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# High-Order Thermal Radiative Transfer

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Los Alamos National Laboratory

14 September 2017

# Research objectives

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- 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

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- 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

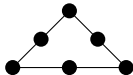
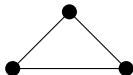
$$T(\mathbf{x}) \approx \sum_j T_j b_j(\mathbf{x})$$

- Low-order (1<sup>st</sup>-order) basis functions assume flat (linear) shape:

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

- High-order (2<sup>nd</sup>-order) basis function allow for solution curvature:

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



# Thermal radiation transport

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The nonlinear thermal radiative transport (TRT) equations:

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

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

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

# Thermal radiation transport

The linearized thermal radiative transport (TRT) equations:

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

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

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

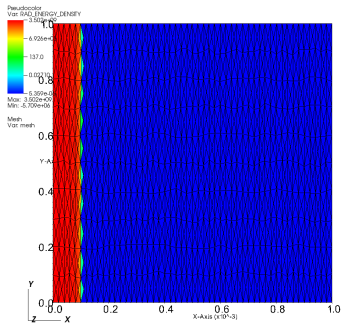
$$\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t} + \mathbf{\Omega} \cdot \nabla I^{n+1} + \sigma_t I^{n+1} = \frac{\sigma_s}{4\pi} E^{n+1} + \sigma_a B^{n+1} + S_0^{n+1},$$

Linearized equations susceptible to maximum principle violations.



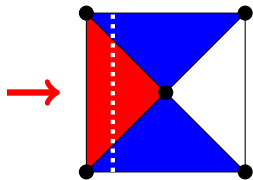
# Test problem: Marshak wave

- 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.

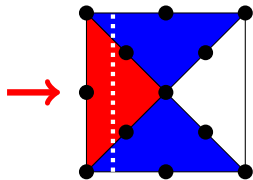


# High-order finite elements - conceptual mass averaging

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



(a) 1<sup>st</sup>-order FEM.



(b) 2<sup>nd</sup>-order FEM.

# Linearized thermal radiation transport test definitions

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

Remember: odds are odd, evens are even.

# Linearized TRT case matrix - $\Delta t$ and $\Delta x$ are part of sufficient conditions to adhere to maximum principle

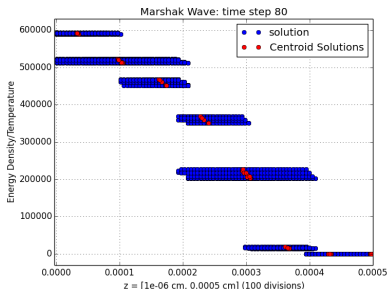
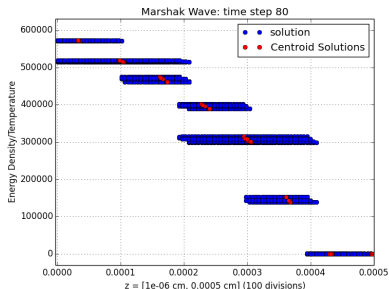
Case matrix for refining the time step and mesh

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

$\Delta t$ (sec.)	no. of mesh zones			
	100	400	1600	6400
$8 \times 10^{-10}$				
$8 \times 10^{-11}$	1, 3			
$8 \times 10^{-12}$	1, 2, 3, 4	1, 2, 3, 4	2	
$8 \times 10^{-13}$	1, 2, 3, 4	1, 2, 3, 4	1, 2, 3, 4	1, 2, 3, 4
$8 \times 10^{-14}$	1, 2, 3, 4	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

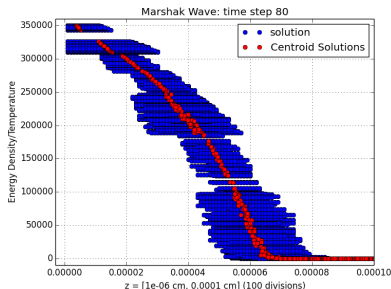
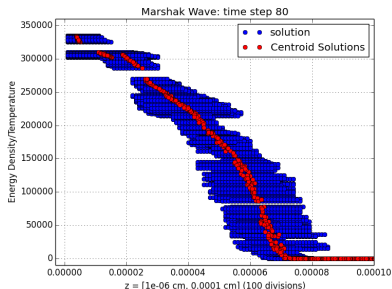
Electron temperatures from linearized system on meshes with 100 zones for  $\Delta t = 8 \times 10^{-12}$  seconds at time step 80.



