A Temperature-Extrapolation Method For Implicit Monte Carlo Radiation-Hydrodynamics Calculations

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Radiative Transfer Problems

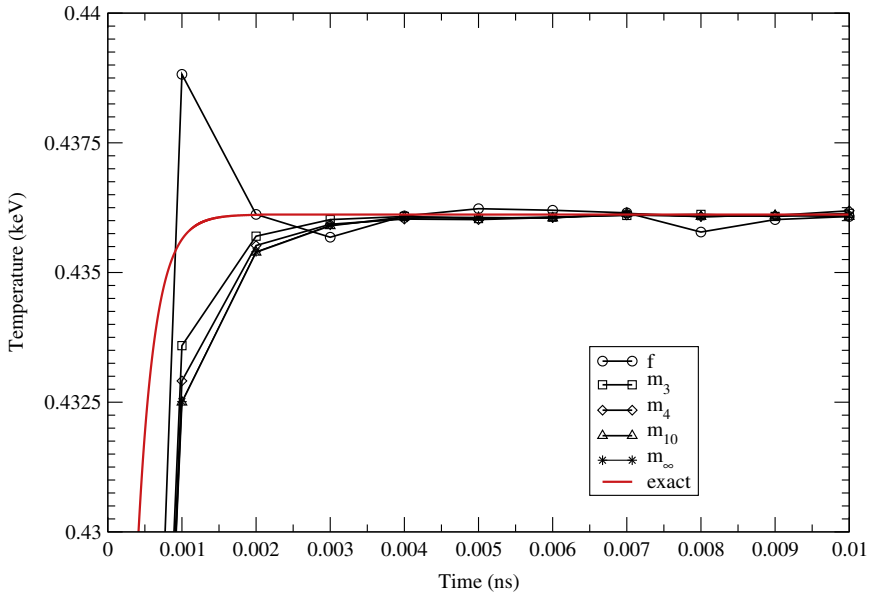
- **Here we're solving transport problems for thermal x-rays as part of a radiation hydrodynamics simulation.**
  - These x-rays behave like particles (or at least we pretend they do).
- **The difference is that when the x-rays are absorbed, they heat up the background material.**
- **The material also 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.**
- **This work is an extension of work presented at the ANS winter meeting last year.**

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

- **Implicit Monte Carlo (IMC) has been around since the 1970'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
  - α = 1 is fully implicit, α = 0 is explicit, and α = ½ is formally second-order
- **In practice, α=1 is almost always used because it is the most robust.**
  - The lack of robustness for α = 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 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,**

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

- **Which we can solve for**

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

- **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**

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

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**

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

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

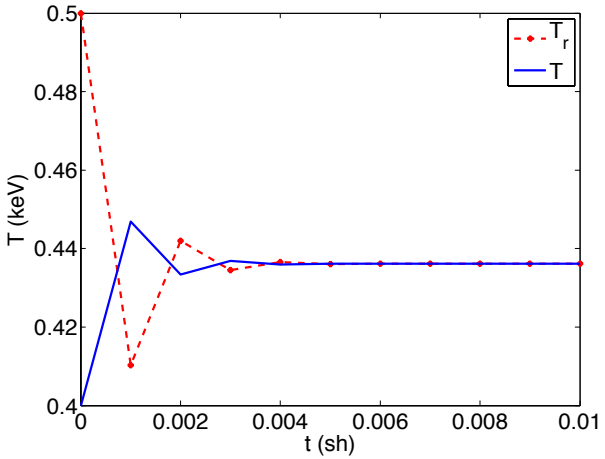
- **Test problem with**

$$C_{\mathrm{v}} = 0.01 \text{ GJ/cm}^3\text{-keV}, \ \sigma(T) = 100 \text{ cm}^{-1}$$

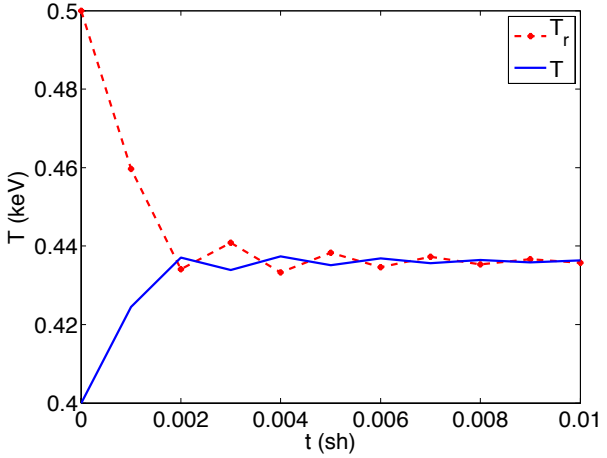
- **Initial conditions of T_r = 0.5 keV, and T_m = 0.4 keV.**
- **This is the same problem solved by Densmore and Larsen (2004) and McClarren and Urbatsch (2009).**
- **This problem has a constant opacity, so including the opacity derivative has no effect.**

