3T Capabilities in FLASH

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RAL Tutorial
May 2012

I define a 1T simulation as one in which separate ion, electron, or radiation energy equations are not evolved

- **In the absence of source terms, the hydrodynamic equations are:**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0,$$

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v} \boldsymbol{v}) + \nabla P_{\mathrm{tot}} = 0,$$

$$\frac{\partial}{\partial t}(\rho E_{\mathrm{tot}}) + \nabla \cdot [(\rho E_{\mathrm{tot}} + P_{\mathrm{tot}})\, \boldsymbol{v}] = 0,$$

$$e_{\mathrm{tot}} = E_{\mathrm{tot}} - \frac{v^2}{2}$$

$$E_{\mathrm{tot}} = \frac{v^2}{2} + e_{\mathrm{tot}},$$

$$e_{\mathrm{tot}} = e_{\mathrm{ion}} + e_{\mathrm{ele}} + e_{\mathrm{rad}}$$

- **These equations are closed using an equation of state (EOS):**

$$P_{\mathrm{tot}} = \mathrm{EOS}(\rho, e_{\mathrm{tot}})$$

- **Since separate ion/electron/radiation energies are not tracked, the 1T EOS units typically make an *assumption* about the temperatures:**

$$T_{ele} = T_{ion} = T_{rad} \quad \text{or} \quad T_{ele} = T_{ion},\ T_{rad} = 0$$

When is a 1T simulation not adequate?

- Source terms may preferentially heat electrons, ions, or the radiation field creating different temperatures
  - Shocks preferentially heat ions
  - Laser preferentially heats electrons
- The difference in temperatures may be important for:
  - Evaluating transport coefficients (conductivity, resistivity, …)
  - Evaluating the EOS
- Thus, it is necessary to evolve the electron, ion, and radiation state so that we can keep track of the different electron/ion/radiation internal energies, temperatures, etc...
- All laser driven HEDP experiments should use the 3T version of FLASH, to activate just specify the following setup option:
  - Split Hydrodynamics Solver: `+3t`
  - Unsplit Hydrodynamics Solver: `+uhd3t`
  - Staggered Mesh Unsplit MHD Solver: `+usm3t`

The 3T version of FLASH solves the following equations

- **The same 1T hydrodynamic equations:**

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) &= 0, \\
\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) + \nabla P_{\mathrm{tot}} &= 0, \\
\frac{\partial}{\partial t}(\rho E_{\mathrm{tot}}) + \nabla \cdot \left[(\rho E_{\mathrm{tot}} + P_{\mathrm{tot}})\, \boldsymbol{v}\right] &= 0, \\
e_{\mathrm{tot}} = E_{\mathrm{tot}} - \frac{v^2}{2}
\end{aligned}
$$

- **Separate equations for ion, electron, radiation internal energy:**

$$
\frac{\partial}{\partial t}(\rho e_{\mathrm{ion}}) + \nabla \cdot (\rho e_{\mathrm{ion}} \boldsymbol{v}) + P_{\mathrm{ion}} \nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,\mathrm{ele}}}{\tau_{ei}} (T_{\mathrm{ele}} - T_{\mathrm{ion}}),
$$

$$
\frac{\partial}{\partial t}(\rho e_{\mathrm{ele}}) + \nabla \cdot (\rho e_{\mathrm{ele}} \boldsymbol{v}) + P_{\mathrm{ele}} \nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,\mathrm{ele}}}{\tau_{ei}} (T_{\mathrm{ion}} - T_{\mathrm{ele}}) - \nabla \cdot \boldsymbol{q}_{\mathrm{ele}} + Q_{\mathrm{abs}} - Q_{\mathrm{emis}} + Q_{\mathrm{las}},
$$

$$
\frac{\partial}{\partial t}(\rho e_{\mathrm{rad}}) + \nabla \cdot (\rho e_{\mathrm{rad}} \boldsymbol{v}) + P_{\mathrm{rad}} \nabla \cdot \boldsymbol{v} = \nabla \cdot \boldsymbol{q}_{\mathrm{rad}} - Q_{\mathrm{abs}} + Q_{\mathrm{emis}},
$$

