlinear thermal radiative transport (TRT) equations:

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t} + \boldsymbol{\Omega} \cdot \nabla I^{n+1} + \sigma_t I^{n+1} = \frac{\sigma_s}{4\pi} E^{n+1} + \sigma_a B^{n+1} + S_0^{n+1},$$

$$\rho C_v \frac{T^{n+1} - T^n}{\Delta t} = \int \int c \sigma_a (I^{n+1} - B^{n+1}) d\nu d\Omega',$$

$$B^{n+1} = \frac{2h\nu^3}{c^2} \left(e^{h\nu/kT_e^{n+1}} - 1 \right)^{-1}$$

Thermal radiation transport

The linearized thermal radiative transport (TRT) equations:

$$B^{n+1} \approx B^n + \left. \frac{\partial B}{\partial T} \right|_{T^n} \delta T$$

$$\rho C_v \frac{\delta T}{\Delta t} = \int \int c \sigma_a (I^{n+1} - B^{n+1}) d\nu d\Omega',$$

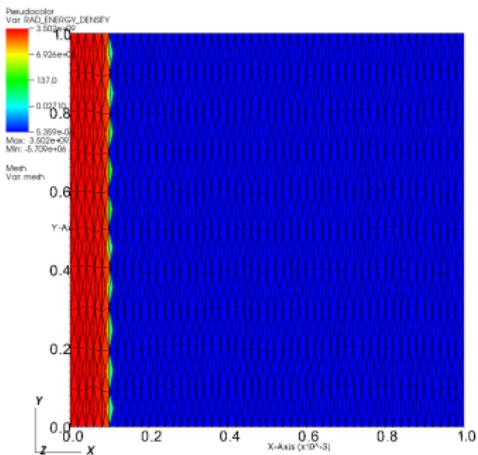
$$B^{n+1} \approx B^n + \left. \frac{\partial B}{\partial T} \right|_{T^n} \delta T$$

$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t} + \Omega \cdot \nabla I^{n+1} + \sigma_t I^{n+1} = \frac{\sigma_s}{4\pi} E^{n+1} + \sigma_a B^{n+1} + S_0^{n+1},$$

Linearized equations susceptible to maximum principle violations.

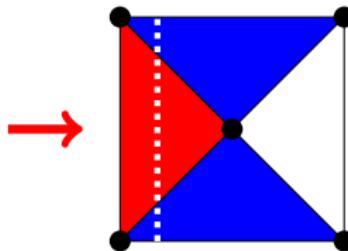
Test problem: Marshak wave

- 1-D, time dependent, material coupled, gray
- $\sigma_t = 10^6 \left(\frac{0.001}{T}\right)^3$
- $C_v = 1.3784 \times 10^{14}$ erg/keV/g
- Gray boundary source 0.150 keV
- As thermal wave propagates, incident radiation penetrates further into the material.

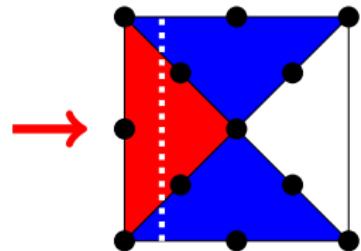


High-order finite elements - conceptual mass averaging

- Higher-order elements have better resolution within each mesh zone.
- Cell average temperature is better mass weighted.



(a) 1st-order FEM.



(b) 2nd-order FEM.

Linearized thermal radiation transport test definitions

1. Linearized system, structured mesh, 1st-order elements
2. Linearized system, structured mesh 2nd-order elements
3. Linearized system, unstructured mesh, 1st-order elements
4. Linearized system, unstructured mesh 2nd-order elements
5. Nonlinear system, structured mesh, 1st-order elements
6. Nonlinear system, structured mesh 2nd-order elements
7. Nonlinear system, unstructured mesh, 1st-order elements
8. Nonlinear system, unstructured mesh 2nd-order elements

Remember: odds are odd, evens are even.