Infinite Medium Tests, temperature vs. time

IMC

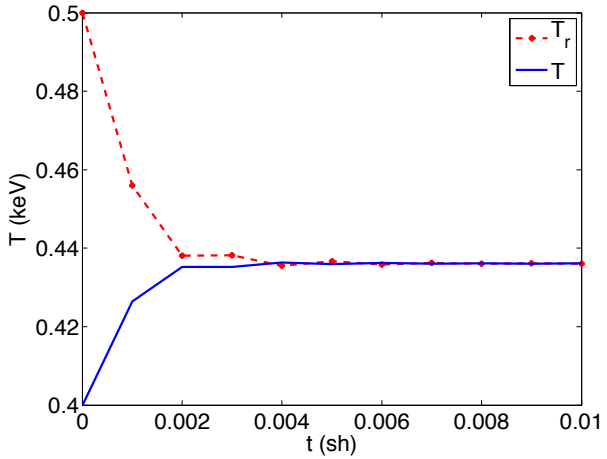


(a) IMC



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

BDF-2
Θ=2/3



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

BDF-2
Θ=1

Infinite Medium Test: temperature dependent opacity

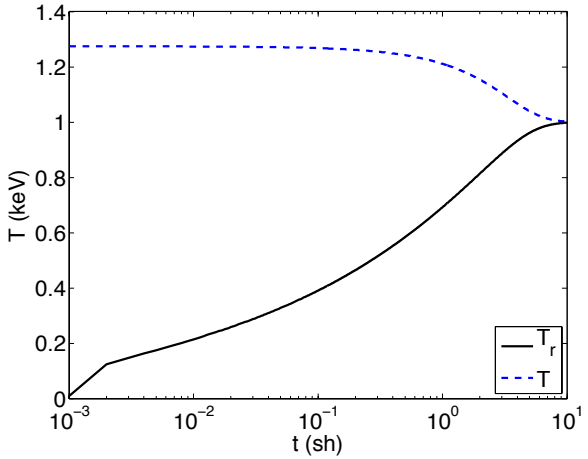
- **Problem introduced by Gentile (2011):**

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

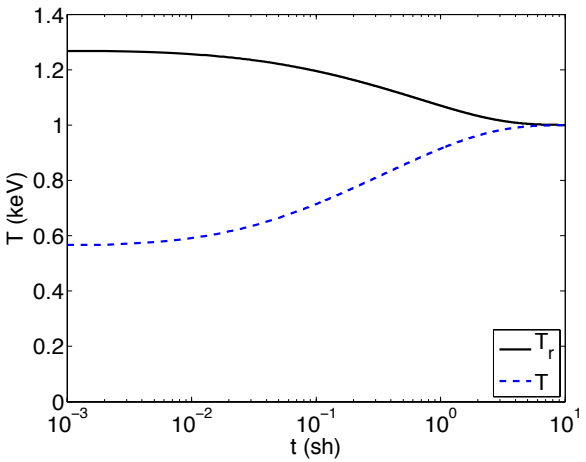
- **Initially,**
  - Radiation T_r = 1.465122 keV,
  - Material T_m = 0.01 keV
  - (chosen so that the equilibrium temperature is 1 keV).

Infinite Medium: temperature-dependent opacity

IMC



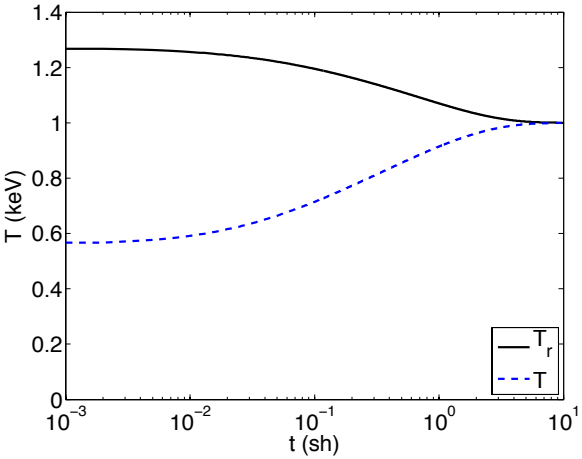
(a) IMC



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

BDF-2
Θ=1
w/deriv

- **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.



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

BDF-2
Θ=1
No deriv

Implementation in Cassio

- **We implemented a prototype of the BDF-2-based extrapolation method in the Cassio code to test it on an ICF problem.**
- **The Cassio code is an Inertial Confinement Fusion (ICF) code in Los Alamos National Laboratory's Eulerian Applications Project.**
- **The code uses a Godunov hydrodynamics scheme in an Eulerian frame on a unit-aspect ratio adaptive-mesh-refinement (AMR) mesh.**
- **Cassio can simulate thermal radiation transport with a diffusion approximation, IMC, or, nearly in production, Sn.**
  - The IMC is the Wedgehog Implicit Monte Carlo package, based on the Fleck and Cummings method, from the LANL's Jayenne Project.

Implementation in Cassio

- Cassio uses an operator split approach where the hydrodynamics solve comes before the radiation solve within each timestep.
- After the hydrodynamics solve, the temperature that is sent to the radiation package was considered to be the beginning-of-timestep temperature that we saved for the next cycle and that we used to extrapolate into the current timestep.
- The old temperature vector needed to be remapped to the newly refined/coarsened AMR mesh at the end of each timestep after the radiation solve.

