Spartan Test Problem Results

Michael L. Hall
Transport Methods Group
Unstructured Mesh Radiation Transport Team
Los Alamos National Laboratory
Los Alamos National Laboratory, NM 87545

Email: `hall@lanl.gov`

Available on-line at
`http://www.lanl.gov/Spartan`

Outline

- Code Package Description
- Method Overview
  - Spartan
  - Augustus
- Equation Set
  - SP_N
  - Diffusion
- Algebraic Solution
- Problem Description
- Diffusion Results
- Results Discussion

Spartan/Augustus Code Package Description

Spartan:	SP_N, 2 T + Multi-Group, Even-Parity Photon Transport Package with v/c corrections
Augustus:	P_1 (Diffusion) Package
JTpack:	Krylov Subspace Iterative Solver Package (by John Turner, ex-LANL)
UMFPACK:	Unstructured Multifrontal Solver Package (an Incomplete Direct Method by Tim Davis, U of FL)
LINPACK:	Direct Dense Linear Equation Solver Package
BLAS:	Basic Linear Algebra Subprograms

Method Overview: Spartan

- Energy/Temperature Discretization
  - Solves 2 T + Multi-Group Even-Parity Equations
  - Can yoke T_e and T_i together to make 1 T
  - Can use a single-group radiation treatment to make 3 T
- Angular Discretization
  - Uses Simplified Spherical Harmonics — SP_N
  - Can do a P_1 (diffusion-like) solution
- Spatial Discretization
  - SP_N decouples equations into many diffusion equations
  - Diffusion equations are solved by Augustus
- Temporal Discretization
  - Linearized implicit discretization
  - Equivalent to one pass of a Newton solve
  - Iteration strategy:
    * Source iteration
    * DSA acceleration
    * LMFG acceleration

Method Overview: Augustus

- Spatial Discretization
  - Morel asymmetric diffusion discretization
  - Support Operator symmetric diffusion discretization
- Temporal Discretization
  - Backwards Euler implicit discretization
- Matrix Solution
  - Krylov Subspace Iterative Methods
    - JTpack: GMRES, BCGS, TFQMR
    - Preconditioners:
      - JTpack: Jacobi, SSOR, ILU
      - Low-order version of Morel or Support Operator discretization that is a smaller, symmetric system and is solved by CG with SSOR (from JTpack)
  - Incomplete Direct Method - UMFPACK

Simplified Spherical Harmonics (SP_N) Even-Parity Equation Set

Radiation transport equations:

$$\frac{1}{c}\frac{\partial}{\partial t}\xi_{m,g} + \overrightarrow{\nabla}\cdot\overrightarrow{\Gamma}_{m,g} + \sigma_g^t \xi_{m,g} = \sigma_g^s \phi_g + \sigma_g^e B_g + \mathcal{C}_g^s \ ,$$

$$\frac{1}{c}\frac{\partial}{\partial t}\overrightarrow{\Gamma}_{m,g} + \mu_m^2 \overrightarrow{\nabla}\xi_{m,g} + \sigma_g^t \overrightarrow{\Gamma}_{m,g} = \overrightarrow{\mathcal{C}}^v_{m,g}$$

for $m = 1, M$, and $g = 1, G$.

Temperature equations:

$$\begin{aligned} C_{vi}\frac{\partial T_i}{\partial t} &= \alpha\left(T_e - T_i\right) + Q_i \ , \\ C_{ve}\frac{\partial T_e}{\partial t} &= \alpha\left(T_i - T_e\right) + Q_e + \sum_{g=1}^{G}\left(\sigma_g^a \phi_g^{(0)} - \sigma_g^e B_g\right) \ , \end{aligned}$$

where

$$\begin{aligned} \xi_{m,g} &= \text{Even-parity pseudo-angular energy intensity,} \\ \overrightarrow{\Gamma}_{m,g} &= \text{Even-parity pseudo-angular energy current,} \end{aligned}$$

Simplified Spherical Harmonics (SP_N) Even-Parity Equation Set (cont)

$$
\begin{aligned}
\mathcal{C}_g^s &= \left(\sigma_g^a - \sigma_g^s\right) \overrightarrow{F}_g^{(0)} \cdot \frac{\overrightarrow{v}}{c} \,, \\
\overrightarrow{\mathcal{C}}_{m,g}^{v} &= 3\mu_m^2 \sigma_g^t \left(P_g + \phi_g\right) \frac{\overrightarrow{v}}{c} \,, \\
\phi_g &= \sum_{m=1}^{M} \xi_{m,g}\, w_m \,, \\
P_g &= \sum_{m=1}^{M} \xi_{m,g}\, \mu_m^2\, w_m \,, \\
\overrightarrow{F}_g &= \sum_{m=1}^{M} \overrightarrow{\Gamma}_{m,g}\, w_m \,, \\
\phi_g^{(0)} &= \phi_g - 2\, \overrightarrow{F}_g^{(0)} \cdot \frac{\overrightarrow{v}}{c} \,, \\
\overrightarrow{F}_g^{(0)} &= \overrightarrow{F}_g - \left(P_g + \phi_g\right) \frac{\overrightarrow{v}}{c} \,, \\
M &= \left(N + 1\right)/2 \,.
\end{aligned}
$$

