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Title: Development and Implementation of Rad-Hydro Verification Test Problems

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Development and Implementation of Rad-Hydro Verification Test Problems

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Outline

- xRAGE
- Goals
- Coggeshall Problems
 - Coggeshall 9 and 11 (Cog9 and Cog11)
 - Heat conduction Invariance
 - Conserved vs. Unconserved quantities
- Verification and Validation
- Convergence
- Calculation of Error
- Results

What is xRAGE?

- One of LANL's main production codes
- Eulerian code that solves radiation-hydrodynamics problems
 - Adaptive mesh refinement
 - Variable time step
- Coggeshall Simplified Rad-Hydro equations:

Conservation of Mass

$$\rho_t + \frac{2\rho u}{r^2} + \rho_r u + \rho u_r = 0$$

Conservation of Momentum

$$\vec{u}_t + \vec{u}\vec{u}_r + \frac{\Gamma\rho_r T}{\rho} + \Gamma T_r = 0$$

Conservation of Energy

$$\frac{\Gamma}{\gamma - 1} (T_t + \vec{u}T_r) + \Gamma T\vec{u}_r + \frac{2\Gamma T\vec{u}}{r} + \frac{\vec{F}_r}{\rho} + \frac{2\vec{F}}{\rho r} = 0$$

$$P = \Gamma\rho T$$

$$e = \left[\frac{\Gamma}{\gamma - 1} \right] T$$

P = pressure

e = specific energy

γ = adiabatic exponent

Γ = gas constant

ρ = density

u = velocity

T = temperature

$\vec{F}$ = radiation heat flux

Goals

- Implement Cog9 and Cog11 for xRAGE
- Verify second-order convergence in space
- Investigate the effect of the heat conduction module
- Determine which cell-averaging method is better: conserved or unconserved

History of the Coggeshall Problems

- A set of 22 analytical solutions
- Developed using Lie group analysis of the PDEs
- Coggeshall #8 has been implemented in the test problem suite for xRAGE

Coggeshall's Heat Flux

- Radiation Flux: Fick's law and Stefan-Boltzmann law.

- Fick's Law:

$$\vec{J} = -D\nabla\phi$$

$\phi = \text{concentration}$

$D = \text{diffusion coefficient}$

$\vec{J} = \text{flux}$

- Stefan-Boltzmann Law:

$$\vec{F} = -D\nabla T^4$$

- Radiation Flux:

$$\lambda(\rho, T) = \lambda_0 \rho^\alpha T^\beta$$

$\alpha, \beta = \text{experimental quantities}$

$$D = \frac{1}{3} c \lambda(\rho, T) a$$

$c = \text{speed of light}$

$\lambda = \text{radiation mean free path}$

$a = \text{radiation constant}$

$$\vec{F} = -\left(\frac{c\lambda(\rho, T)a}{3}\right)\nabla T^4$$

Coggeshall #9 and #11

Cog9 {

$$\rho(r, t) = \rho_0 r^{-\frac{(2\beta+k+7)}{\alpha}} t^{-\frac{2[\alpha(k+1)-2\beta-k-7]}{\alpha[2+(\gamma-1)(k+1)]}}$$

$$u(r, t) = \frac{2r}{t[2 + (\gamma - 1)(k + 1)]} \quad k = \text{geometry factor}$$

$$T(r, t) = \frac{2\alpha(\gamma - 1)(k + 1)r^2}{t^2 \Gamma[2 + (\gamma - 1)(k + 1)]^2 (2\alpha - 2\beta - k - 7)}$$

Cog11 {

$$\rho(r, t) = \rho_0 r^{(\gamma-1)(k+1)-2} t^{1-k-(\gamma-1)(k+1)}$$

$$u(r, t) = \frac{r}{t}$$

$$T(r, t) = T_0 r^{2-(\gamma-1)(k+1)} t^{-2}$$

$$\alpha = \beta + 4 + (k - 1)/[2 - (\gamma - 1)(k + 1)]$$

Coggeshall #9 (Cog9)

$\alpha = -1, \beta = 2, k = 2$ (Spherical),

$$\gamma = 5/3$$

$$\rho(r, t) = \rho_0 \frac{r^{13}}{t^8}$$

$$u(r, t) = \frac{r}{2t}$$

$$T(r, t) = \frac{r^2}{60\Gamma t^2}$$

Coggeshall #11 (Cog11)