Peculiarities with the implementation

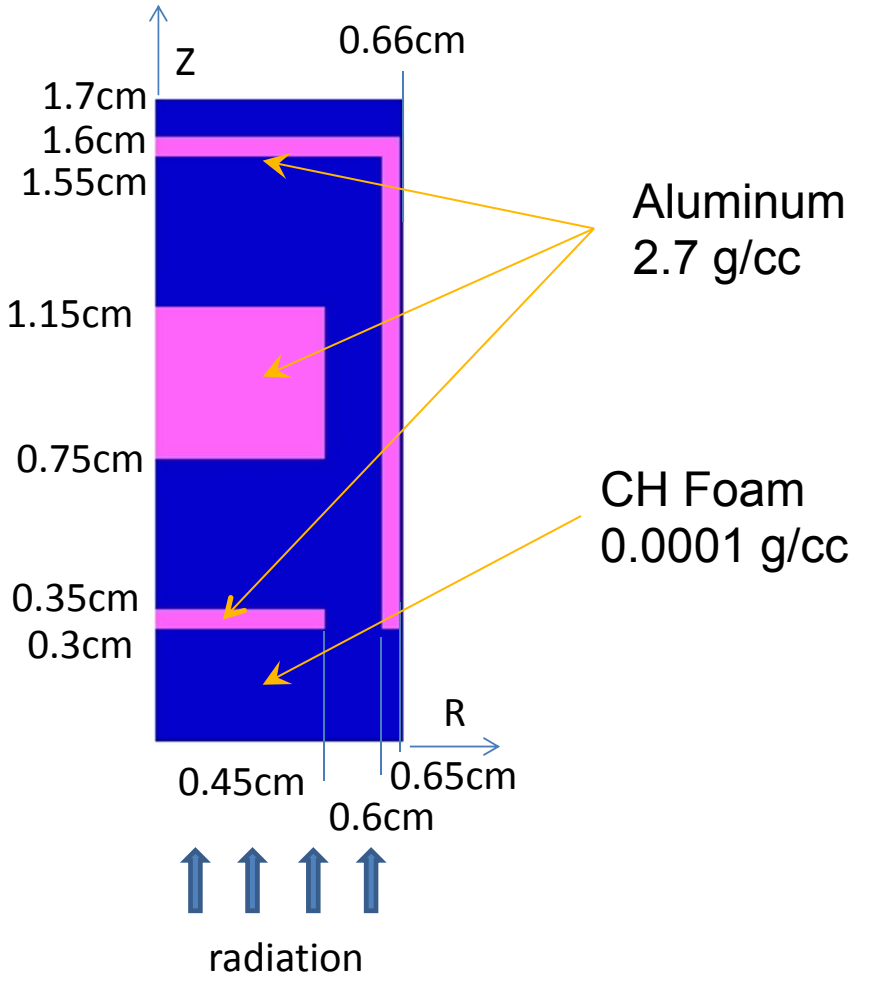
- We used regular IMC for the first cycle.
- The emission and opacity were evaluated at the extrapolated temperature, but the heat capacity was not.
- No opacity derivatives were considered.
- We used time lumping, setting the implicitness to 1.0
- The extrapolated temperature was optionally limited to some fraction of the beginning-of-time step temperature. Considerations were 20%, 100%, and no ceiling along with a cold floor to avoid negativities.
- The old temperature vector was not advected with the hydrodynamics step.

Timestep Control

- The timestep control in Cassio considers many different constraints and selects the minimum value.
- One timestep control is some fraction of the Courant timestep limit for the hydro.
- Thus, a refined mesh anywhere in the problem reduces the timestep.
- The implication is that this BDF-2-based extrapolation will become relatively less necessary and effective as a given mesh is refined.
- If there were no detriment to the hydrodynamics, loosening the cell-size-based timestep controls could result in the BDF-2-based extrapolation showing more benefit, but then any errors from not advecting the old temperature vector could become larger.

