An Implicit Monte Carlo method based on BDF-2 Time Integration for Simulating Nonlinear Radiative Transfer

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Radiative Transfer Problems

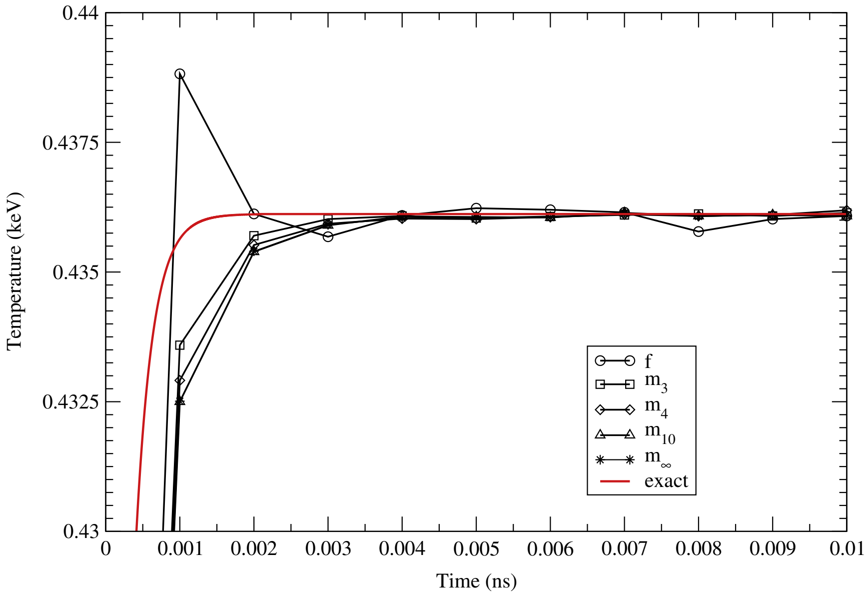
- **Here we're solving transport problems for thermal x-rays**
  - These x-rays behave like particles (or at least we pretend they do).
- **The difference is that when the x-rays are absorbed, they heat up the background material.**
- **The material also emits x-rays (i.e., acts as a source) depending on its temperature.**
  - This is what makes it nonlinear
- **The problems are also typically time dependent.**

Implicit Monte Carlo is not the truth. (shhh, don't tell anyone)

- **Implicit Monte Carlo (IMC) has been around since the 1980's and it can give accurate solutions when run correctly.**
- **Nevertheless, IMC has errors**
  - Even in the limit of an infinite number of particles (phauxtons)
  - Mesh Errors, time discretization errors, linearization errors.
- **Some of the errors are weird**
  - In diffusive media, IMC can give better answers with larger mesh cells and time steps
    - If the number of particles is not increased.
- **Given all this IMC is the method that refuses to die, despite much effort at improvement at LANL, LLNL, AWE, and beyond.**
- **This talk will detail an approach to deal with time and linearization errors.**

What can these errors do?

- The figure on the right shows how IMC behaves in a simple, infinite medium problem.
- In this problem, initially the radiation temperature is 0.5 keV, and the material temperature is 0.4 keV.
- Note how IMC (the "f" line) oscillates around the exact solution.
- The main problem here is that IMC is linearizing about the previous time step's temperature (implying not enough emission).



McClarren and Urbatsch, 2009.

What is going on in IMC

- **IMC takes the emission term in the radiative transfer equations and "linearizes" about a suitably appropriate time averaged value of the emission source.**
  - The time averaging can be switched from semi-implicit to fully explicit using the, implicitness parameter, α
  - $\alpha = 1$ is fully implicit, $\alpha = 0$ is explicit, and $\alpha = ½$ is formally second-order
- **In practice, α=1 is almost always used because it is the most robust.**
  - The lack of robustness for $\alpha = ½$ was pointed out in the original Fleck and Cummings paper.
- **This lack of robustness comes from the fact that IMC linearizes about the previous time step's emission source.**
- **In effect, the material does not know if the emission term will increase or decrease during a time step (thereby over or undershoots can occur).**
- **Moreover, the important quantity is σT^4.**

Linearizing about a different time

- **The idea that we explore in this work is to use the two previous time-steps' temperatures to center the linearization about a mid-time temperature.**
- **We do this based on the BDF-2 method**
  - A time integration method that implicitly computes a second-order update by differently differencing the time derivative operator.
- **This also allows us to evaluate the opacity at a mid-time-step temperature.**
- **Also, this change looks the same as IMC**
  - With a slight change to the Fleck factor,
  - And temperatures evaluated at an average of the previous two time steps.

The BDF-2 Method

- **Consider the differential equation,**

$$\frac{du(t)}{dt} = f(u(t))$$

- **The BDF-2 discretization (for a constant time step) is**

$$\frac{u^{n+1} - \frac{4}{3}u^n + \frac{1}{3}u^{n-1}}{\Delta t} = \frac{2}{3}f(u^{n+1})$$

- **This method is both second-order and L-stable**
  - L-stability meaning that any size of time step is stable and that oscillations are damped in time.
- **This method is not "self-starting" (i.e. for the first time step we can't use BDF-2).**
- **In practice, we will deal with this by taking a standard IMC step to the mid of the first time step, and use that to start the calculation.**

Applying BDF-2 to the IMC equations

- **The gray radiative transfer equations are**

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \Omega \cdot \nabla \psi + \sigma(T)\psi = \frac{\sigma(T)acT^4}{4\pi} + \frac{Q}{4\pi},$$

$$\frac{\partial E_{\mathrm{m}}}{\partial t} = c\sigma(T)(E_{\mathrm{r}} - aT^4),$$