Diffusion (P_1) Equation Set:

$$\alpha\frac{\partial\Phi}{\partial t} - \overrightarrow{\nabla}\cdot D\overrightarrow{\nabla}\Phi + \overrightarrow{\nabla}\cdot\overrightarrow{J} + \sigma\Phi = S$$

Which can be written

$$\alpha\frac{\partial\Phi}{\partial t} + \overrightarrow{\nabla}\cdot\overrightarrow{F} + \sigma\Phi = S$$

$$\overrightarrow{F} = -D\overrightarrow{\nabla}\Phi + \overrightarrow{J}$$

Where

Φ	=	Intensity
$\overrightarrow{F}$	=	Flux
D	=	Diffusion Coefficient
α	=	Time Derivative Coefficient
σ	=	Removal Coefficient
S	=	Intensity Source Term
$\overrightarrow{J}$	=	Flux Source Term

Algebraic Solution

- Main Matrix System (Asymmetric Method):
  - Asymmetric – must use an asymmetric solver like GMRES, BCGS or TFQMR
  - Size is $(3n_c + n_b/2)$ squared
  - Maximum of 7 non-zero elements per row

- Main Matrix System (Support Operator Method):
  - Symmetric – can use CG to solve
  - Size is $(3n_c + n_b/2)$ squared
  - Maximum of 9 non-zero elements per row

- Preconditioner for Krylov Space methods is a Low-Order Matrix System:
  - Assume orthogonal: drop out minor directions in flux terms
  - Symmetric – can use standard CG solver
  - Size is n_c squared
  - Maximum of 5 non-zero elements per row

Problem Description

- Mesh:
  - Kershaw, $\{r, z\}$ Mesh over 1 cm $\times$ 1 cm area
  - Grid size - $51 \times 51 = 2601$ nodes, 2500 cells
- Physics:
  - Two temperature, P_1 run
  - No removal or sources
  - Initial temperature of $\sqrt[4]{10^5} = 0.05623413$ keV
- Boundary Conditions:
  - Black-body source at 1 keV at $z = 0$ cm
  - Vacuum boundary condition at $z = 1$ cm
  - Reflective boundaries at $r = 0$ cm and $r = 1$ cm
- Physical Constants:
  - No scattering
  - Absorption, emission and total cross sections defined via $\sigma = 30\, T_{mat}^{-3}$ cm^{-1}
  - Specific heat corresponds to an ideal gas with a density of 3 g/cc and $\overline{a} = 1$, giving a value of $C_v = 0.4310461$ jerks/cm^3/keV

Problem Description (cont)

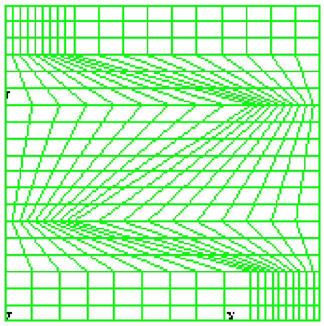
- Opacity Evaluation:
  - Node opacities = Average of neighbor faces
  - Face opacities evaluated at average of cell center temperatures
  - Vacuum boundary face opacity equal to cell center opacity
  - Black-body source boundary face opacity evaluated at source temperature
- Solution Methods:
  - Morel Asymmetric Method, Support Operator Method
  - UMFPACK solver - an incomplete direct method
  - Time step limited so that the norm of the relative changes of T_{mat}, T_r, and ϕ are kept less than 0.03
  - Temperature floor set to 0.056 keV

Results

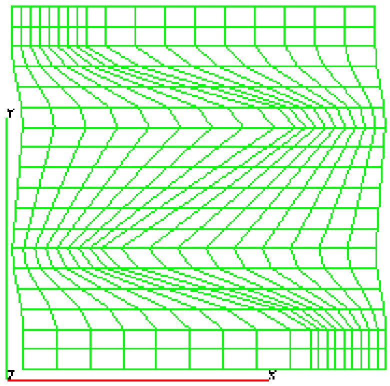
- Morel Asymmetric Method
  - Decreasing intensity (like an intensity sink) starts when wave reaches skewed part of the mesh
  - Fix-up: when radiation temperature dips below the temperature floor, use low-order scheme in that cell
  - Fix-up eliminates positive off-diagonals in matrix, which would guarantee a positive solution if done over entire mesh
  - Fix-up was successful: problem runs until steady-state
  - All plots are from this method
- Support Operator Method
  - Instabilities:
    * grow without bound from roundoff values
    * located at the skewed parts of the mesh
    * begin at $t \approx 6 \times 10^{-7}$ sh, before the wave has reached the area
    * could be a coding error?
  - Fix-up has no effect