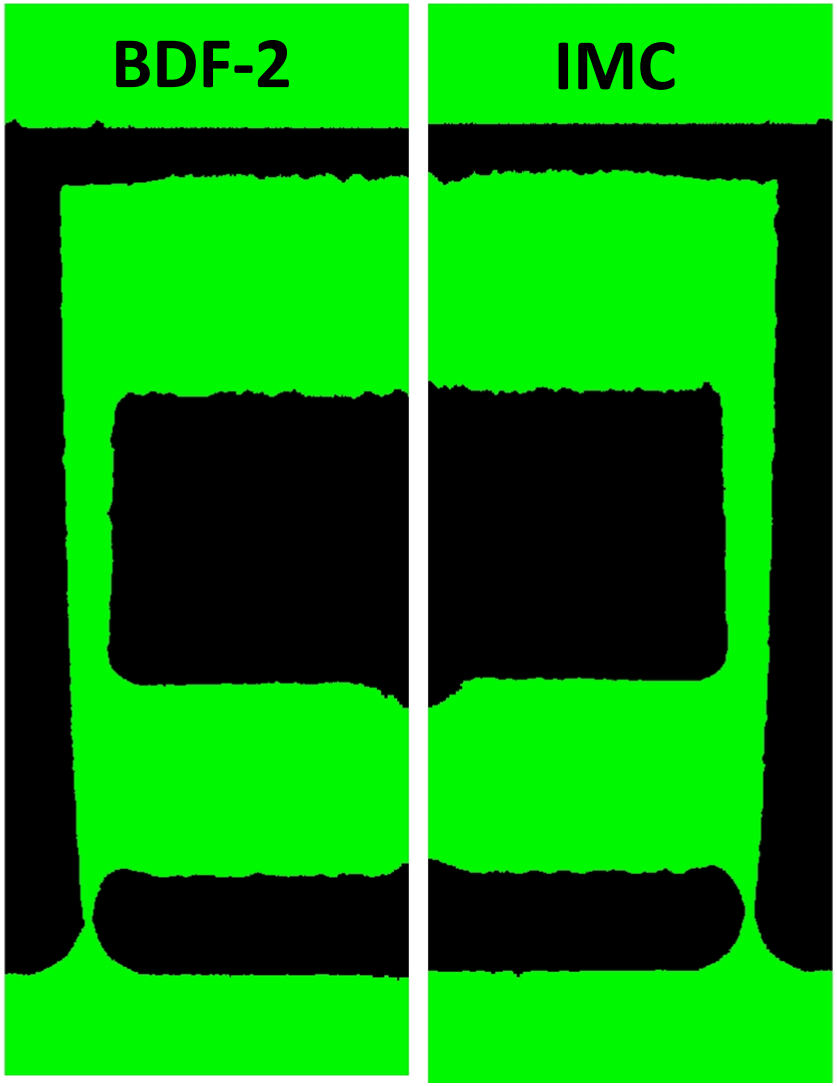
Holhraum Problem

- **This problem has radiation striking a hohlraum with an annular opening.**
- **The radiation is a blackbody source at 400 eV.**
- **We used 102 logarithmically spaced energy groups.**
- **Ramping linearly in time from 1e5 particles to 1e6 particles over about a nanosecond, a [Router/r]^2 source bias model was applied over each cell in the entire problem.**

