Spartan Test Problem Results

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

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

$$\frac{1}{c} \frac{\partial}{\partial t} \vec{\Gamma}_{m,g} + \mu_m^2 \nabla \cdot \vec{\xi}_{m,g} + \sigma_g^t \vec{\Gamma}_{m,g} = \vec{C}_{m,g},$$

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

Temperature equations:

$$C_{vi} \frac{\partial T_i}{\partial t} = \alpha (T_e - T_i) + Q_i,$$

$$C_{ve} \frac{\partial T_e}{\partial t} = \alpha (T_i - T_e) + Q_e + \sum_{g=1}^{G} \left( \sigma_{g}^a \phi_{g}^{(0)} - \sigma_{g}^e B_g \right),$$

where

$$\xi_{m,g} = \text{Even-parity pseudo-angular energy intensity},$$

$$\vec{\Gamma}_{m,g} = \text{Even-parity pseudo-angular energy current},$$
Simplified Spherical Harmonics ($SP_N$) Even-Parity Equation Set (cont)

\[
C_g^s = \left( \sigma_{g}^{a} - \sigma_{g}^{s} \right) \vec{F}_g^{(0)} \cdot \frac{\vec{v}}{c},
\]

\[
\vec{C}_{\mathbf{m},g}^{\mathbf{v}} = 3\mu_m^2\sigma_{g}^{t}(P_g + \phi_g) \frac{\vec{v}}{c},
\]

\[
\phi_g = \sum_{m=1}^{M} \xi_{m,g} w_m,
\]

\[
P_g = \sum_{m=1}^{M} \xi_{m,g} \mu_m^2 w_m,
\]

\[
\vec{F}_g = \sum_{m=1}^{M} \vec{\Gamma}_{m,g} w_m,
\]

\[
\phi_g^{(0)} = \phi_g - 2\vec{F}_g^{(0)} \cdot \frac{\vec{v}}{c},
\]

\[
\vec{F}_g^{(0)} = \vec{F}_g - (P_g + \phi_g) \frac{\vec{v}}{c},
\]

\[
M = \frac{(N + 1)}{2}.
\]
**Diffusion \((P_1)\) Equation Set:**

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

Which can be written

\[
\alpha \frac{\partial \Phi}{\partial t} + \nabla \cdot F + \sigma \Phi = S
\]

\[
F = -D \nabla \Phi + J
\]

Where

\[
\Phi = \text{Intensity} \\
F = \text{Flux} \\
D = \text{Diffusion Coefficient} \\
\alpha = \text{Time Derivative Coefficient} \\
\sigma = \text{Removal Coefficient} \\
S = \text{Intensity Source Term} \\
J = \text{Flux Source Term}
\]
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 \( \sqrt[4]{10^3} = 0.05623413 \text{ keV} \)

- **Boundary Conditions:**
  - Black-body source at 1 keV at \( z = 0 \text{ cm} \)
  - Vacuum boundary condition at \( z = 1 \text{ cm} \)
  - Reflective boundaries at \( r = 0 \text{ cm} \) and \( r = 1 \text{ cm} \)

- **Physical Constants:**
  - No scattering
  - Absorption, emission and total cross sections defined via \( \sigma = 30 T_{\text{mat}}^{-3} \text{ cm}^{-1} \)
  - Specific heat corresponds to an ideal gas with a density of 3 g/cc and \( \overline{a} = 1 \), giving a value of \( C_v = 0.4310461 \text{ jerks/cm}^3/\text{keV} \)
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 $\phi$ 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 $t \approx 6 \times 10^{-7}$ s, before the wave has reached the area
    * could be a coding error?
  - Fix-up has no effect
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 s
$T_{rad}$ Time-Dependent Results

$t = 0.1 \text{ sh}$

$t = 0.2 \text{ sh}$

$t = 0.4 \text{ sh}$

$t = 0.6 \text{ sh}$

$t = 0.8 \text{ sh}$

$t = 1.0 \text{ sh}$
Time-Dependent Results (cont)

$t = 2.0 \text{ sh}$

$t = 3.0 \text{ sh}$

$t = 4.0 \text{ sh}$

$t = 5.0 \text{ sh}$

$t = 6.0 \text{ sh}$

$t = 7.0 \text{ sh}$
T_{mat} Time-Dependent Results

\[ t = 0.1 \text{ sh} \] \hspace{1cm} \[ t = 0.2 \text{ sh} \]

\[ t = 0.4 \text{ sh} \] \hspace{1cm} \[ t = 0.6 \text{ sh} \]

\[ t = 0.8 \text{ sh} \] \hspace{1cm} \[ t = 1.0 \text{ sh} \]
$T_{mat}$ Time-Dependent Results (cont)

\begin{align*}
& t = 2.0 \text{ sh} & & t = 3.0 \text{ sh} \\
& t = 4.0 \text{ sh} & & t = 5.0 \text{ sh} \\
& t = 6.0 \text{ sh} & & t = 7.0 \text{ sh}
\end{align*}
Steady-State Results: Time = 29.6 sh

$T_{\text{rad}}$

$T_{\text{mat}}$
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