- **With the relations**

$$\frac{\partial E_{\mathrm{m}}}{\partial t} = C_{\mathrm{v}}(T)\frac{\partial T}{\partial t}. \qquad E_{\mathrm{r}}(r,t) = \frac{1}{c}\int_{4\pi} \psi(r,\Omega,t)\, d\Omega.$$

- **Applying the BDF-2 method to the material energy equation gives**

$$\frac{C_{\mathrm{v}}}{\Delta t}\left(T^{n+1} - \frac{4}{3}T^{n} + \frac{1}{3}T^{n-1}\right) = \frac{2c}{3}\sigma\left(T^{n+1}\right)\left(E_{\mathrm{r}}^{n+1} - a(T^{n+1})^4\right).$$

Applying BDF-2 to the IMC equations (cont.)

- **Next, we expand the emission term on the LHS about the n+½ time step to get**

$$\sigma\left(T^{n+1}\right) a(T^{n+1})^4 = \sigma\left(T^{n+1/2}\right) a(T^{n+1/2})^4 + \frac{\Delta t}{2}\frac{\partial}{\partial t}\left[\sigma(T)\, aT^4\right]_{t=t^{n+1/2}}$$

$$= \sigma\left(T^{n+1/2}\right) a(T^{n+1/2})^4 + \left(T^{n+1} - T^{n+1/2}\right)\frac{\partial}{\partial T}\left[\sigma(T)\, aT^4\right]_{T=T^{n+1/2}}$$

- **The temperature derivative is then written as**

$$\frac{\partial}{\partial T}\left[\sigma(T)\, aT^4\right]_{T=T^{n+1/2}} = 4a\sigma(T^{n+1/2})\left(T^{n+1/2}\right)^3 + a(T^{n+1/2})^4 \left.\frac{\partial \sigma}{\partial T}\right|_{T=T^{n+1/2}}$$

- **We then write the mid-step temperature as**

$$T^{n+1/2} = \frac{4}{3}T^n - \frac{1}{3}T^{n-1}$$

Applying BDF-2 to the IMC equations (cont.)

- **Upon substituting this average we get,**

$$\sigma\left(T^{n+1}\right) a(T^{n+1})^4 = \sigma\left(\frac{4}{3}T^n - \frac{1}{3}T^{n-1}\right) a\left(\frac{4}{3}T^n - \frac{1}{3}T^{n-1}\right)^4$$

$$+\left(T^{n+1} - \frac{4}{3}T^n + \frac{1}{3}T^{n-1}\right)\left(4a\sigma\left(\frac{4}{3}T^n - \frac{1}{3}T^{n-1}\right)\left(\frac{4}{3}T^n - \frac{1}{3}T^{n-1}\right)^3 + a\left(\frac{4}{3}T^n - \frac{1}{3}T^{n-1}\right)^4 \left.\frac{\partial\sigma}{\partial T}\right|_{T=T^{n+1/2}}\right)$$

- **Which we can solve for**

$$\left(T^{n+1} - \frac{4}{3}T^n + \frac{1}{3}T^{n-1}\right) = \frac{\sigma\left(T^{n+1}\right) a(T^{n+1})^4 - \sigma\left(T^{n+1/2}\right) a(T^{n+1/2})^4}{4a\sigma\left(T^{n+1/2}\right)\left(T^{n+1/2}\right)^3 + a\left(T^{n+1/2}\right)^4 \left.\frac{\partial\sigma}{\partial T}\right|_{T=T^{n+1/2}}}$$

- **This allows us to solve for**

$$a(T^{n+1})^4 = ma\left(T^{n+1/2}\right)^4 + (1-m)E_{\mathrm{r}}$$

- **Where**

$$m = \frac{1}{1 + \frac{2}{3}\beta c\sigma\left(T^{n+1/2}\right)\Delta t} \qquad \beta = \frac{4a\left(T^{n+1/2}\right)^3}{C_{\mathrm{v}}} + \frac{\left(T^{n+1/2}\right)^4}{C_{\mathrm{v}}}\left.\frac{d}{dT}\log(\sigma)\right|_{T=T^{n+1/2}}$$

Applying BDF-2 to the IMC equations (cont.)

- The final result is then

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \Omega \cdot \nabla \psi + \sigma\left(T^{n+1/2}\right)\psi = \frac{(1-m)c\,\sigma\left(T^{n+1/2}\right)E_{\mathrm{r}}}{4\pi} + \frac{m\,\sigma\left(T^{n+1/2}\right)ac\left(T^{n+1/2}\right)^4}{4\pi} + \frac{Q}{4\pi}$$

$$\frac{\partial E_{\mathrm{m}}}{\partial t} = mc\,\sigma\left(T^{n+1/2}\right)\left(E_{\mathrm{r}} - a\left(T^{n+1/2}\right)^4\right),$$

- Notice that these equations are the same as the standard IMC equations except for the Fleck factor and the fact that we evaluate the opacity and emission terms at the middle of the time step.