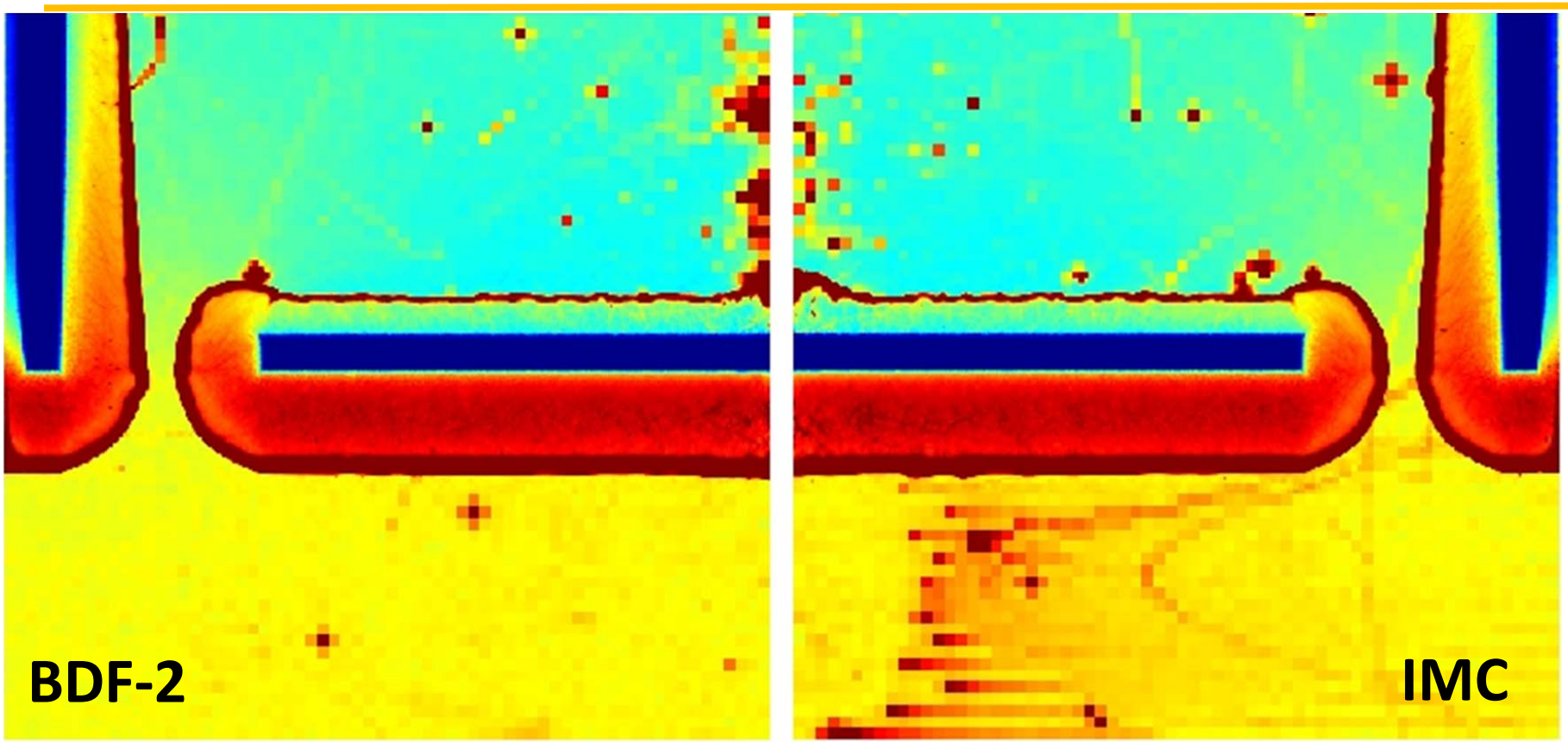


Material Locations @ 1ns

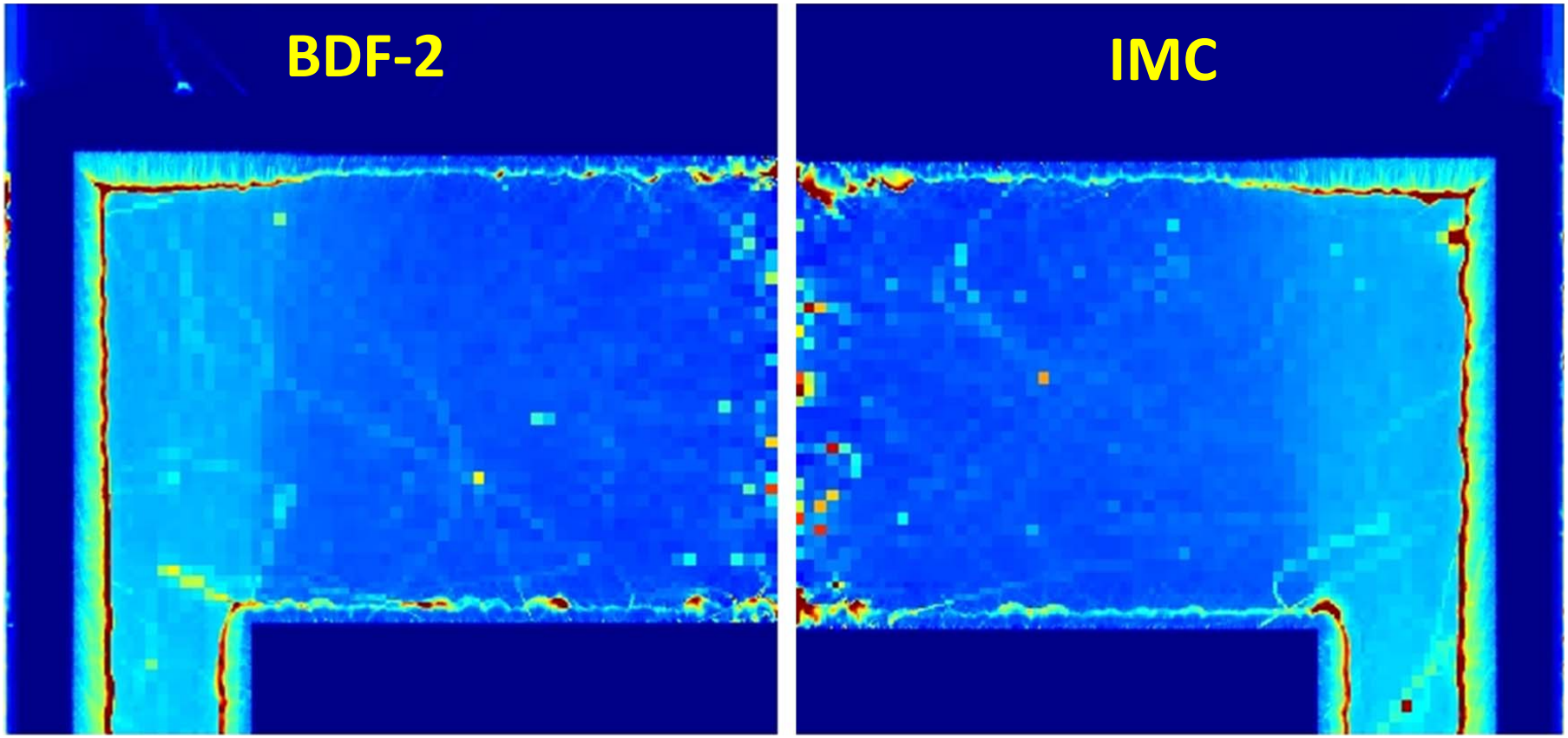
- Aluminum is black
- CH Foam is green
- The BDF-2 solution appears to be slightly smoother along the interface.