Plotting Anomaly

Actual Mesh (Cell Nodes)



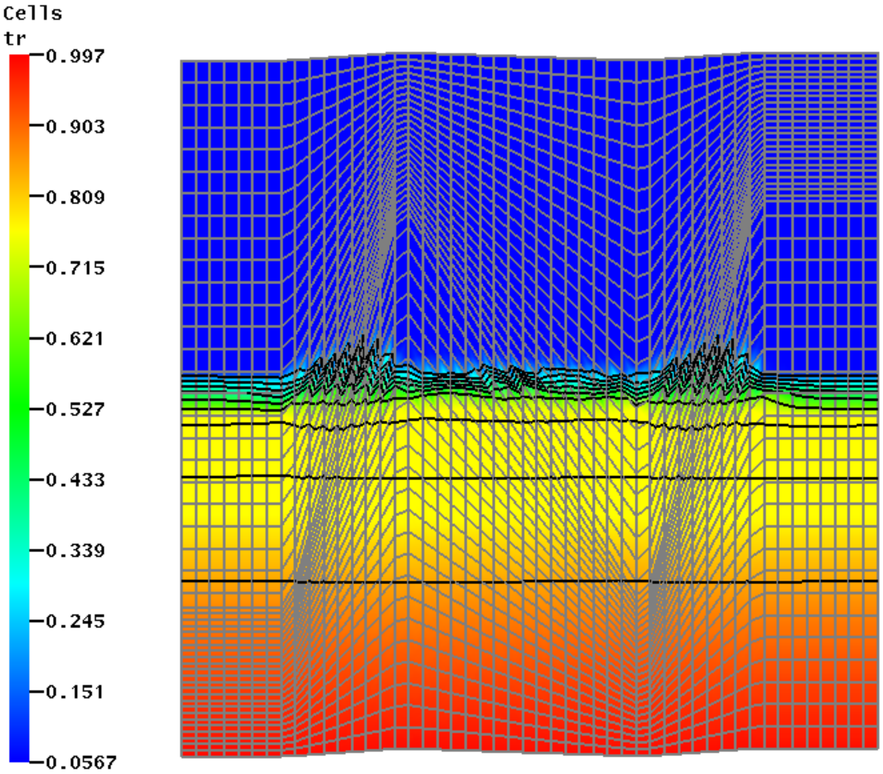
Dual Mesh (Cell Centers)



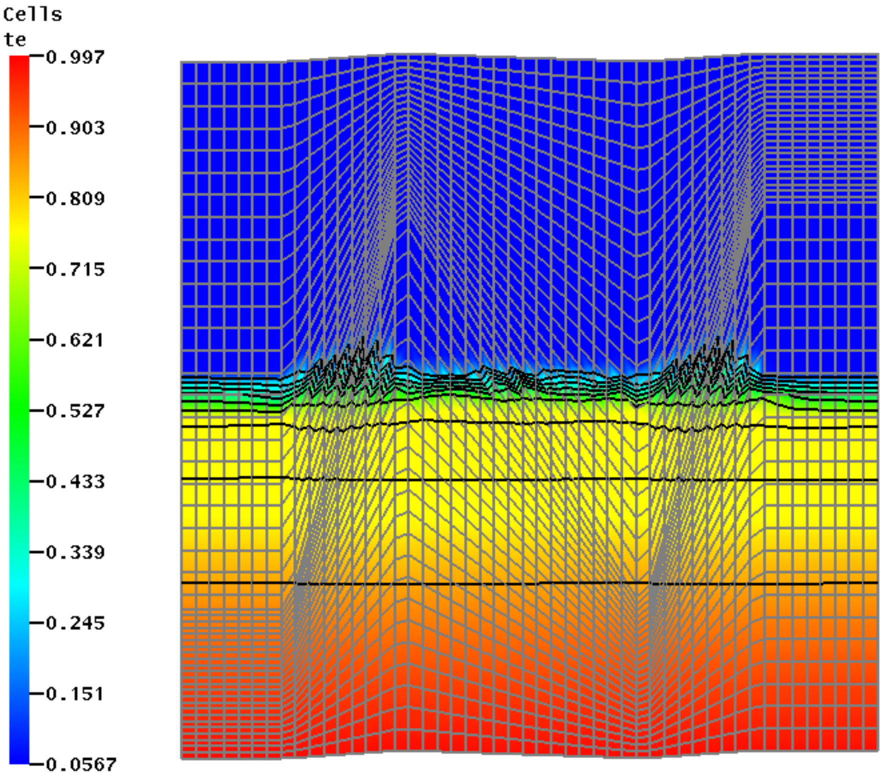
In order to plot contour lines, the cell centers are treated like node values. This gives an irregular boundary shape, but you should consider that a plotting anomaly only.