Linearized TRT case matrix - Δt and Δx are part of sufficient conditions to adhere to maximum principle

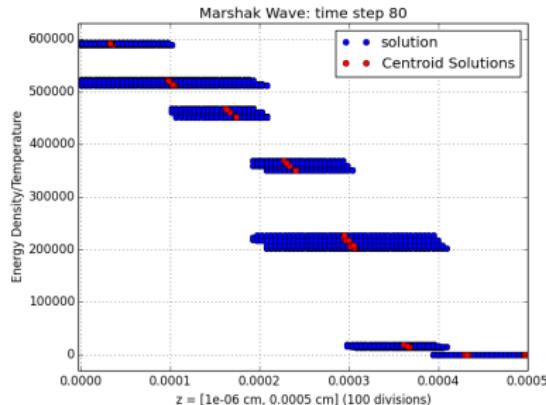
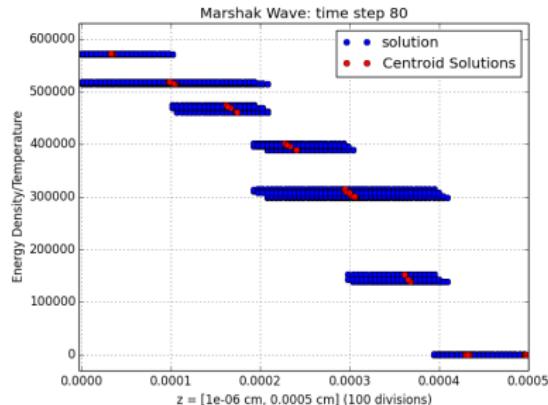
Case matrix for refining the time step and mesh

- Populated with test numbers that adhere to the maximum principle, i.e., $T(0 < x' < x, y, t) > T(x, y, t)$

Δt (sec.)	no. of mesh zones			
	100	400	1600	6400
	8×10^{-10}			
	8×10^{-11}	1, 3		
	8×10^{-12}	1, 2, 3, 4	1, 2, 3, 4	2
	8×10^{-13}	1, 2, 3, 4	1, 2, 3, 4	1, 2, 3, 4
	8×10^{-14}	1, 2, 3, 4	1, 2, 3, 4	1, 2, 3, 4

Linearized TRT coarse unstructured mesh - HO FEM does not propagate energy as far as LO

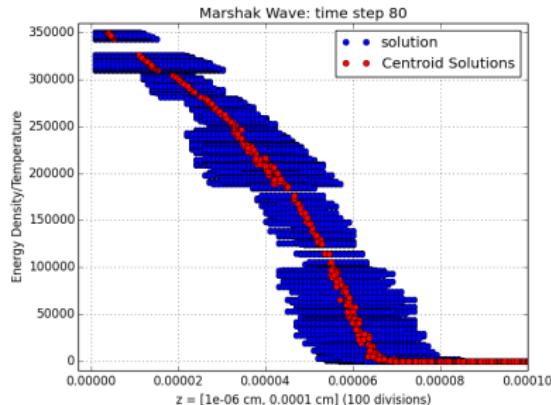
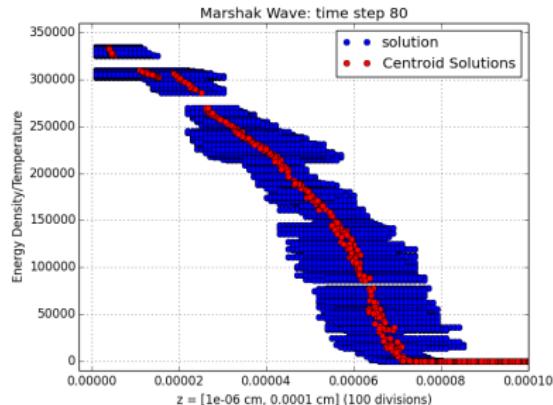
Electron temperatures from linearized system on meshes with 100 zones for $\Delta t = 8 \times 10^{-12}$ seconds at time step 80.



(a) Test 3 (1st-order, unstructured). (b) Test 4 (2nd-order, unstructured).

Linearized TRT refined unstructured mesh - mesh resolution affects continuity of temperature profile

Electron temperatures from linearized system on structured meshes with 6400 zones for $\Delta t = 8 \times 10^{-13}$ seconds at time step 80.



(a) Test 3 (1st-order, unstructured). (b) Test 4 (2nd-order, unstructured).