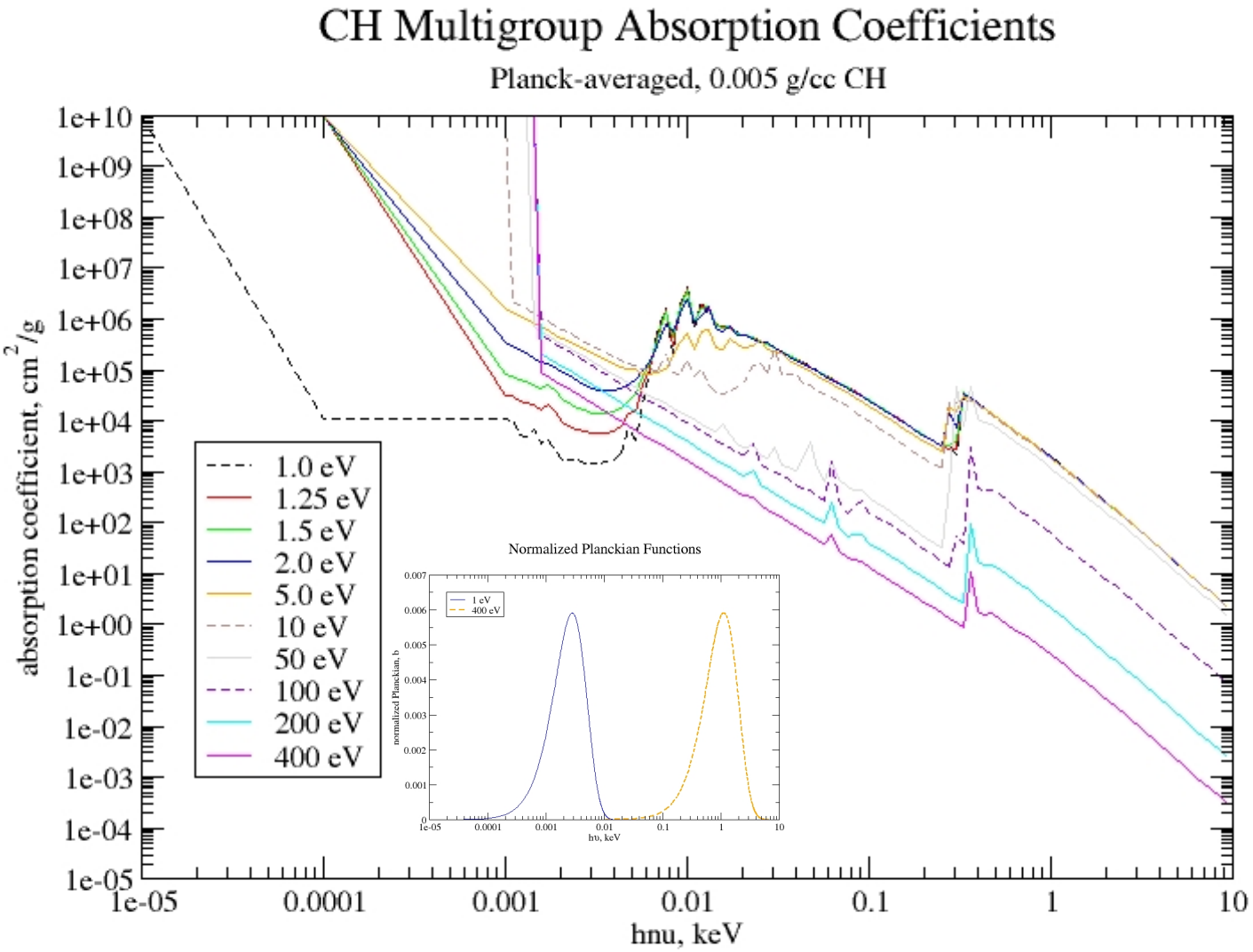
At 1ns, the BDF-2-based extrapolation appears to have less overheating in the CH.



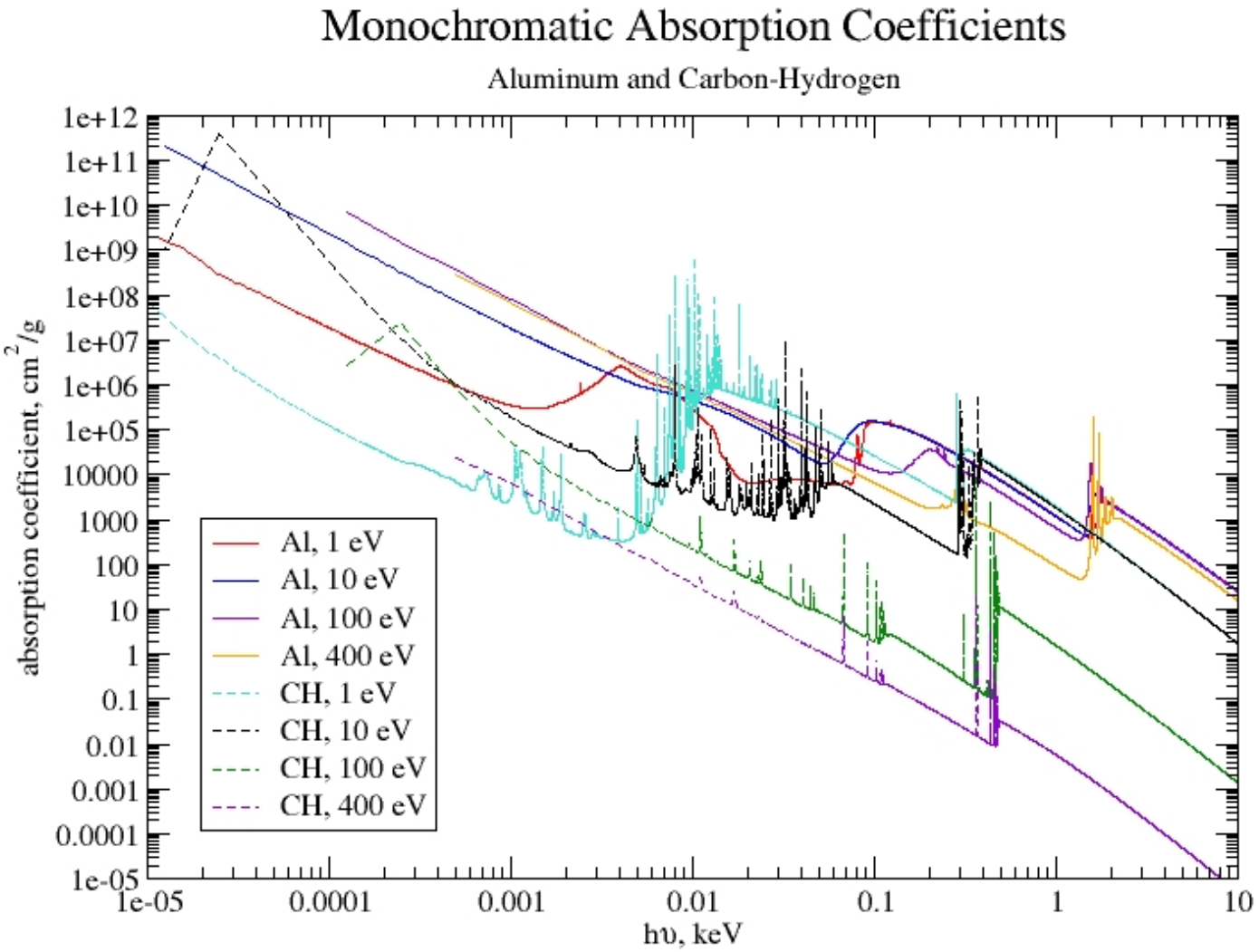
The solution behind the target @ 1ns shows the BDF-2-based extrapolation to be smoother.