The 3T version of FLASH solves the following equations

- **Separate equations for ion, electron, radiation internal energy:**

$$\frac{\partial}{\partial t}(\rho e_{\rm ion}) + \nabla \cdot (\rho e_{\rm ion}\boldsymbol{v}) + P_{\rm ion}\nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,\rm ele}}{\tau_{ei}}(T_{\rm ele} - T_{\rm ion}),$$

$$\frac{\partial}{\partial t}(\rho e_{\rm ele}) + \nabla \cdot (\rho e_{\rm ele}\boldsymbol{v}) + P_{\rm ele}\nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,\rm ele}}{\tau_{ei}}(T_{\rm ion} - T_{\rm ele}) - \nabla \cdot \boldsymbol{q}_{\rm ele} + Q_{\rm abs} - Q_{\rm emis} + Q_{\rm las},$$

$$\frac{\partial}{\partial t}(\rho e_{\rm rad}) + \nabla \cdot (\rho e_{\rm rad}\boldsymbol{v}) + P_{\rm rad}\nabla \cdot \boldsymbol{v} = \nabla \cdot \boldsymbol{q}_{\rm rad} - Q_{\rm abs} + Q_{\rm emis},$$

- **These equations are closed using an EOS, but now, information about the electron, ion, radiation state are known, so the EOS can use this information:**

$$P_{\rm tot}, T_{\rm ion}, T_{\rm ele}, T_{\rm rad} = \mathrm{EOS}(\rho, e_{\rm ion}, e_{\rm ele}, e_{\rm rad})$$

$$P_{\rm tot}, e_{\rm ion}, e_{\rm ele}, e_{\rm rad} = \mathrm{EOS}(\rho, T_{\rm ion}, T_{\rm ele}, T_{\rm rad})$$

- **Typically, for simulations of HEDP experiments, EOS tables are used for each material**

The 3T version of FLASH solves the following equations

- **Separate equations for ion, electron, radiation internal energy:**

$$\frac{\partial}{\partial t}(\rho e_{\text{ion}}) + \nabla\cdot(\rho e_{\text{ion}}\boldsymbol{v}) + P_{\text{ion}}\nabla\cdot\boldsymbol{v} = \rho\frac{c_{v,\text{ele}}}{\tau_{ei}}(T_{\text{ele}} - T_{\text{ion}}),$$

$$\frac{\partial}{\partial t}(\rho e_{\text{ele}}) + \nabla\cdot(\rho e_{\text{ele}}\boldsymbol{v}) + P_{\text{ele}}\nabla\cdot\boldsymbol{v} = \rho\frac{c_{v,\text{ele}}}{\tau_{ei}}(T_{\text{ion}} - T_{\text{ele}}) - \nabla\cdot\boldsymbol{q}_{\text{ele}} + Q_{\text{abs}} - Q_{\text{emis}} + Q_{\text{las}},$$

$$\frac{\partial}{\partial t}(\rho e_{\text{rad}}) + \nabla\cdot(\rho e_{\text{rad}}\boldsymbol{v}) + P_{\text{rad}}\nabla\cdot\boldsymbol{v} = \nabla\cdot\boldsymbol{q}_{\text{rad}} - Q_{\text{abs}} + Q_{\text{emis}},$$

- **$q_{qele} = - K_{ele}\, \nabla T_{ele}$ represents the electron heat flux, where K_{ele} is the electron conductivity**
- **A flux-limiter is used to limit the electron heat flux in regions where the temperature gradient is steep**
- **The Spitzer conductivity is primarily used in FLASH simulations, although the next release will include the Lee-More conductivity**

Electron thermal conduction (q_{ele}) is advanced in the `Diffuse` unit. It is solved implicitly using the HYPRE parallel linear algebra library

- To access the implicit HYPRE based diffusion solver include the following line in your `Config` file:

```
REQUESTS physics/Diffuse/DiffuseMain/Unsplit
```

- FLASH solves the following equation to model electron thermal conduction:

$$\rho c_{v,\mathrm{ele}} \frac{dT_{\mathrm{ele}}}{dt} = \nabla \cdot K_{\mathrm{ele}} \nabla T_{\mathrm{ele}}^*$$

- Typically the Sptizer conductivity is used. To access it, include:

```
REQUESTS physics/materialProperties/Conductivity/ConductivityMain/SpitzerHighZ
```

$$K_{\mathrm{ele}} = \left(\frac{8}{\pi}\right)^{3/2} \frac{k_B^{7/2}}{e^4 \sqrt{m_{\mathrm{ele}}}} \left(\frac{1}{1 + 3.3/\bar{z}}\right) \frac{T_{\mathrm{ele}}^{5/2}}{\bar{z} \ln \Lambda_{ei}}$$