- If the time step is changing, then we use

$$T^{n+1/2} = \left(1 + \frac{\rho^2}{3}\right)T^n - \frac{\rho^2}{3}T^{n-1} \qquad\qquad \rho = \frac{\Delta t^n}{\Delta t^{n-1}}.$$

Time Lumping

- **We can modify the definition of *m*, with θ in [$^2/_3$, 1], as**

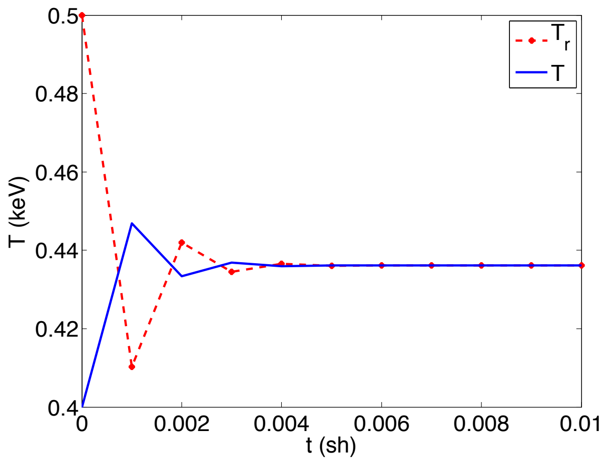
$$m = \frac{1}{1 + \theta\beta c\sigma\left(T^{n+1/2}\right)\Delta t}$$

- **When θ=$^2/_3$, we recover the BDF-2 factor.**
- **In practice we have noticed that setting θ=1 is more robust, though formally this will not be second-order.**
- **We call this effect time lumping, because we sacrifice an order of accuracy for robustness**
  - Similar to techniques used in finite element methods when dealing with spatial stencils.

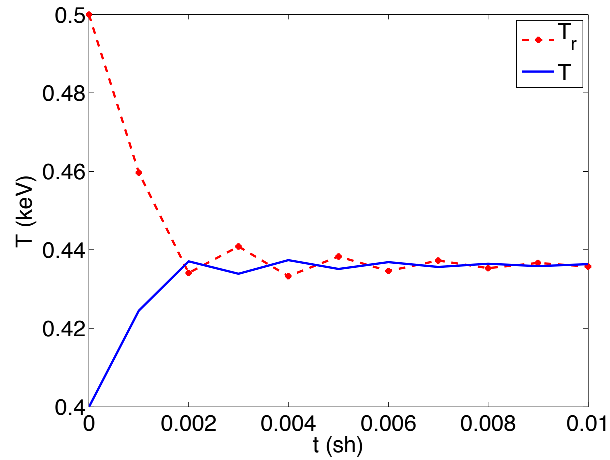
Infinite Medium Tests

- Test problem with $C_{\mathrm{v}} = 0.01\ \mathrm{GJ/cm^3\text{-}keV},\ \sigma(T) = 100\ \mathrm{cm}^{-1}$.
- Initial conditions of T_r = 0.5 keV, and T_m = 0.4 keV.
- This is the same problem solved by Densmore and Larsen (2004) and McClarren and Urbatsch (2009).
- This problem has a constant opacity, so including the opacity derivative has no effect.

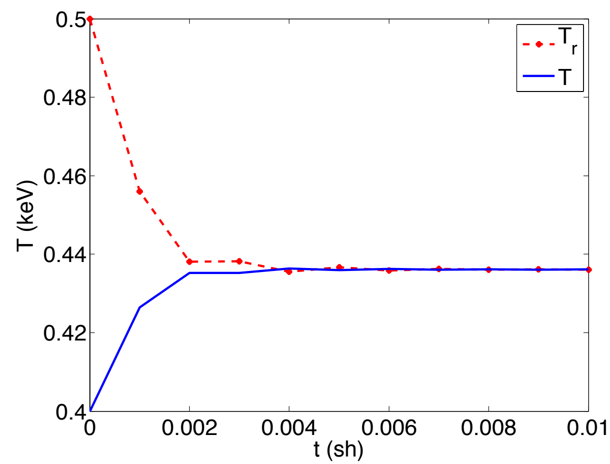
Infinite Medium Tests



(a) IMC



(b) BDF-2, $\theta = \frac{2}{3}$



(c) BDF-2, $\theta = 1$

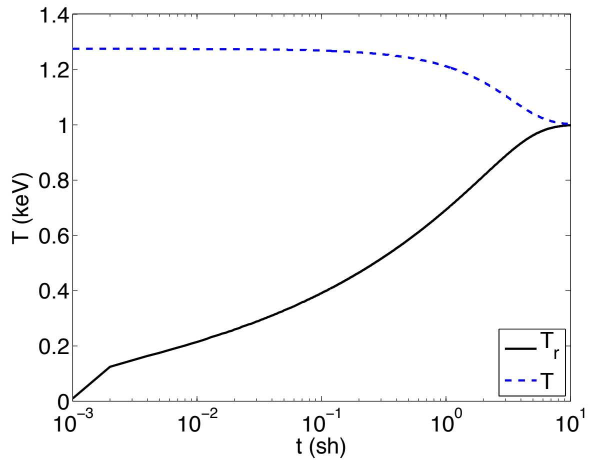
Infinite Medium Test: temperature dependent opacity

- **Problem introduced by Gentile (2011):**

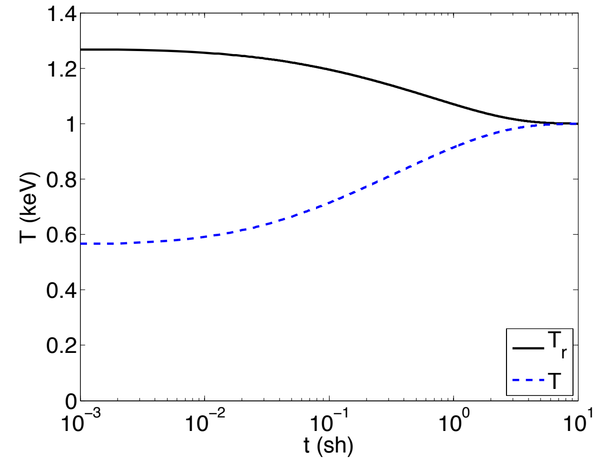
$$C_{\mathrm{v}} = 0.05 \text{ GJ/cm}^3\text{-keV}, \ \sigma(T) = 0.001T^{-5} \text{ cm}^{-1} \text{ with } T \text{ in keV}$$