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

# Nonlinear TRT test definitions

---

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

$\Delta t$ (sec.)	no. of mesh zones			
	100	400	1600	6400
$8 \times 10^{-10}$				
$8 \times 10^{-11}$	5, 7			
$8 \times 10^{-12}$	5, 6, 7, 8	5, 6, 7, 8	5, 7	5, 7
$8 \times 10^{-13}$	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8
$8 \times 10^{-14}$	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8	5, 6, 7, 8

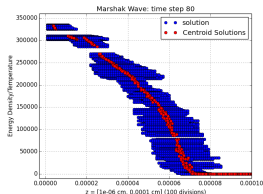


# Nonlinear TRT refined unstructured mesh - LO FEM is affected by linearization

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

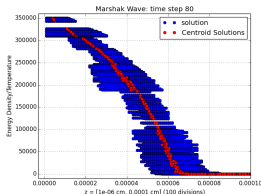
Test 3

(linearized,  
1<sup>st</sup>-order,  
unstructured).



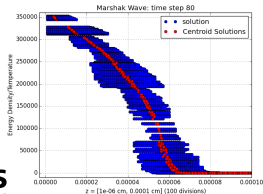
Test 4

(linearized,  
2<sup>nd</sup>-order,  
unstructured).



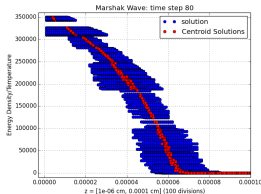
Test 7

(nonlinear,  
1<sup>st</sup>-order,  
unstructured).



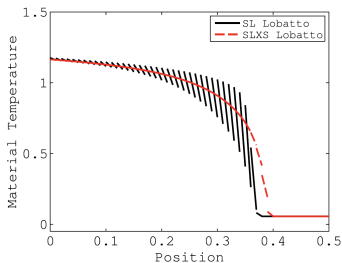
Test 8

(nonlinear,  
2<sup>nd</sup>-order,  
unstructured).



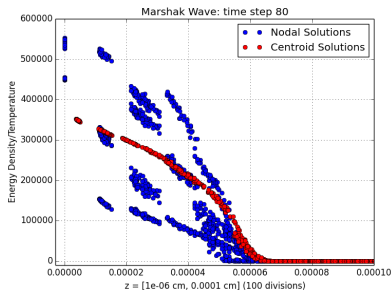
# Serrano vs. Hidalgo: opacities and heat capacities evaluated at nodal temperatures

- 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.

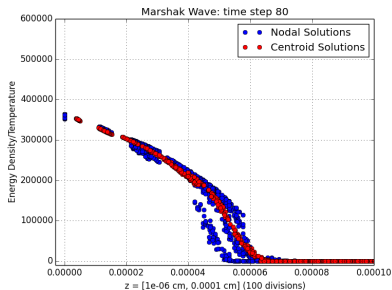


Maginot et al. (2016).

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

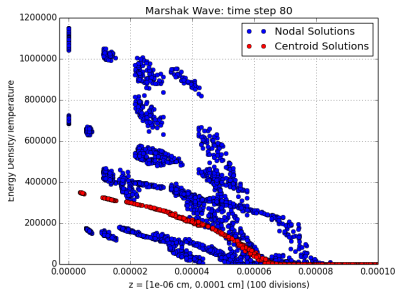


(a) Test 7 (nonlinear, 1<sup>st</sup>-order, unstructured) with Serrano.

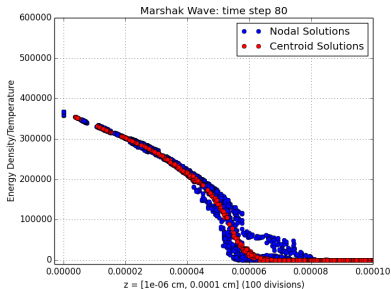


(b) Test 7 (nonlinear, 1<sup>st</sup>-order, unstructured) with Hidalgo.

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



(a) Test 8 (nonlinear, 2<sup>nd</sup>-order, unstructured) with Serrano.



(b) Test 8 (nonlinear, 2<sup>nd</sup>-order, unstructured) with Hidalgo.

# Conclusions

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- 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

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- 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?

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Thank you!

Matt Cleveland

Ryan Wollaeger

Jim Warsa

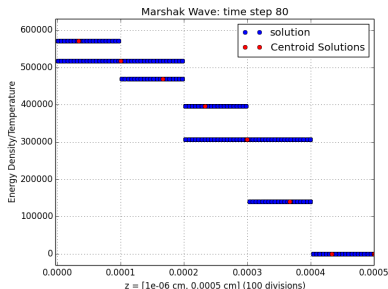


**Oregon State**  
University

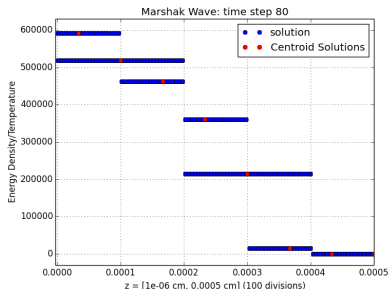
This research was performed by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract XX-XXXX-XXXXXXXXXX.