The 3T version of FLASH solves the following equations

- **Separate equations for ion, electron, radiation internal energy:**

$$\frac{\partial}{\partial t}(\rho e_{\rm ion}) + \nabla\cdot(\rho e_{\rm ion}\boldsymbol{v}) + P_{\rm ion}\nabla\cdot\boldsymbol{v} = \rho\frac{c_{v,\rm ele}}{\tau_{ei}}(T_{\rm ele} - T_{\rm ion}),$$

$$\frac{\partial}{\partial t}(\rho e_{\rm ele}) + \nabla\cdot(\rho e_{\rm ele}\boldsymbol{v}) + P_{\rm ele}\nabla\cdot\boldsymbol{v} = \rho\frac{c_{v,\rm ele}}{\tau_{ei}}(T_{\rm ion} - T_{\rm ele}) - \nabla\cdot\boldsymbol{q}_{\rm ele} + Q_{\rm abs} - Q_{\rm emis} + Q_{\rm las},$$

$$\frac{\partial}{\partial t}(\rho e_{\rm rad}) + \nabla\cdot(\rho e_{\rm rad}\boldsymbol{v}) + P_{\rm rad}\nabla\cdot\boldsymbol{v} = \nabla\cdot\boldsymbol{q}_{\rm rad} - Q_{\rm abs} + Q_{\rm emis},$$

- **The ion/electron equilibration term causes the electron/ion temperatures to relax over time due to collisions**
- $\boldsymbol{\tau_{ei}}$ **is the ion/electron collision frequency. Most simulations use the Spizter form for this term**

Ion/electron equilibration is advanced by the `HeatExchange` unit

- To access ion/electron equilibration using the Spitzer collision time, include:

```
REQUESTS physics/sourceTerms/Heatexchange/HeatexchangeMain/Spitzer
```

- FLASH solves the following equations to model ion/electron equilibration:

$$\frac{\partial e_{\text{ion}}}{\partial t} = \frac{c_{v,\text{ele}}}{\tau_{ei}}(T_{\text{ele}} - T_{\text{ion}}),$$
$$\frac{\partial e_{\text{ele}}}{\partial t} = \frac{c_{v,\text{ele}}}{\tau_{ei}}(T_{\text{ion}} - T_{\text{ele}}).$$

- The ion/electron equilibration time is:

$$\tau_{ei} = \frac{3k_B^{3/2}}{8\sqrt{2\pi}e^4} \frac{(m_{\text{ion}}T_{\text{ele}} + m_{\text{ele}}T_{\text{ion}})^{3/2}}{(m_{\text{ele}}m_{\text{ion}})^{1/2}\,\bar{z}^2 n_{\text{ion}} \ln \Lambda_{ei}}$$

The 3T version of FLASH solves the following equations

- **Separate equations for ion, electron, radiation internal energy:**

$$\frac{\partial}{\partial t}(\rho e_{\rm ion}) + \nabla \cdot (\rho e_{\rm ion}\boldsymbol{v}) + P_{\rm ion}\nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,{\rm ele}}}{\tau_{ei}}(T_{\rm ele} - T_{\rm ion}),$$

$$\frac{\partial}{\partial t}(\rho e_{\rm ele}) + \nabla \cdot (\rho e_{\rm ele}\boldsymbol{v}) + P_{\rm ele}\nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,{\rm ele}}}{\tau_{ei}}(T_{\rm ion} - T_{\rm ele}) - \nabla \cdot \boldsymbol{q}_{\rm ele} + Q_{\rm abs} - Q_{\rm emis} + Q_{\rm las},$$

$$\frac{\partial}{\partial t}(\rho e_{\rm rad}) + \nabla \cdot (\rho e_{\rm rad}\boldsymbol{v}) + P_{\rm rad}\nabla \cdot \boldsymbol{v} = \nabla \cdot \boldsymbol{q}_{\rm rad} - Q_{\rm abs} + Q_{\rm emis},$$

- **$Q_{\rm las}$ represents the energy source due to laser energy deposition. This is computed using a ray-tracing algorithm (this will be discussed in detail tomorrow)**

- **The user can specify the location of multiple beams which illuminate the target**

- **The laser energy is absorbed using the common inverse Bremsstrahlung absorption coefficient**