Results: Time = 2.0 sh

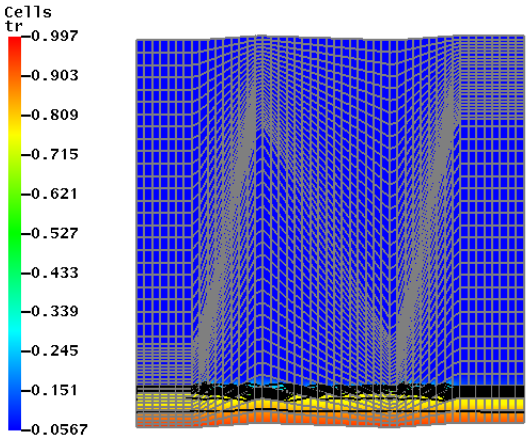
T_{rad}



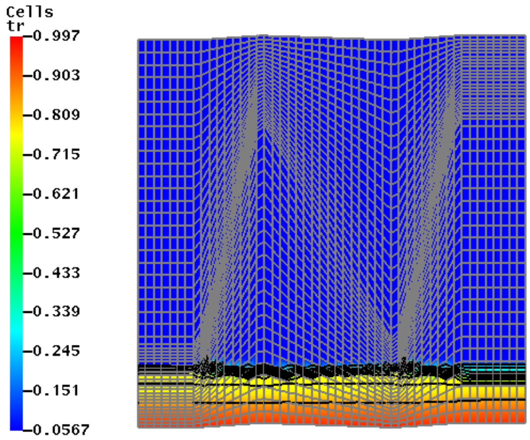
T_{mat}



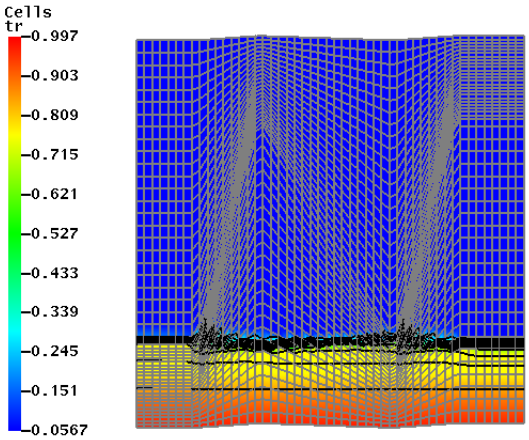
T_{rad} Time-Dependent Results



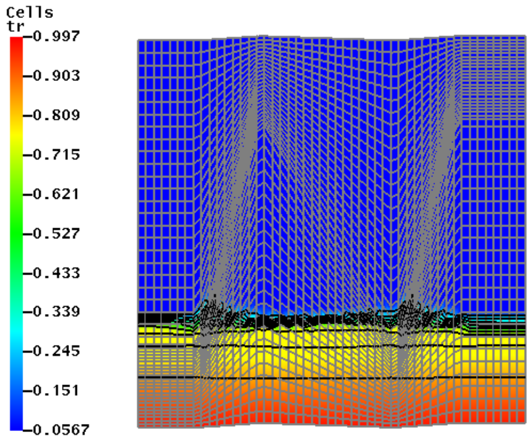
$t = 0.1$ sh



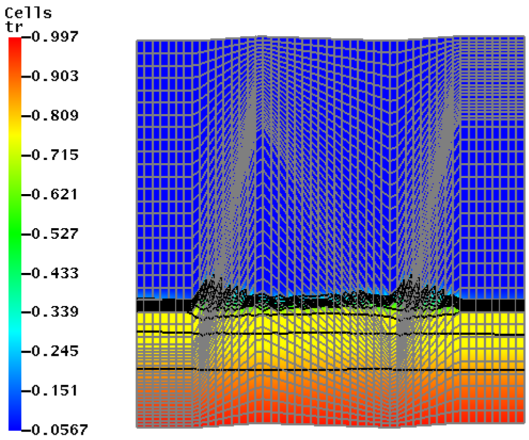
$t = 0.2$ sh



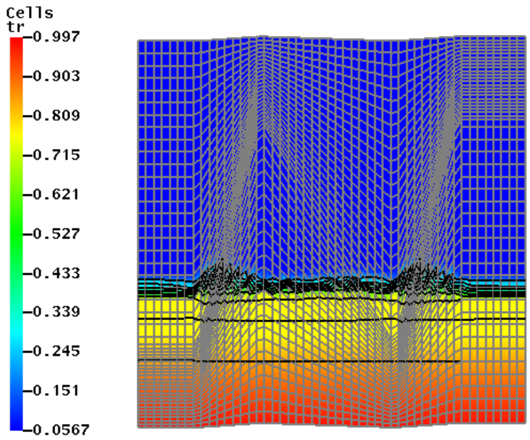
$t = 0.4$ sh



$t = 0.6$ sh

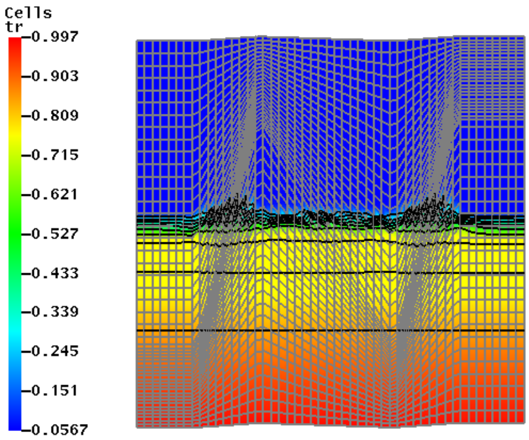


$t = 0.8$ sh

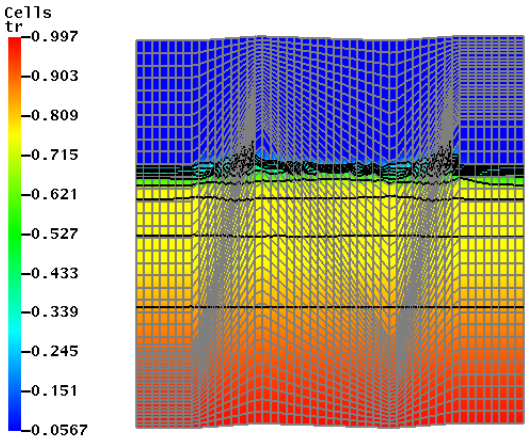


$t = 1.0$ sh

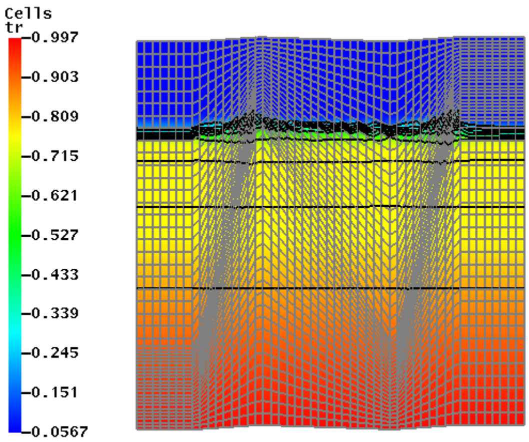
T_{rad} Time-Dependent Results (cont)