# 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 (1<sup>st</sup>-order, structured).

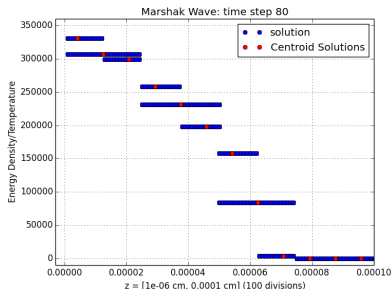


(b) Test 2 (2<sup>nd</sup>-order, structured).

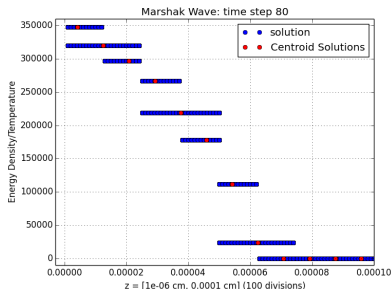


# Linearized TRT refined structured mesh - HO FEM has higher temperature near boundary

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 (1<sup>st</sup>-order, structured).

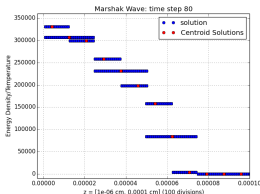


(b) Test 2 (2<sup>nd</sup>-order, structured).

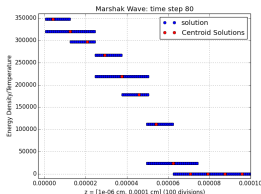
# Nonlinear TRT refined structured mesh - LO FEM is affected by linearization

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

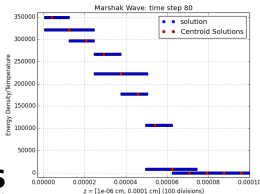
Test 1  
(linearized,  
1<sup>st</sup>-order,  
structured).



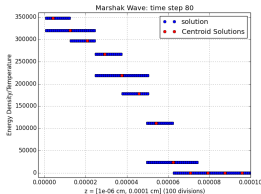
Test 2  
(linearized,  
2<sup>nd</sup>-order,  
structured).



Test 5  
(nonlinear,  
1<sup>st</sup>-order,  
structured).



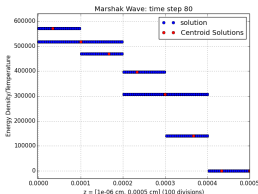
Test 6  
(nonlinear,  
2<sup>nd</sup>-order,  
structured).



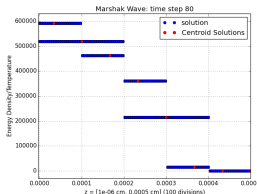
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Electron temperatures from linearized system on meshes with 100 zones for  $\Delta t = 8 \times 10^{-12}$  seconds at time step 80.

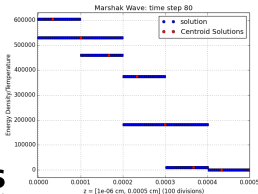
Test 1  
(linearized,  
1<sup>st</sup>-order,  
structured).



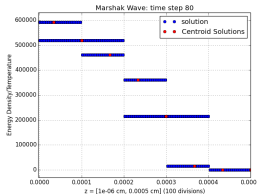
Test 2  
(linearized,  
2<sup>nd</sup>-order,  
structured).



Test 5  
(nonlinear,  
1<sup>st</sup>-order,  
structured).



Test 6  
(nonlinear,  
2<sup>nd</sup>-order,  
structured).

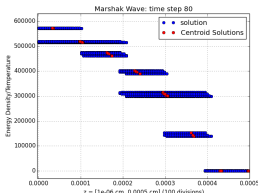


# Nonlinear TRT coarse unstructured mesh - nonlinear LO propagates less energy than HO

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

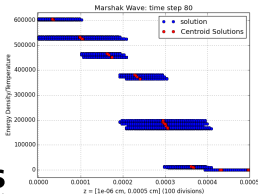
Test 3

(linearized,  
1<sup>st</sup>-order,  
unstructured).



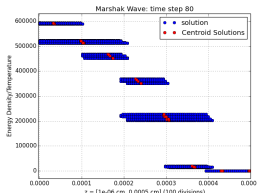
Test 7

(nonlinear,  
1<sup>st</sup>-order,  
unstructured).



Test 4

(linearized,  
2<sup>nd</sup>-order,  
unstructured).



Test 8

(nonlinear,  
2<sup>nd</sup>-order,  
unstructured).