The 3T version of FLASH solves the following equations

- **Separate equations for ion, electron, radiation internal energy:**

$$\frac{\partial}{\partial t}(\rho e_{\text{ion}}) + \nabla \cdot (\rho e_{\text{ion}} \boldsymbol{v}) + P_{\text{ion}} \nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,\text{ele}}}{\tau_{ei}} (T_{\text{ele}} - T_{\text{ion}}),$$

$$\frac{\partial}{\partial t}(\rho e_{\text{ele}}) + \nabla \cdot (\rho e_{\text{ele}} \boldsymbol{v}) + P_{\text{ele}} \nabla \cdot \boldsymbol{v} = \rho \frac{c_{v,\text{ele}}}{\tau_{ei}} (T_{\text{ion}} - T_{\text{ele}}) - \nabla \cdot \boldsymbol{q}_{\text{ele}} + Q_{\text{abs}} - Q_{\text{emis}} + Q_{\text{las}},$$

$$\frac{\partial}{\partial t}(\rho e_{\text{rad}}) + \nabla \cdot (\rho e_{\text{rad}} \boldsymbol{v}) + P_{\text{rad}} \nabla \cdot \boldsymbol{v} = \nabla \cdot \boldsymbol{q}_{\text{rad}} - Q_{\text{abs}} + Q_{\text{emis}},$$

- **The third equation above represents the change in the radiation energy density where q_{rad} is the radiation energy flux, Q_{emis} is the radiation energy emission, and Q_{abs} is the absorption of energy**

- **The flux is computed using flux-limited multigroup diffusion with tabulated opacities. This will be discussed in detail tomorrow**

FLASH solves the 3T equations by operator splitting the source terms from the “hydrodynamic” terms. Each source term is advanced by a different code unit...

- Electron thermal conduction (q_{ele}) is advanced in the `Diffuse` unit. It is solved implicitly using the HYPRE parallel linear algebra library
- Laser energy deposition is computed in the `EnergyDeposition` unit
- Radiation emission, absorption, and energy flux is advanced in the `RadTrans` unit. This is also evaluated implicitly using HYPRE
- Ion/electron equilibration is advanced by the `HeatExchange` unit
- The `Eos` unit computes the 3T equation of state
- The remaining terms in the energy equations represent hydrodynamic work and advection of internal energy by the fluid; these effects are included by the `Hydro` unit

FLASH solves the 3T equations by operator splitting the source terms from the “hydrodynamic” terms, we are left with:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0,$$
$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) + \nabla P_{\mathrm{tot}} = 0,$$
$$\frac{\partial}{\partial t}(\rho E_{\mathrm{tot}}) + \nabla \cdot [(\rho E + P_{\mathrm{tot}})\, \boldsymbol{v}] = 0,$$
$$\frac{\partial}{\partial t}(\rho e_{\mathrm{ion}}) + \nabla \cdot (\rho e_{\mathrm{ion}} \boldsymbol{v}) + P_{\mathrm{ion}} \nabla \cdot \boldsymbol{v} = 0,$$
$$\frac{\partial}{\partial t}(\rho e_{\mathrm{ele}}) + \nabla \cdot (\rho e_{\mathrm{ele}} \boldsymbol{v}) + P_{\mathrm{ele}} \nabla \cdot \boldsymbol{v} = 0,$$
$$\frac{\partial}{\partial t}(\rho e_{\mathrm{rad}}) + \nabla \cdot (\rho e_{\mathrm{rad}} \boldsymbol{v}) + P_{\mathrm{rad}} \nabla \cdot \boldsymbol{v} = 0,$$

- **Solving these equations can be difficult for an Eulerian code, the work terms are NOT written as the divergence of a flux**
- **Worse, they include the divergence of velocity, which is discontinuous at a shock**

The electron, ion, radiation, internal energy equations cannot be directly evaluated, a work around is needed...