- **Initially, T_r = 1.465122 keV, T_m = 0.01 keV (chosen so that the equilibrium temperature is 1 keV).**
- **In the standard IMC results, the material and radiation temperatures "flip" in the first time step and *never* revert.**
- **In other words, after the first time step the material is hotter than the radiation until equilibrium is reached**
  - This is clearly incorrect.

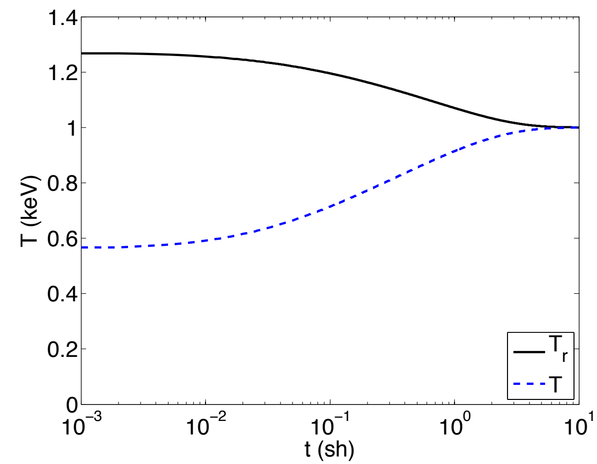
Infinite Medium: temperature dependent opacity



(a) IMC



(b) BDF-2, $\theta = 1$, with derivative of $\sigma(T)$ term in β



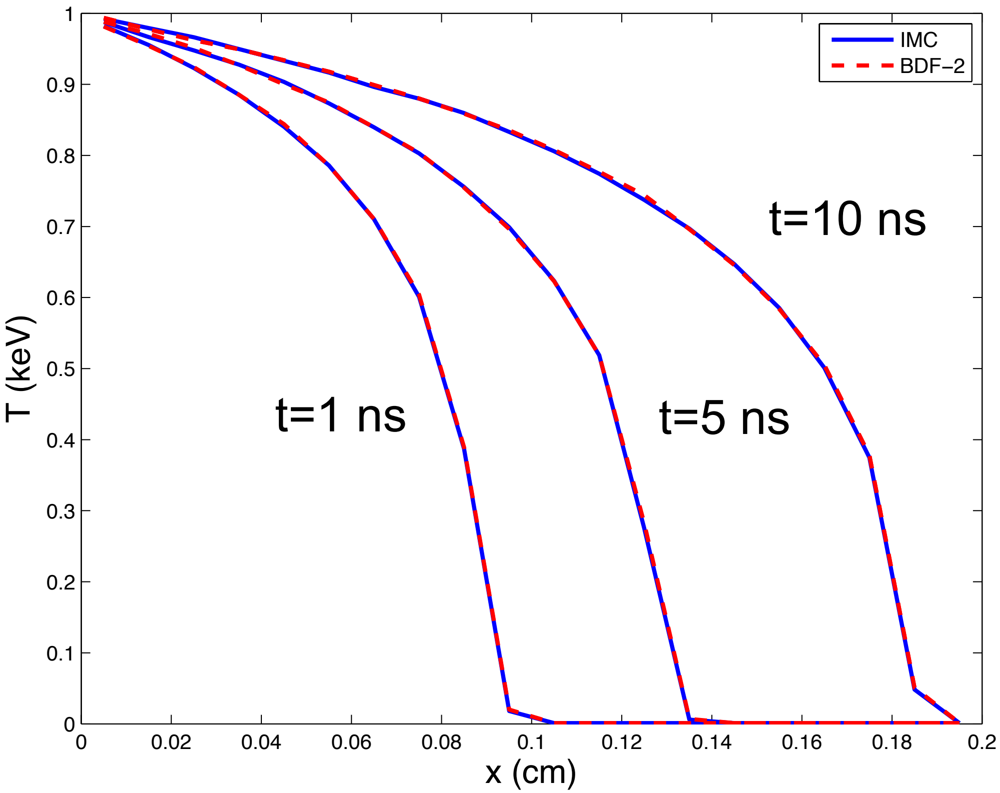
(c) BDF-2, $\theta = 1$, without derivative of $\sigma(T)$ term in β