Looking at the multigroup CH absorption coefficient, we see different dependencies on temperature.



We see that certain parts of the opacity spectrum have a stronger temperature dependence, where the extrapolation could help.

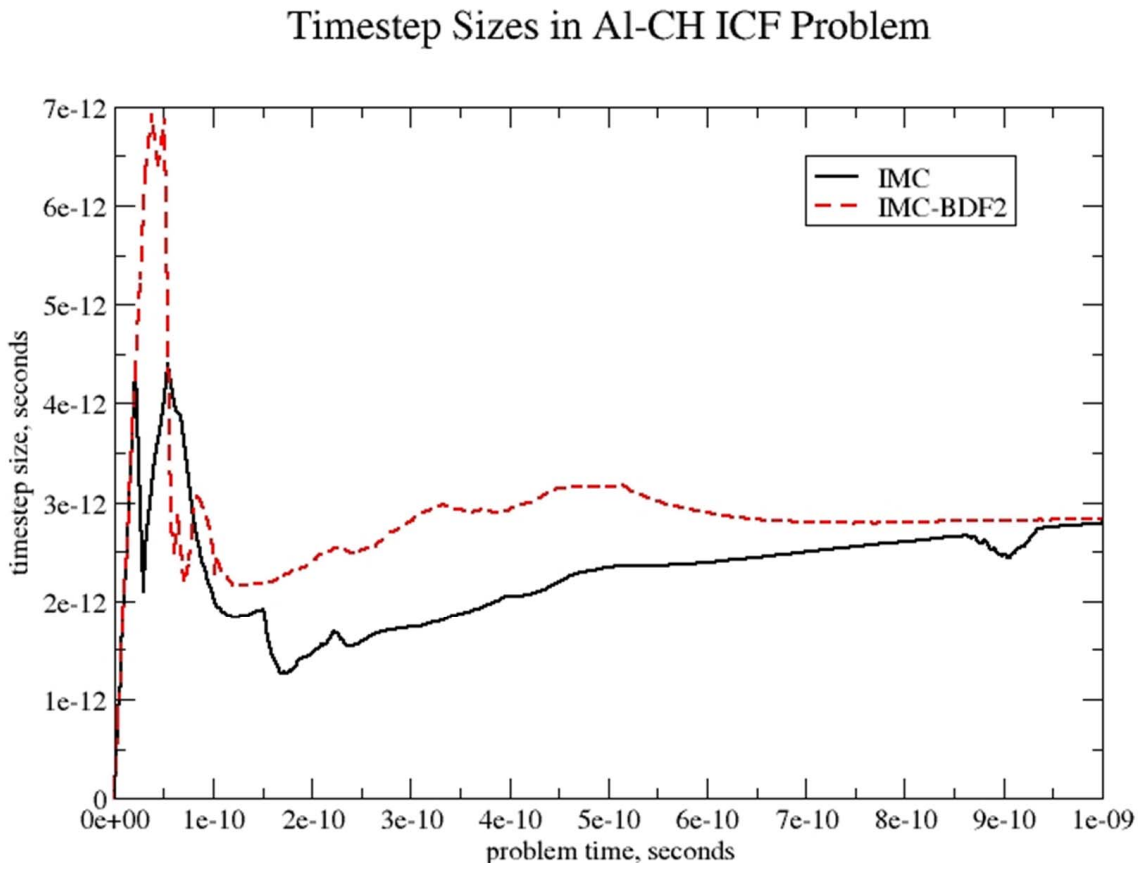


BDF-2-based extrapolation allowed larger timesteps for a large portion of the runtime