Nonlinear TRT test definitions

1. Linearized system, structured mesh, 1st-order elements
2. Linearized system, structured mesh 2nd-order elements
3. Linearized system, unstructured mesh, 1st-order elements
4. Linearized system, unstructured mesh 2nd-order elements
5. Nonlinear system, structured mesh, 1st-order elements
6. Nonlinear system, structured mesh 2nd-order elements
7. Nonlinear system, unstructured mesh, 1st-order elements
8. Nonlinear system, unstructured mesh 2nd-order elements

Remember: odds are odd, evens are even.

Nonlinear TRT case matrix - nonlinear solver convergence restricted by time step size

Case matrix for refining the time step and mesh

- Populated with test numbers that provide “reasonable” solutions

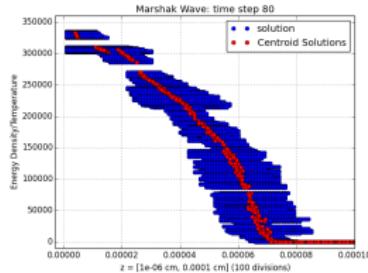
Δt (sec.)	no. of mesh zones			
	100	400	1600	6400
8×10^{-10}				
8×10^{-11}	5, 7			
8×10^{-12}	5, 6, 7, 8	5, 6, 7, 8	5, 7	5, 7
8×10^{-13}	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8
8×10^{-14}	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8

Nonlinear TRT refined unstructured mesh - LO FEM is affected by linearization

Electron temperatures from linearized system on structured meshes with 6400 zones for $\Delta t = 8 \times 10^{-13}$ seconds at time step 80.

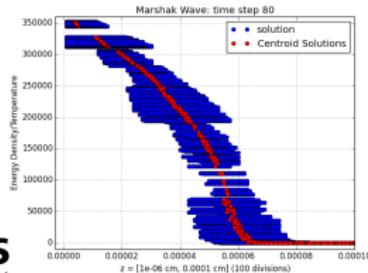
Test 3

(linearized,
1st-order,
unstructured).



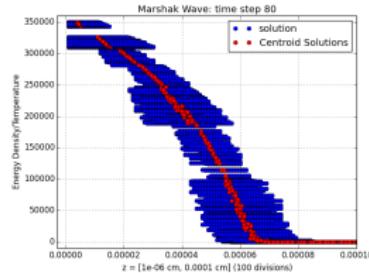
Test 7

(nonlinear,
1st-order,
unstructured).



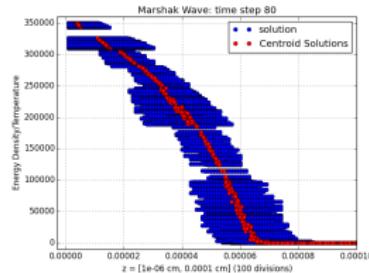
Test 4

(linearized,
2nd-order,
unstructured).



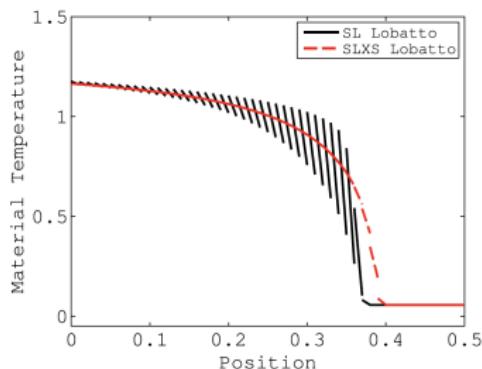
Test 8

(nonlinear,
2nd-order,
unstructured).



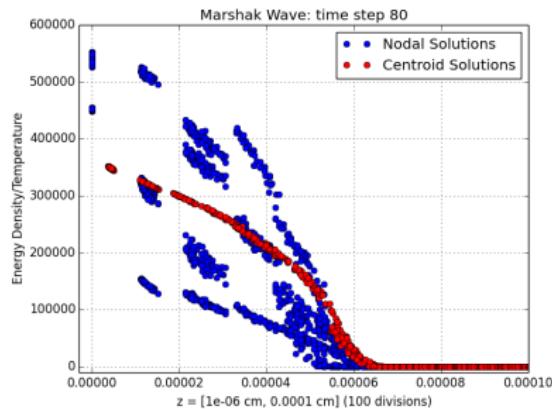
Serrano vs. Hidalgo: opacities and heat capacities evaluated at nodal temperatures

- Serrano solves using cell-wise average opacities and heat capacities.
- Maginot (2016) and Luke Cornejo showed the nodal solutions are discontinuous.
- Evaluating material properties at nodal temperatures greatly smooths out nodal solutions.