1-D Marshak Wave Solutions

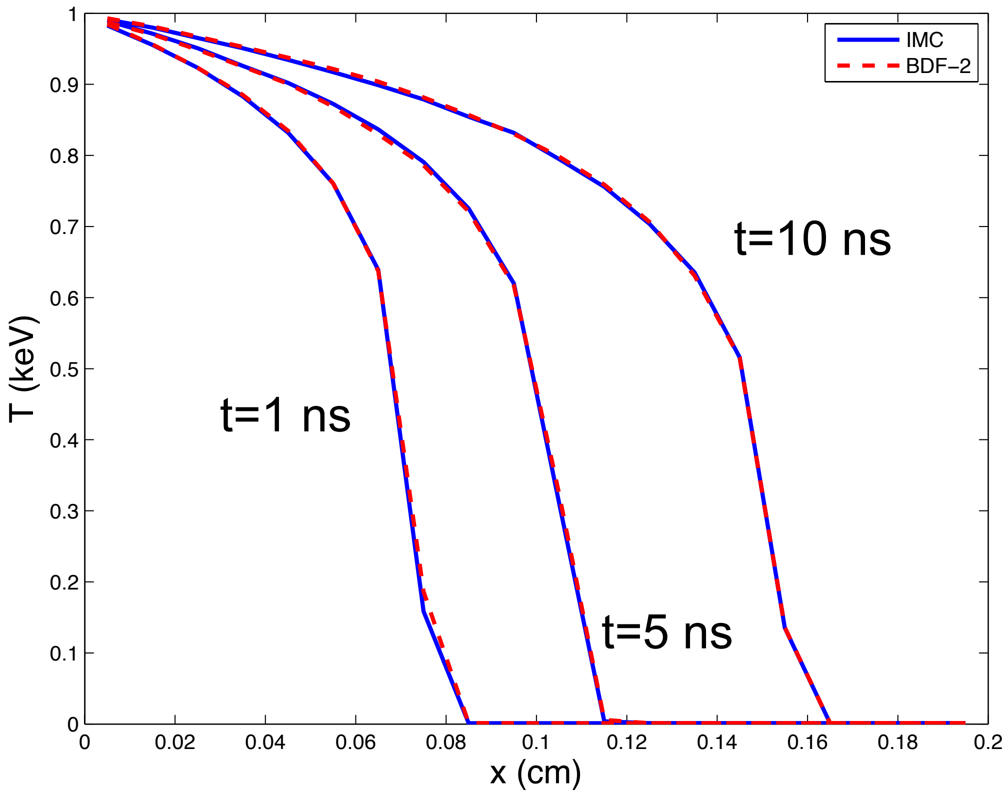
- This standard problem* has an isotropic incident boundary condition at x=0 corresponding to a blackbody at T=1 keV.
- The material has a heat capacity of 0.3 GJ/(keV cm^3), and an opacity of σ = 300/T^3 for T in keV.
- These results were generated by Alex Long in his research IMC code.
- The code limited $T^{n+1/2}$ so that the emission σT^4 would not change by more than 125%.

*See, for instance, McClarren, Evans, et al., JCP, 2008

1-D Marshak Wave Solutions ($\Delta t = 10^{-4}$ ns)

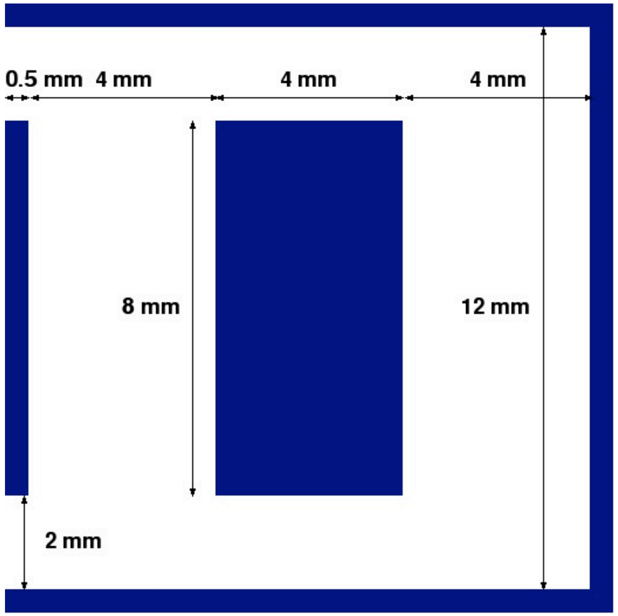


1-D Marshak Wave Solutions ($\Delta t = 5 \times 10^{-4}$ ns)