- In general, there are three hydrodynamic effects which alter the ion, electron, radiation, and total internal energy:
  - Advection
  - Work
  - Shock heating
- The normal 1T hydrodynamics solver updates the total internal energy. The change in internal energy in a given cell must then be divided among the ions, electrons, and radiation field
- For example, the total work done on a cell (or by a cell) is divided among the ions, electrons, and radiation field in proportion to their pressures

One work around involves treating the electrons adiabatically (no shock heating for electrons)

- **To do this, you replace the electron internal energy equation with an advection equation for the electron entropy**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0,$$

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) + \nabla P_{\rm tot} = 0,$$

$$\frac{\partial}{\partial t}(\rho E_{\rm tot}) + \nabla \cdot [(\rho E + P_{\rm tot})\, \boldsymbol{v}] = 0,$$

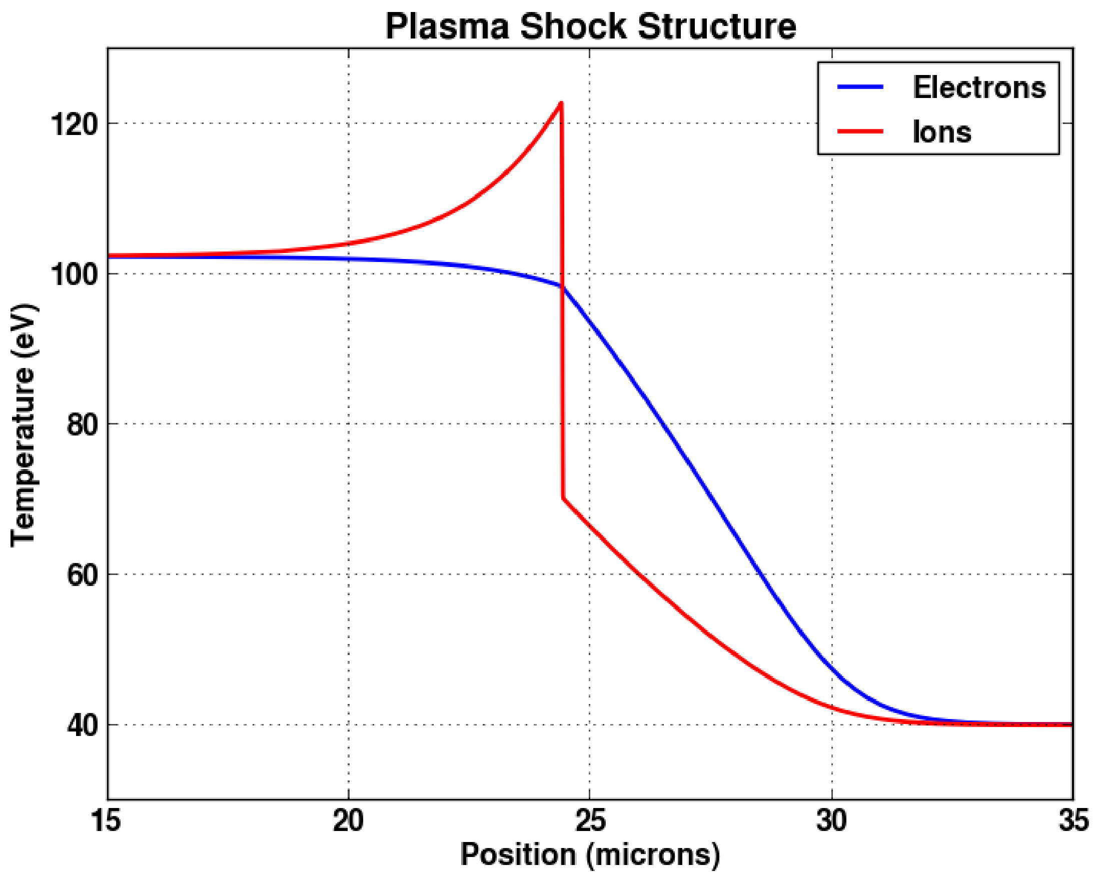
$$\frac{\partial}{\partial t}(\rho s_{\rm ele}) + \nabla \cdot (\rho s_{\rm ele} \boldsymbol{v}) = 0,$$

$$e_{\rm tot} = E_{\rm tot} - \frac{v^2}{2},$$

$$P_{\rm tot}, e_{\rm ion}, T_{\rm ele}, T_{\rm ion}, e_{\rm ele}, ... = {\rm EOS}(\rho, e_{\rm tot}, s_{\rm ele})$$

- **Unfortunately, the electron entropy method currently only works without radiation and for a fixed-ionization gamma-law EOS**
- **But we (Klaus) are working on extending this so that it works generally!**

Structure of a shock in a plasma with electron thermal conduction and no radiation