To reach 1 ns:

- **IMC:**
  - 495 cycles, 26 min
- **BDF-2:**
  - 396 cycles, 22 min

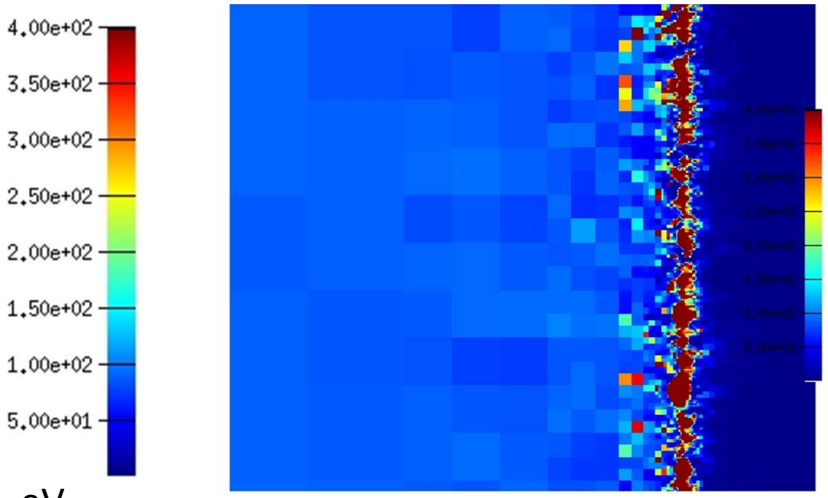
Run on 32 processors of LANL's Tri-Lab Computing Cluster, Moonlight, an Opteron+GPGPU architecture from Appro



1-D Hohlraum problem (in 3-D)

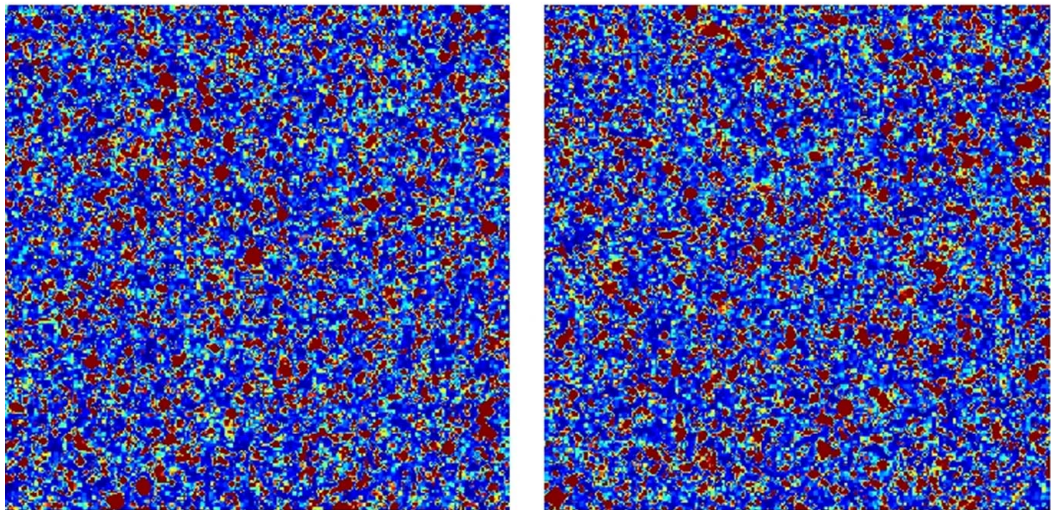
- **We next define a subset of the hohlraum problem, a 1D slab problem of 400-eV Planckian radiation**
- **Traveling through 0.1cm of CH at density 1.0e-3 g/cc and impinging on a 0.02cm-thick aluminum wall.**
- **With a zeroth-level mesh of 0.01cm cubed, we looked at 4, 6, and 8 levels of refinement at the material interface,**
  - This translates to cell widths of 0.00125 cm, 0.0003125 cm, and 0.000078125 cm, respectively.

Whereas the various refinement levels significantly affected the behavior of the simulation, the BDF-2 prototype appeared to have less impact on the solution except that it may be displaying less clumping of hot spots.



Tmat, eV

BDF-2-based extrapolation



IMC

Conclusions

- We have implemented a temperature extrapolation in LANL's Cassio code which calls the Jayenne Project's Wedgehog IMC package.
- The extrapolation is based on a backward difference formulation of order 2 (BDF-2) time-integration method.
- The extrapolation shows some improvement in the radiation-hydrodynamics code Cassio.
- The prototype may benefit from advecting the old temperature each timestep.

Abstract

We have implemented a temperature extrapolation in LANL's Cassio IMC code. The extrapolation is based on a backward difference formulation of order 2 (BDF-2) time-integration method. The extrapolation shows marked improvement in radiation-only test problems and some improvement in the radiation-hydrodynamics code Cassio. We show Cassio results for an Aluminum/Carbon-Hydrogen hohlraum problem whose geometry is based on an existing test problem (but has real materials). We suggest further enhancements that may be necessary to improve this particular implementation.