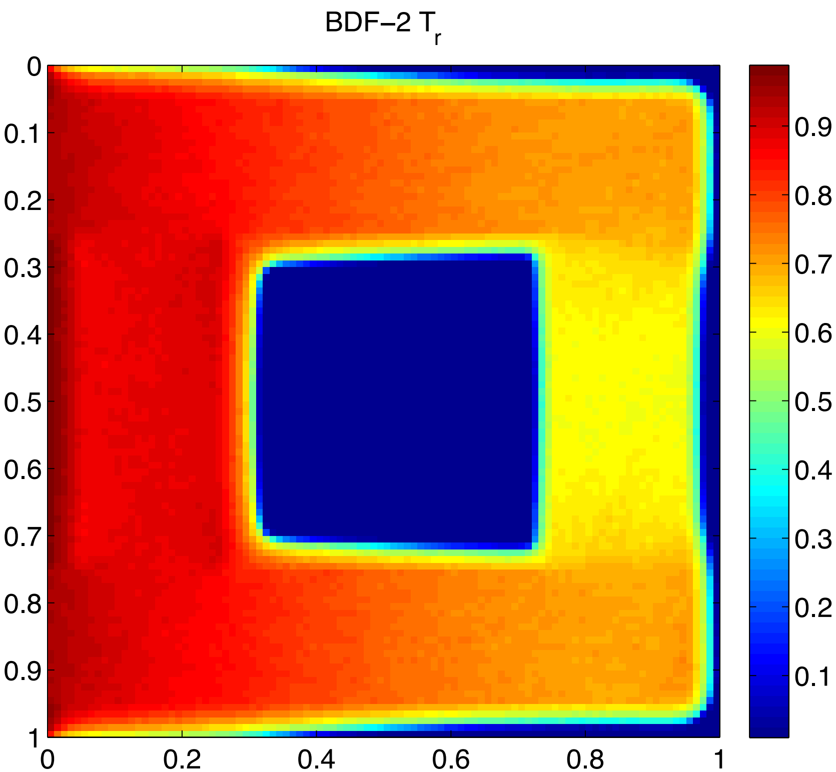


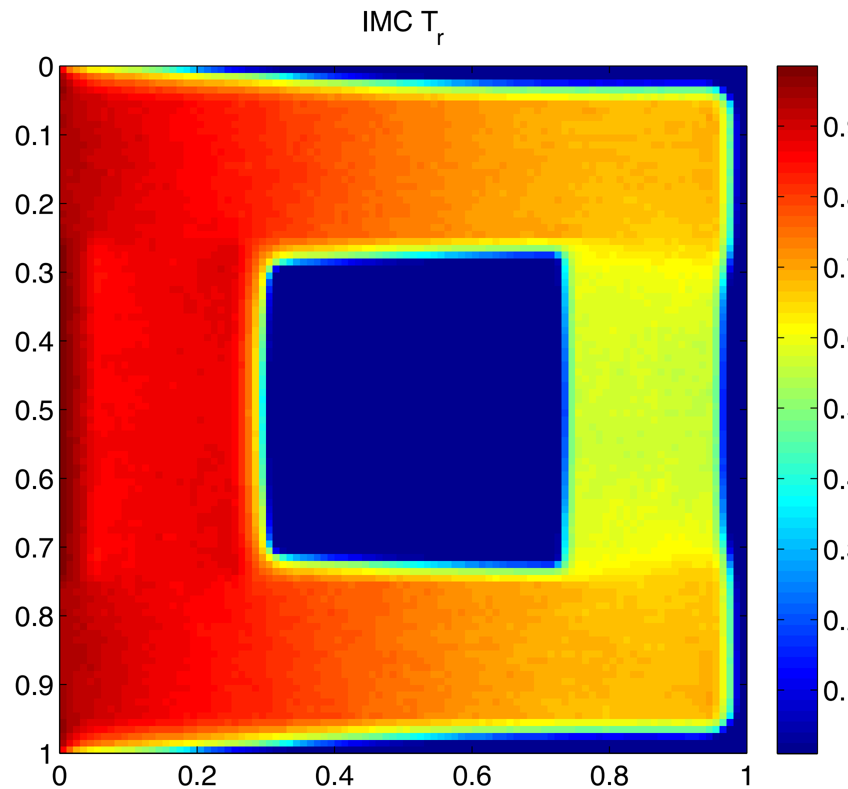
2-D Results: Cartesian Holhraum Problem

- A modification of a problem originally designed by Brunner.
- This is an xy Cartesian problem (i.e., infinite in and out of the page).
- There is a 1 keV source on the left side of the problem.
- The blue areas have $\sigma = 300/T^3$
- The white areas are vacuum.