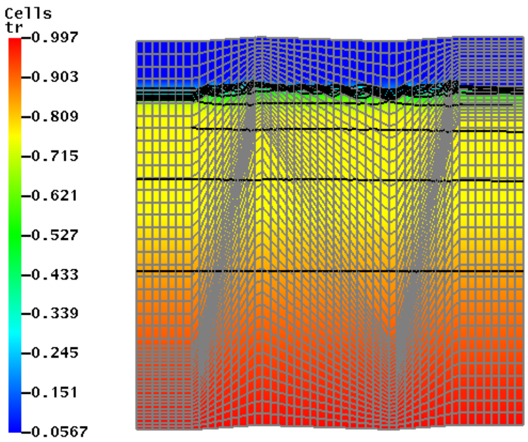
$t = 2.0$ sh



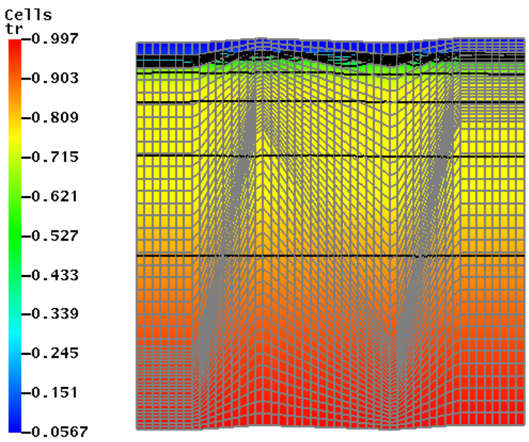
$t = 3.0$ sh



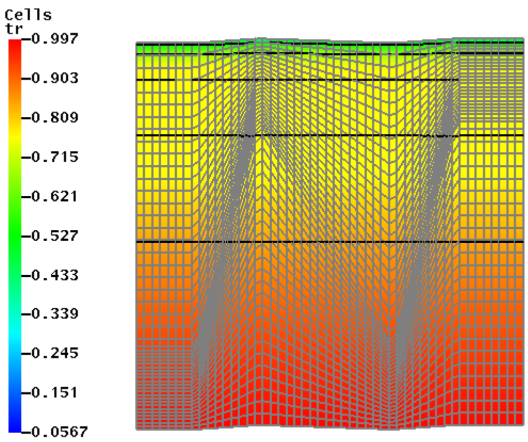
$t = 4.0$ sh



$t = 5.0$ sh

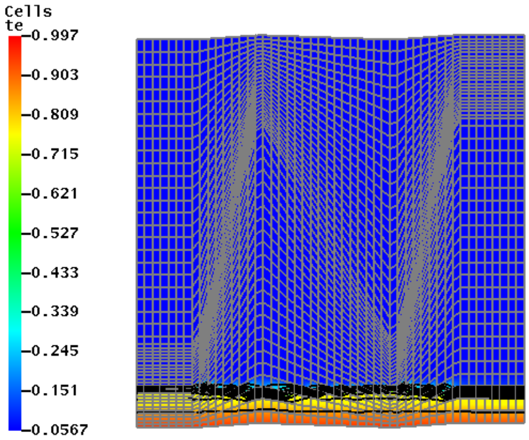


$t = 6.0$ sh

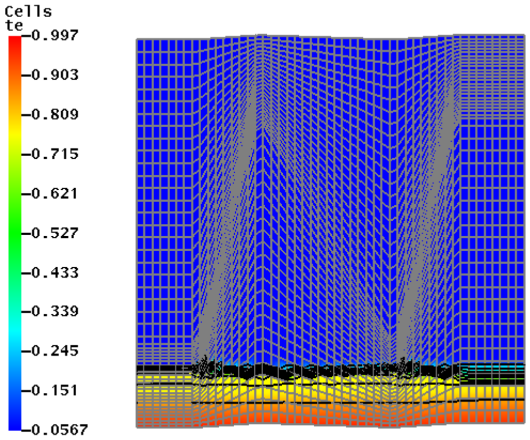


$t = 7.0$ sh

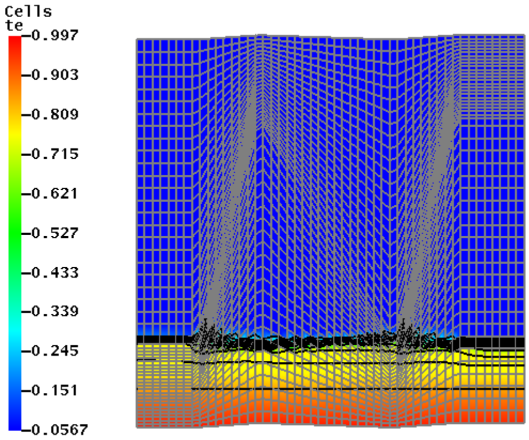
T_{mat} Time-Dependent Results