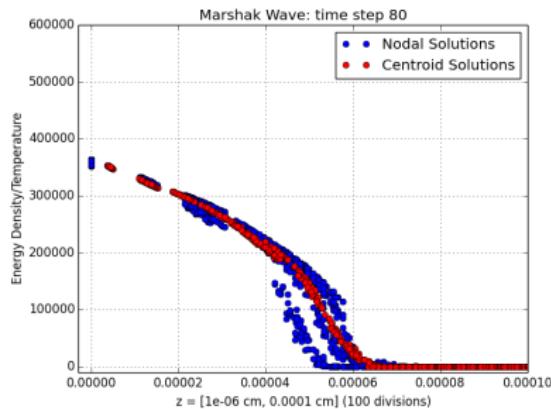


Maginot et al. (2016).

Serrano vs. Hidalgo - nodal solutions are substantially closer to cell average solutions

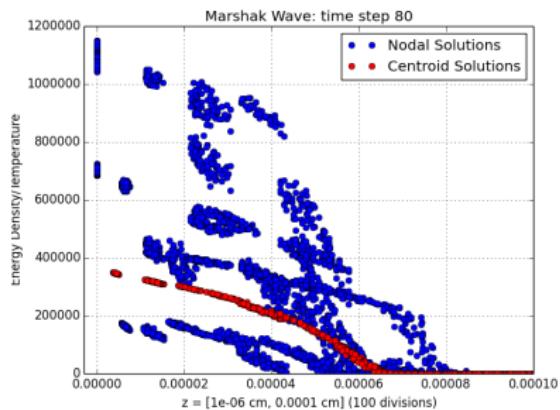


(a) Test 7 (nonlinear, 1st-order, unstructured) with Serrano.

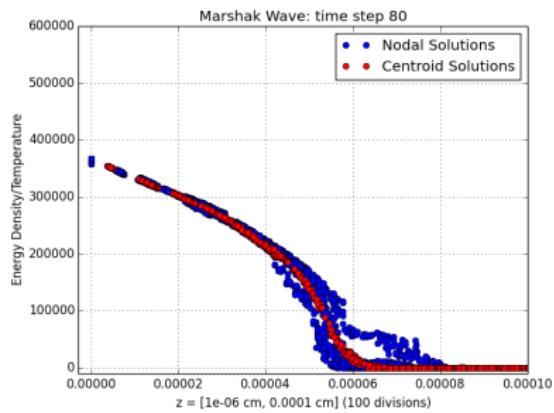


(b) Test 7 (nonlinear, 1st-order, unstructured) with Hidalgo.

Serrano vs. Hidalgo - nodal solutions are substantially closer to cell average solutions



(a) Test 8 (nonlinear, 2nd-order, unstructured) with Serrano.



(b) Test 8 (nonlinear, 2nd-order, unstructured) with Hidalgo.

Conclusions

- Linearization affects the solution
 - Low-order elements are much more sensitive to the linearization
 - Higher-order elements are far less sensitive to the linearization
- Nonlinear low-order elements tend to agree with nonlinear high-order elements
 - Nonlinear low-order may propagate less energy
- Evaluating material properties at the nodal temperatures reduces blading

Future Work

- Finite element analysis for maximum principle
 - Determine the time step size to tolerate the maximum nodal energy deposition before violating the maximum principle
- Refined mesh at boundary may reduce “gaps”
- Time step ramp-up may allow solutions to nonlinear system
- Compare to analytic local thermodynamic equilibrium diffusion solution

QUESTIONS?

Thank you!