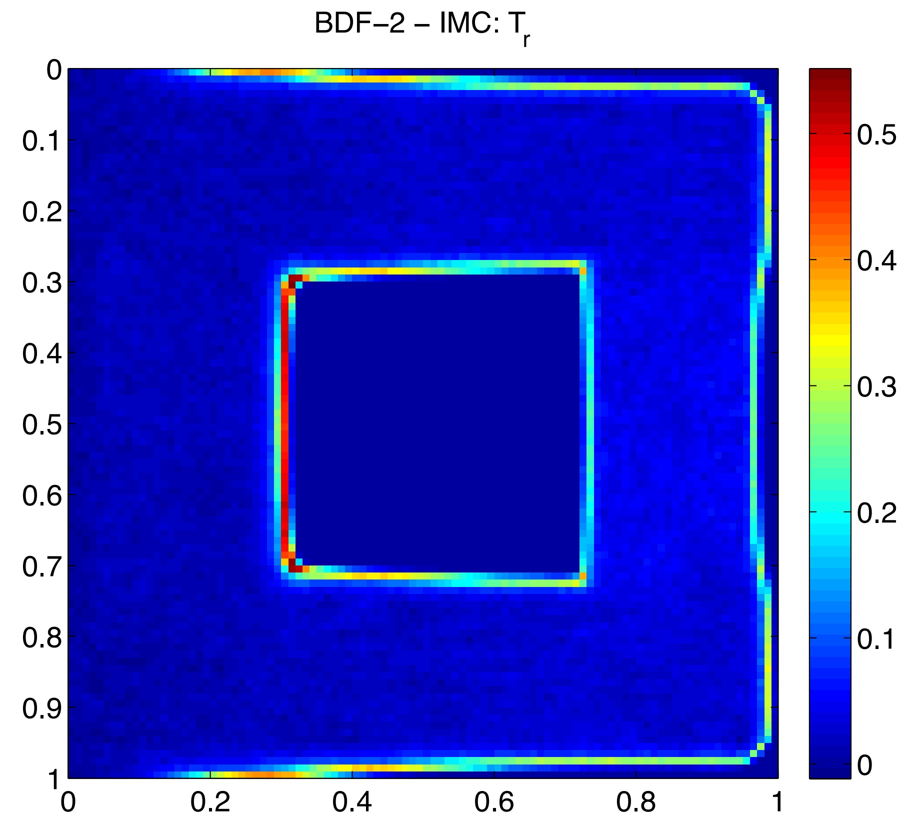


2-D Results at 1 ns

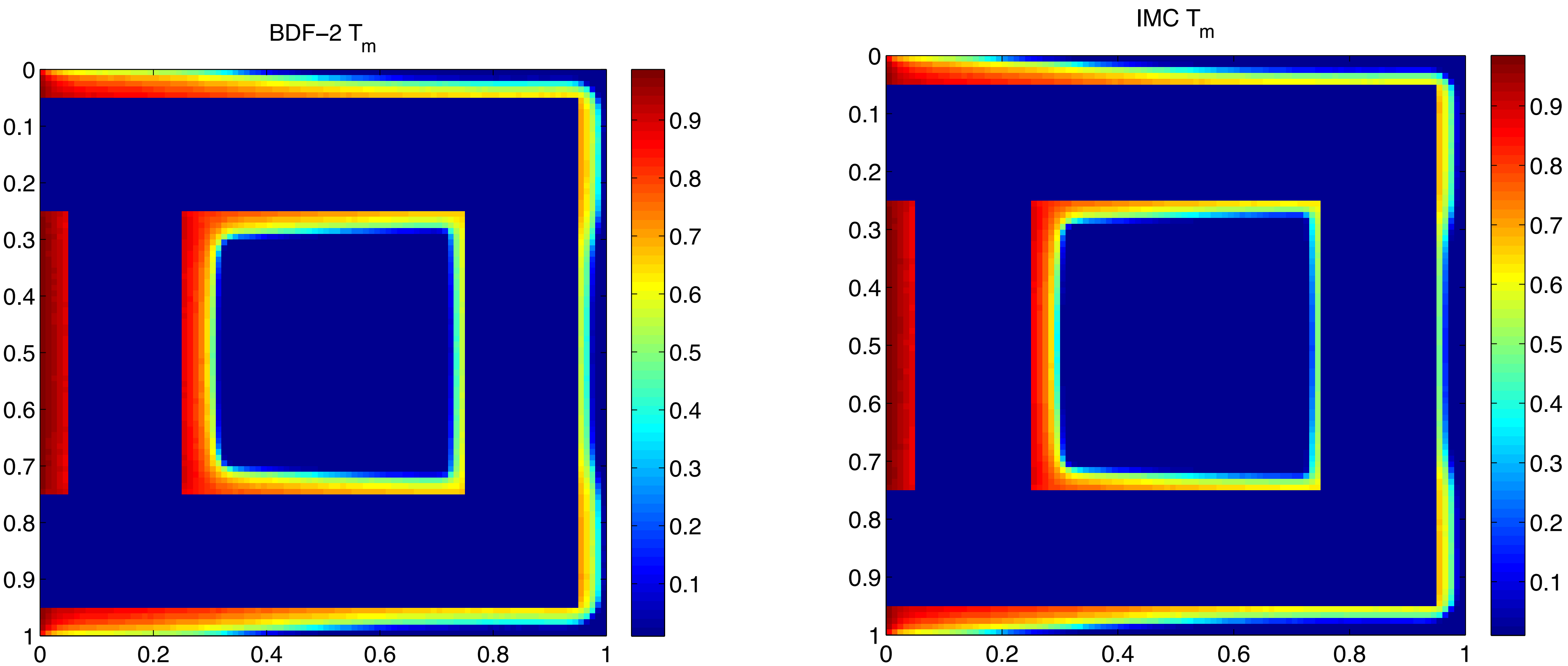




Difference between BDF-2 and IMC



Material Temperature at 1 ns



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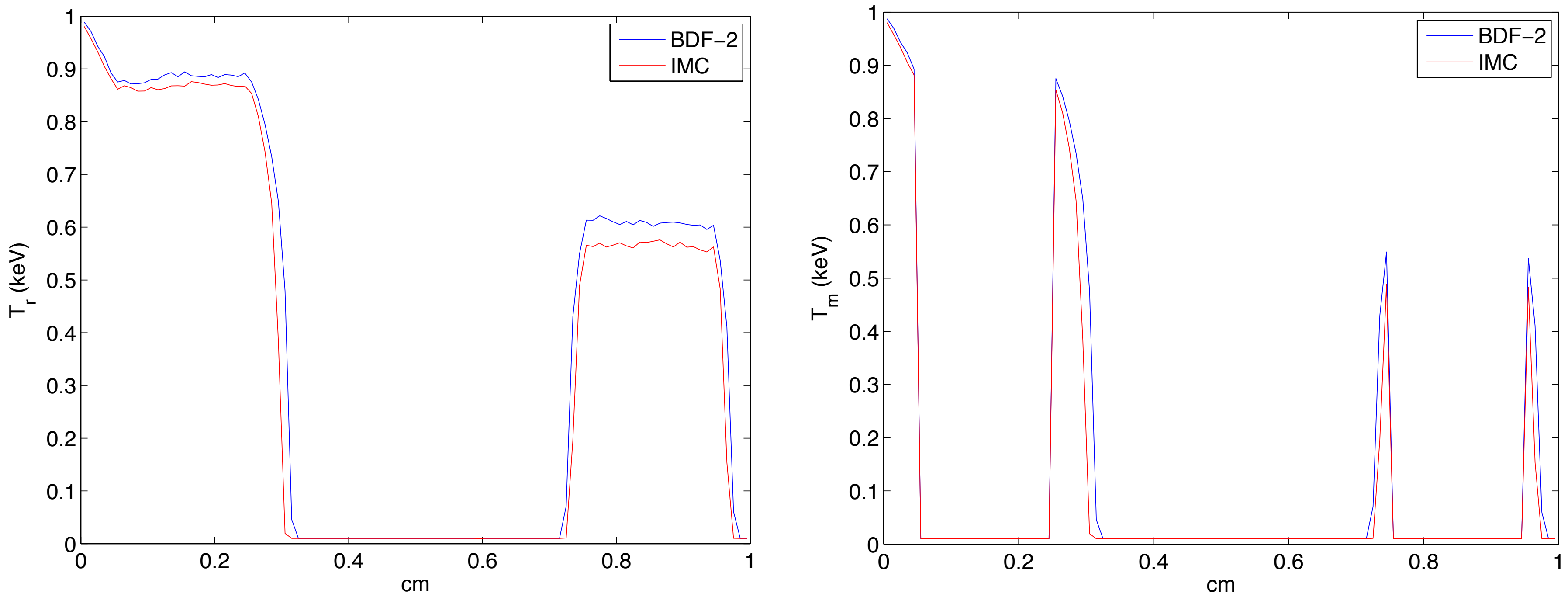
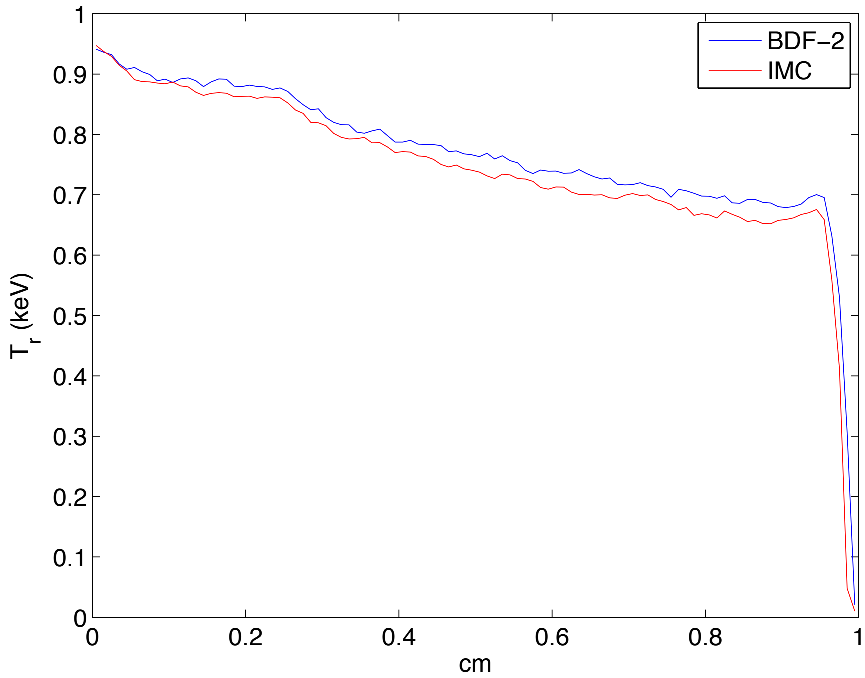
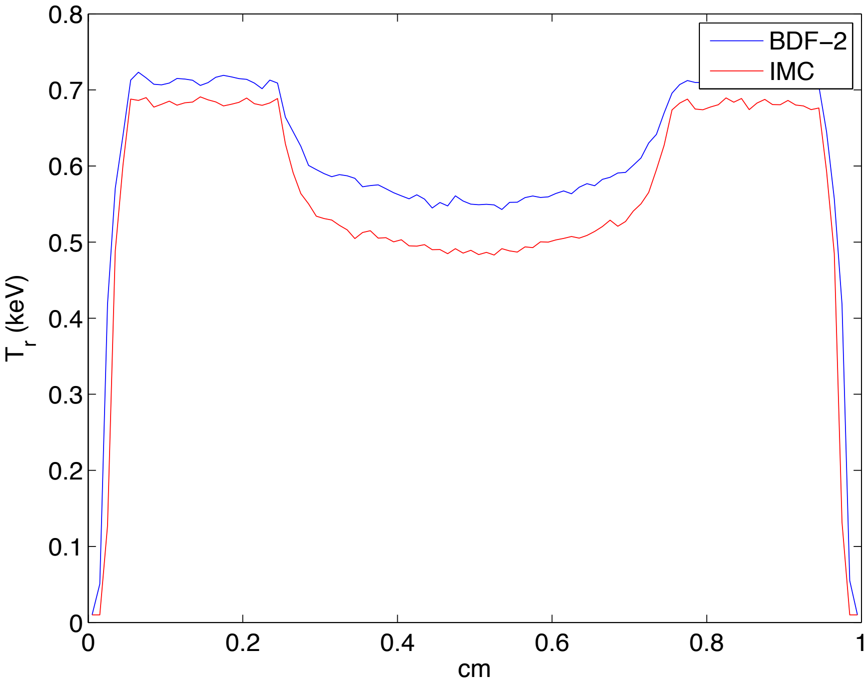
Midline Temperature at 1 ns



T_r in the bottom duct (left) and behind block (right) at 1 ns





Conclusions

- **We've developed a framework for consistently including extrapolation in temperature to the IMC method.**
- **On several problems the methods shows a significant improvement**
  - On others really no difference.
- **In a 2-D problem the BDF-2 results resulted in higher temperatures compared with standard IMC.**
- **In the future we will apply our method to radiation hydrodynamics problems to investigate the effects of temperature extrapolation.**