Helium
ρ = 0.0018 g/cc

Fully Ionized,
Gamma EOS

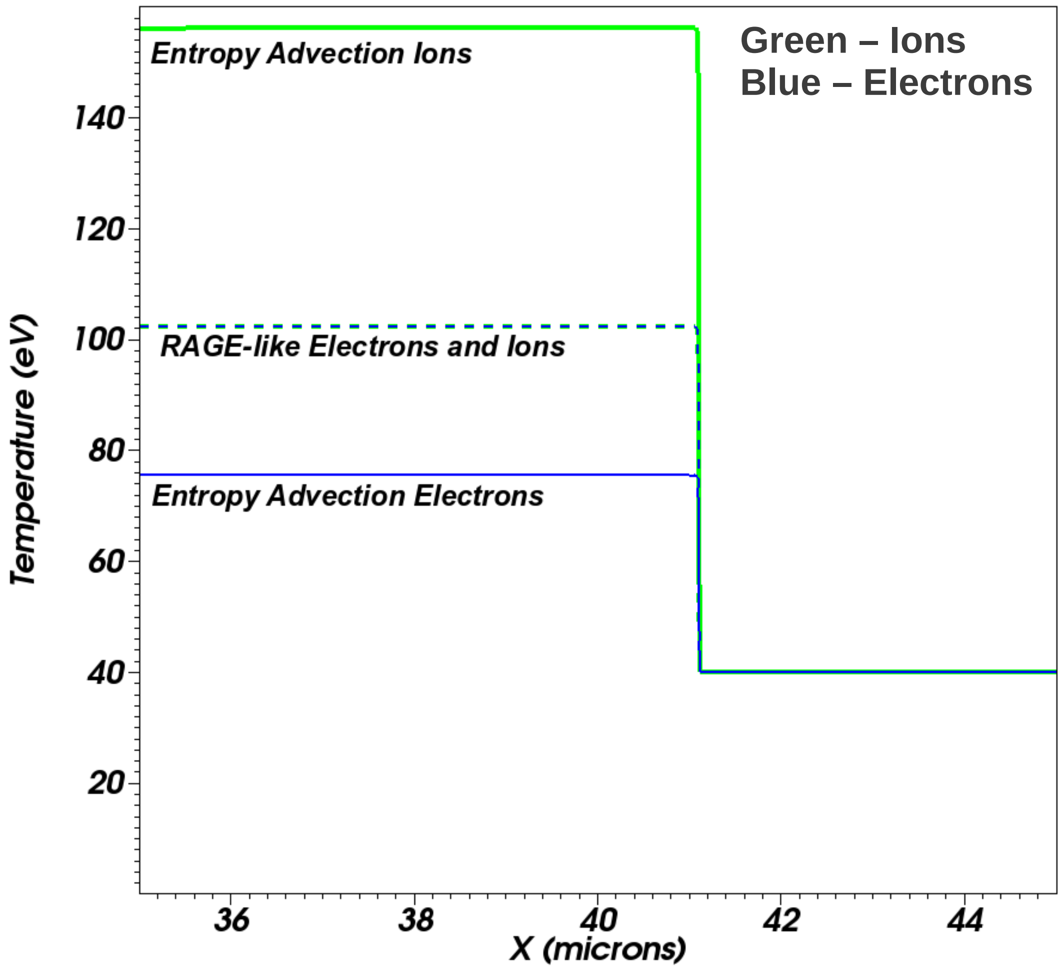
Shock moves from left to right

The “RAGE-like” hydro method is an alternative to entropy-advection, it is less accurate near shocks