Matt Cleveland

Ryan Wollaeger

Jim Warsa



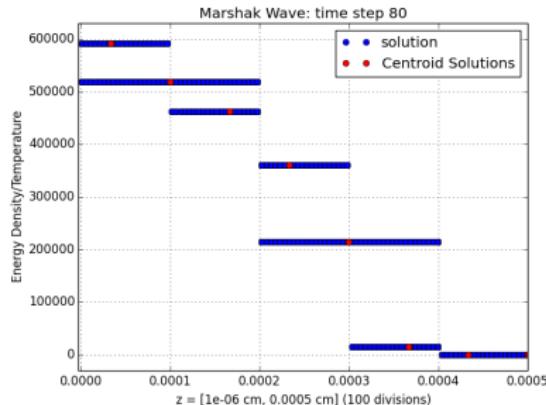
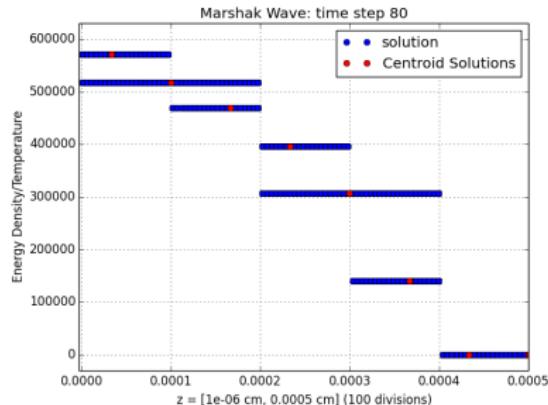
This research was performed by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract XX-XXXX-XXXXXXXXXX.



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Linearized TRT coarse structured mesh - HO FEM does not propagate energy as far as LO

Electron temperatures from linearized system on meshes with 100 zones for $\Delta t = 8 \times 10^{-12}$ seconds at time step 80.

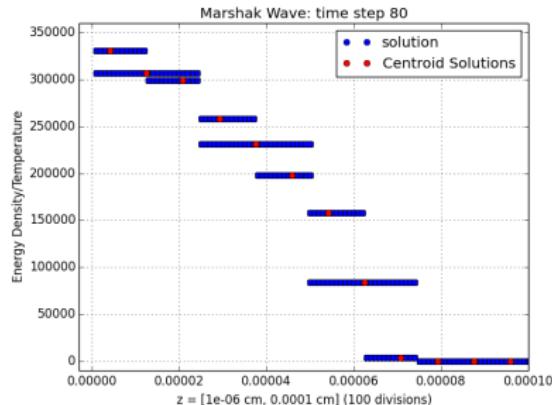


(a) Test 1 (1st-order, structured).

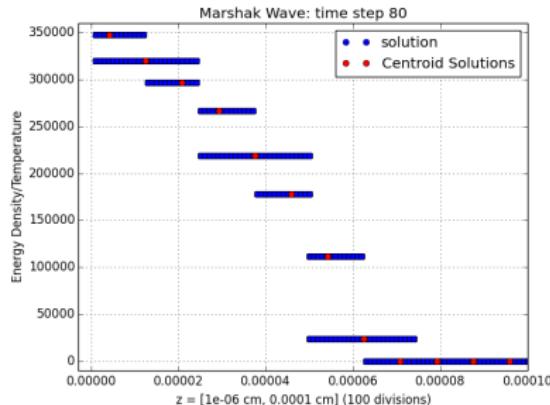
(b) Test 2 (2nd-order, structured).

Linearized TRT refined structured mesh - HO FEM has higher temperature near boundary

Electron temperatures from linearized system on meshes with 6400 zones for $\Delta t = 8 \times 10^{-13}$ seconds at time step 80.



(a) Test 1 (1st-order, structured).

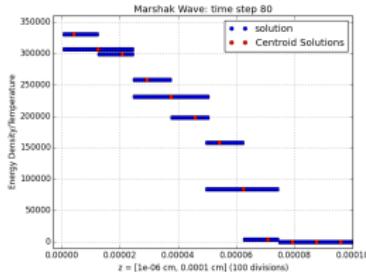


(b) Test 2 (2nd-order, structured).

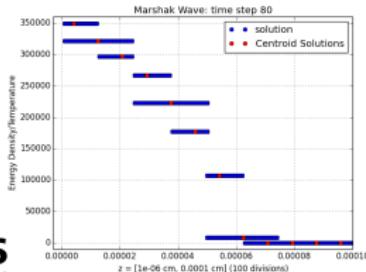
Nonlinear TRT refined structured mesh - LO FEM is affected by linearization

Electron temperatures from linearized system on meshes with 6400 zones for $\Delta t = 8 \times 10^{-13}$ seconds at time step 80.