$\alpha = -1, \beta = 2, k = 2$ (Spherical),
 $\gamma = 12/7$

$$\rho(r, t) = \rho_0 r^{\frac{1}{7}} t^{-\frac{22}{7}}$$

$$u(r, t) = \frac{r}{t}$$

$$T(r, t) = T_0 r^{-1/7} t^{-2}$$

Heat Conduction Invariant

$$dQ_i = dQ_o$$

Heat Conduction Invariant

- Show the heat transferred into the cell is equal to the heat transferred out of the cell

$$4\pi r_1^2 \vec{F}_1 = 4\pi r_2^2 \vec{F}_2$$

- Calculate the divergence of the flux and show that it is zero

$$\nabla \cdot \vec{F} = 0$$

Heat Conduction Invariant

- Cog9

- Cog11

Conserved vs. Unconserved

Conserved vs. Unconserved

- Two methods of calculating cell-averaged quantities:
 - Standard volume weighted mean (unconserved).
 - Conserve mass, momentum, and energy on a cell-by-cell basis (conserved).

Cell-Average	Unconserved	Conserved
Density	$\bar{\rho} = \frac{\int r^2 dr \rho(r)}{\int r^2 dr}$	$\bar{\rho} = \frac{\int r^2 dr \rho(r)}{\int r^2 dr}$
Velocity	$\bar{u} = \frac{\int r^2 dr u(r)}{\int r^2 dr}$	$\bar{u} = \frac{\int r^2 dr \rho(r) u(r)}{\int r^2 dr \rho(r)}$
Specific Internal Energy	$\bar{e} = \frac{\int r^2 dr e(r)}{\int r^2 dr}$	$TE = 4\pi \int r^2 dr \rho(r) [e(r) + \frac{1}{2} u^2(r)]$ $\bar{e} = \frac{\left(\frac{TE}{\bar{\rho}} - \frac{1}{2} \bar{u}^2 \right)}{\int r^2 dr}$

Conserved vs. Unconserved

- Cog9

- Cog11

Verification and Validation

- Verification:
 - Does the code solve the equations correctly?

- Validation:
 - Does the code solve the correct equations?

- We are using convergence as a quantitative way to verify xRAGE

Convergence

- Convergence is the rate at which the numerical methods approximate the solution
- Determine convergence rate of the spatial mesh size

$$E(\Delta x) \approx C\Delta x^n$$

$$\log(E) = n \log(\Delta x) + \log(C)$$

Calculation of Error

$$L_1 = \frac{\int_{x_{min}}^{x_{max}} dV |f_{exact} - f_{xRAGE}|}{\int_{x_{min}}^{x_{max}} dV}$$

$$Global\ Error \equiv L_1 \approx \frac{\sum_{i=1}^N |f_{exact,i} - f_{xRAGE,i}| (x_{max,i}^3 - x_{min,i}^3)}{\sum_{i=1}^N (x_{max,i}^3 - x_{min,i}^3)}$$

Results of Heat Conduction

t = 3.0	Heat Conduction Module	Density	Velocity	Internal Energy	Pressure
Coggeshall #9	On	2.22078	2.2997	1.8986	2.17192
	Off	2.22078	2.2995	1.89866	2.17192
Coggeshall #11	On	2.80453	2.4354	1.86782	2.01101
	Off	3.1982	2.659	1.8974	2.0056

*

- Convergence is approx. 2
- Heat Conduction off gives better convergence

*Using conserved quantities

Results of Conserved vs. Unconserved

*					
t = 3.0	Cell Averages	Density	Velocity	Internal Energy	Pressure
Coggeshall #9	Conserved	2.22078	2.2995	1.89866	2.17192
	Unconserved	2.2165	2.2808	1.89176	2.17158
Coggeshall #11	Conserved	3.1982	2.659	1.8974	2.0056
	Unconserved	2.60006	0.905	2.14088	1.60959

- Majority of the values are second order
- Conserved quantities gives better convergence

*Using heat conduction module off

Conclusions

- Second order spatial convergence was observed
- The heat module did alter the convergence but not at a significant level
- Using conserved quantities generally produced better convergence

Future Work

- Investigate possible causes of third order convergence and less than second order convergence
- Implement solution in 2D geometry
- Investigate convergence of time step
- Different α , β , and γ values

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Questions?