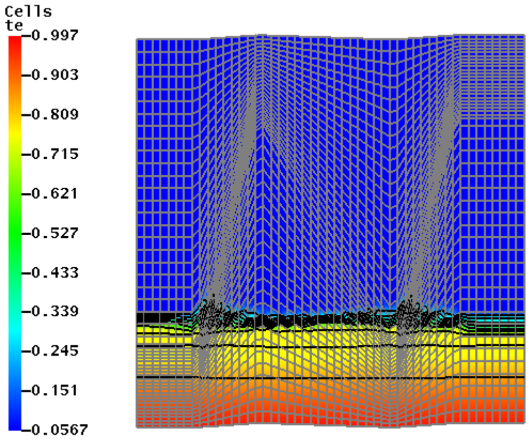
$t = 0.1$ sh



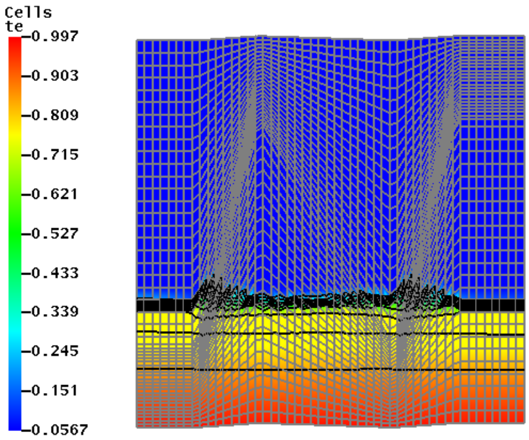
$t = 0.2$ sh



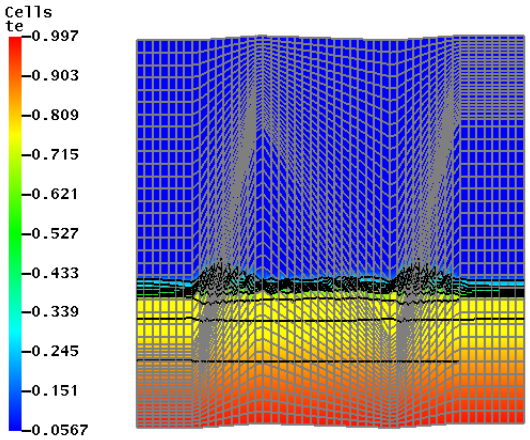
$t = 0.4$ sh



$t = 0.6$ sh

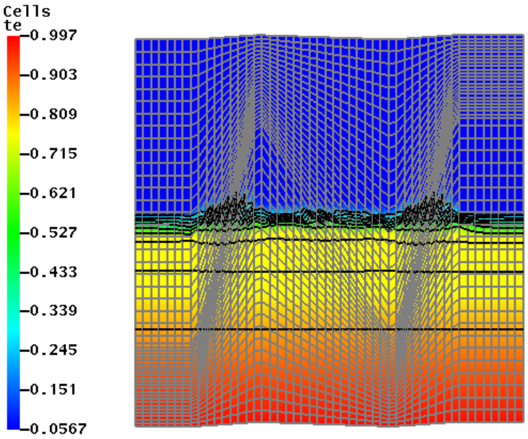


$t = 0.8$ sh

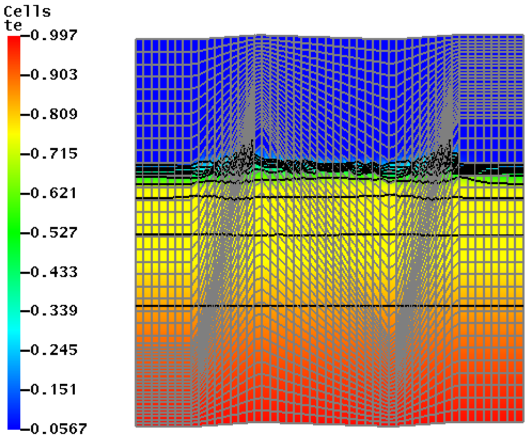


$t = 1.0$ sh

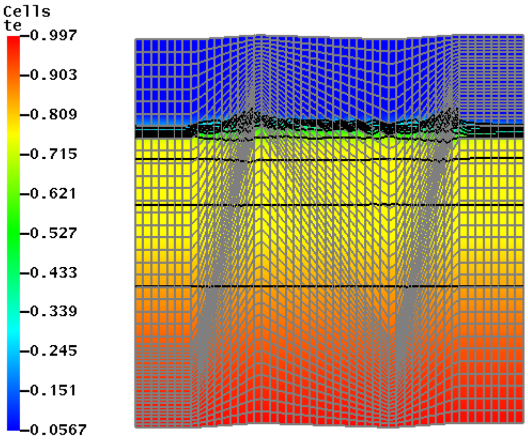
T_{mat} Time-Dependent Results (cont)