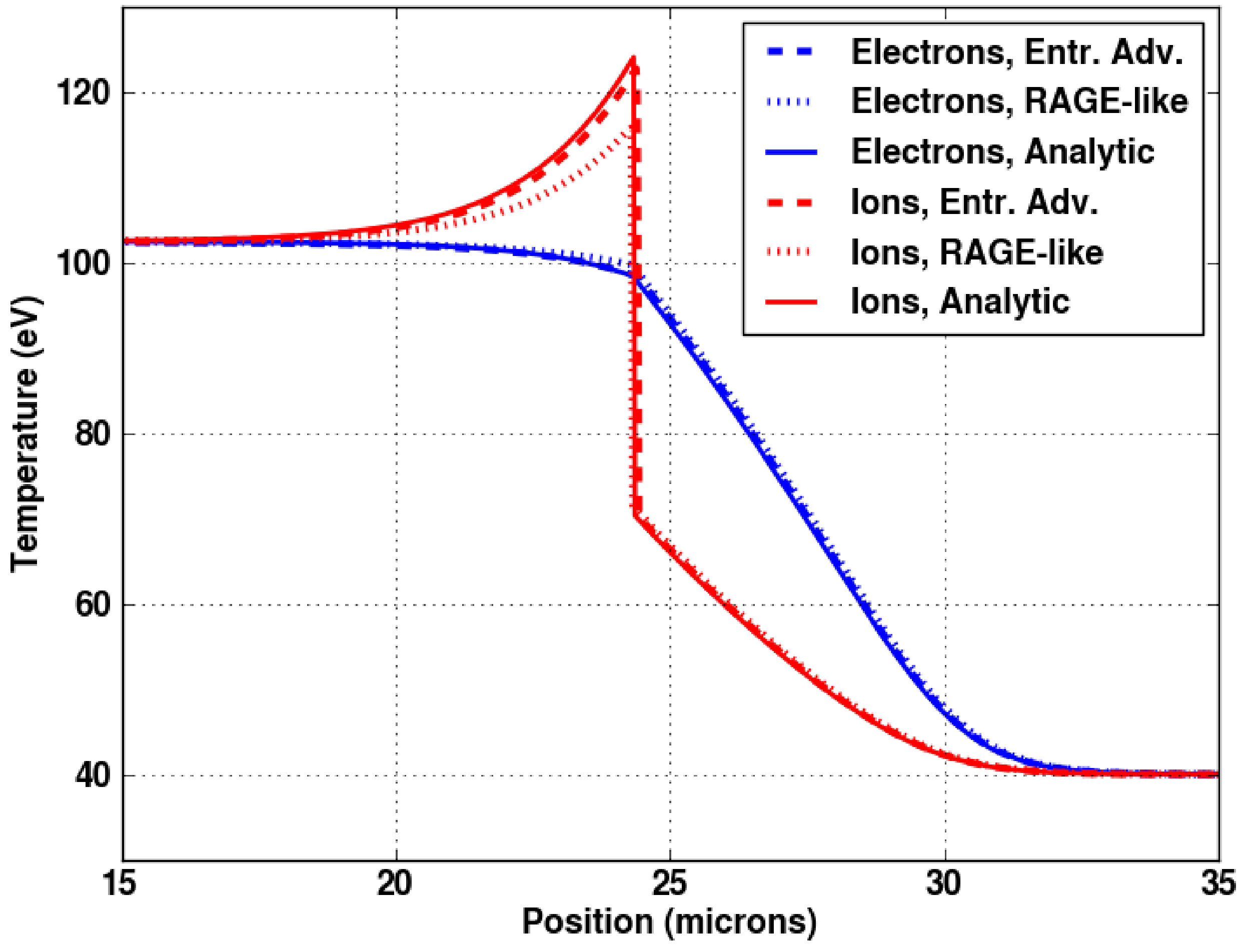
- **The entropy-advection approach treats the electrons adiabatically**
- **An alternative is to divide the shock heating between electrons in exactly the same way as the work – in proportion to the pressure ratios**
  - **This is the “RAGE-like” approach to 3T hydrodynamics in an Eulerian code**
- **In this case, the electrons would be shock heated, but the solution away from shocks should be accurate**
- **This is not necessarily important – in plasmas the ion/electron temperatures equilibrate over time!**
- **RAGE-like hydro is the default method, you can try entropy advection by setting the following parameter in the runtime parameters file (`flash.par`):**

```
hy_eosModeAfter = “dens_ie_sele_gather”
```

There is a large difference between entropy-advection and RAGE-like hydro in the absence of ion/electron equilibration



When Ion/electron equilibration is significant, the difference between RAGE-like hydro and entropy advection is small – even near a shock



FLASH has been extended to support 3T simulations

- 3T should be used for simulations of laser driven HEDP experiments
- A lot of physics relevant to simulating HEDP experiments only works with 3T:
  - Laser
  - Electron thermal conduction
  - Multrigroup radiation diffusion
- 3T hydrodynamics in an Eulerian code is a little tricky because the electrons should be treated adiabatically
- This can affect the electron/ion temperatures near shocks
- We will see some hands on examples and a details on the laser and multigroup diffusion radiation tomorrow!
- For more on 3T simulations, please see user's guide (Ch 13, Sec 25.7.5):

  http://flash.uchicago.edu/site/flashcode/user_support/flash4b_ug/node20.html

  http://flash.uchicago.edu/site/flashcode/user_support/flash4b_ug/node34.html#SECTION08175000000000000000