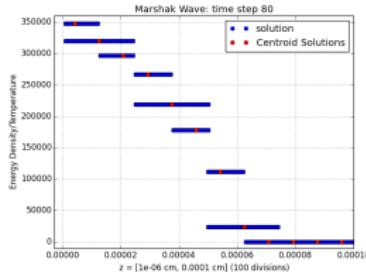
Test 1
(linearized,
1st-order,
structured).



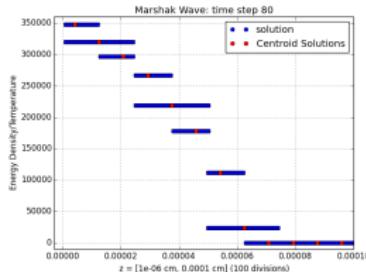
Test 5
(nonlinear,
1st-order,
structured).



Test 2
(linearized,
2nd-order,
structured).



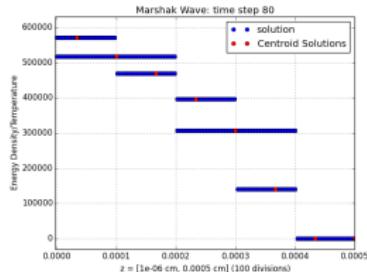
Test 6
(nonlinear,
2nd-order,
structured).



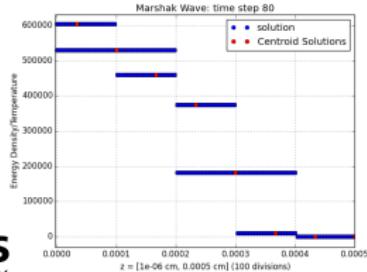
Nonlinear TRT coarse structured mesh - LO FEM affected by linearization

Electron temperatures from linearized system on meshes with 100 zones for $\Delta t = 8 \times 10^{-12}$ seconds at time step 80.

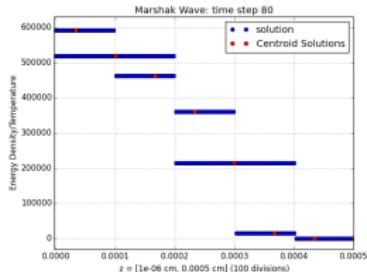
Test 1
(linearized,
1st-order,
structured).



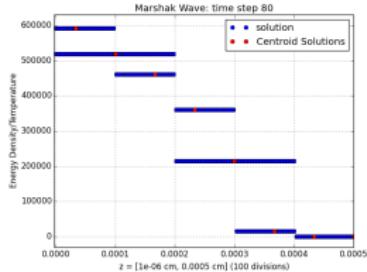
Test 5
(nonlinear,
1st-order,
structured).



Test 2
(linearized,
2nd-order,
structured).



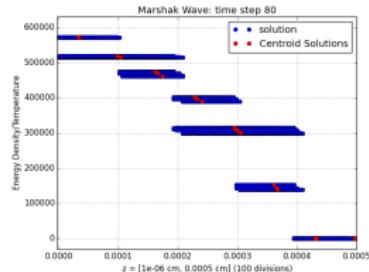
Test 6
(nonlinear,
2nd-order,
structured).



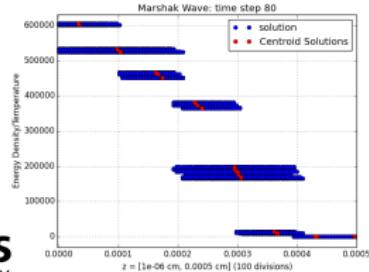
Nonlinear TRT coarse unstructured mesh - nonlinear LO propagates less energy than HO

Electron temperatures from linearized system on meshes with 100 zones for $\Delta t = 8 \times 10^{-12}$ seconds at time step 80.

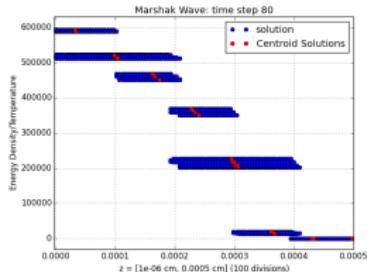
Test 3
(linearized,
1st-order,
unstructured).



Test 7
(nonlinear,
1st-order,
unstructured).



Test 4
(linearized,
2nd-order,
unstructured).



Test 8
(nonlinear,
2nd-order,
unstructured).