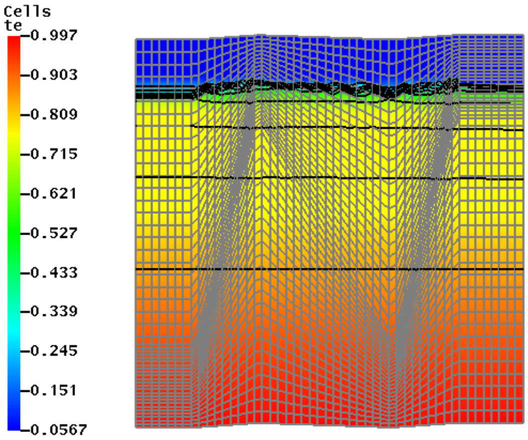
$t = 2.0$ sh



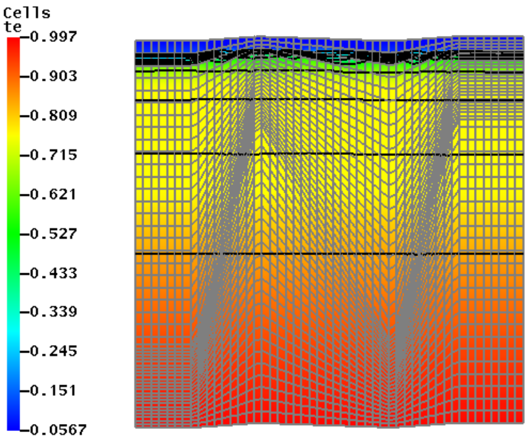
$t = 3.0$ sh



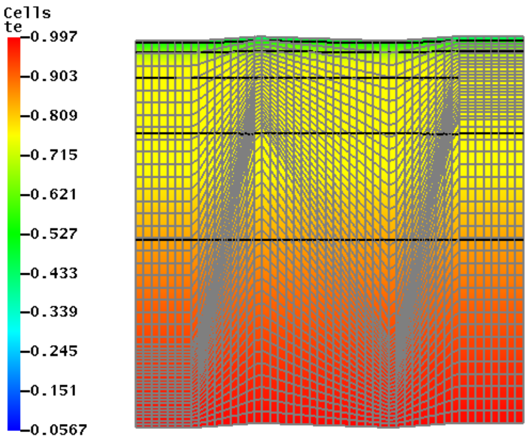
$t = 4.0$ sh



$t = 5.0$ sh



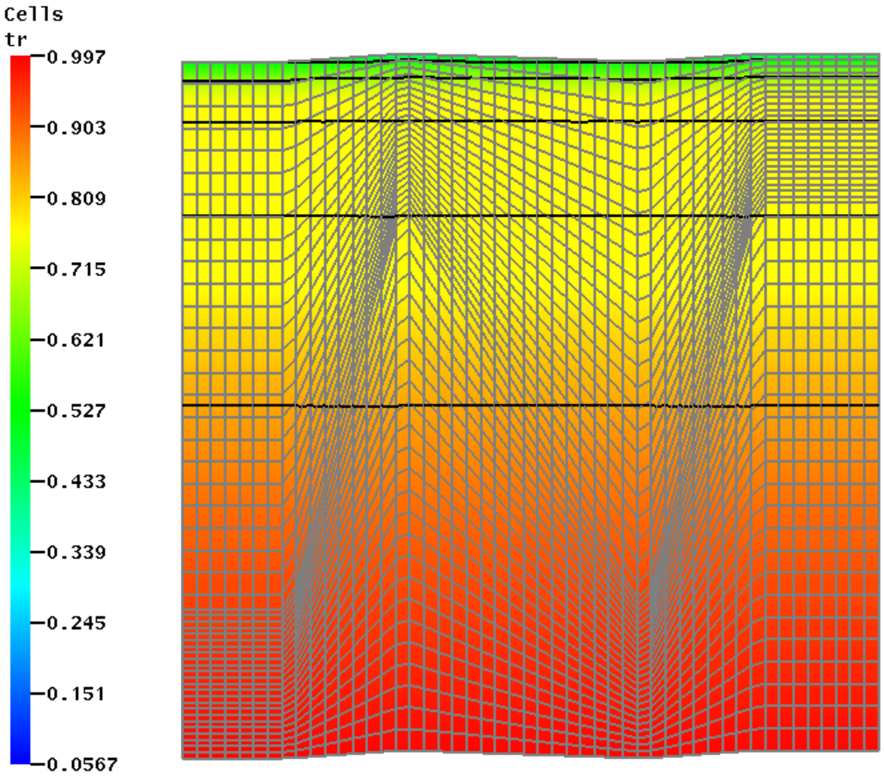
$t = 6.0$ sh



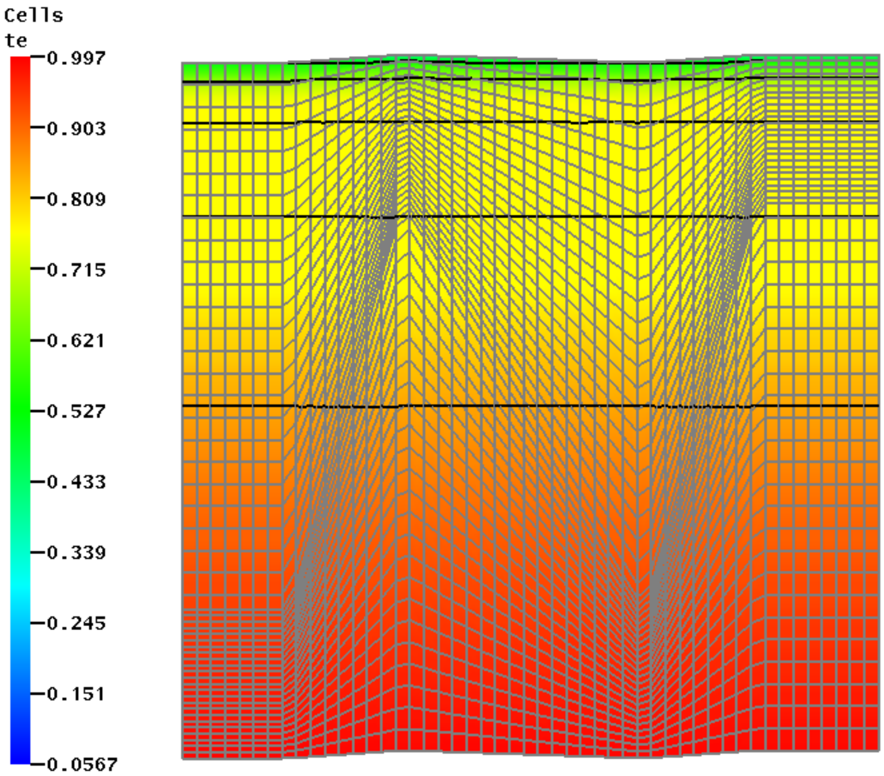
$t = 7.0$ sh

Steady-State Results: Time = 29.6 sh

T_{rad}



T_{mat}



Results Discussion

- Difficulties (instabilities and intensity sinks) are generated by both methods

- A fix-up for the Morel Asymmetric Method was successful

- No solution for the Support Operator Method has been found so far

- For the Morel Asymmetric Method:

  - 28089 time steps, 34.92 hours, 4.47 s / time step on Sun Ultra SPARC 1 Model 170 needed to model 32 shakes of real time
  - Contours are relatively flat for the time-dependent solution, completely flat for the steady-state solution

Future Work

- Parallel version