Numerical simulation of nuclear flame microphysics in type Ia supernovae

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Introduction

- Observation suggests that type Ia supernovae are not pure detonations
- Early stages are low speed nuclear flames (slow relative to local sound speed)
- Late time dynamic behavior requires dramatic acceleration from nuclear flame

$\Rightarrow$ Simulate detailed microphysics of type Ia Supernovae to study potential mechanisms for acceleration

Outline

- Low-Mach number formulation
- Current numerical methodology
- Operator splitting
- Alternative: Deferred corrections algorithm
- Convergence results
- Flame results
- Summary and Future Work

Supernova Modeling

Compressible Navier-Stokes equations:

Conservation of mass

$$\rho_t + \nabla \cdot \rho u = 0$$

Conservation of species abundance

$$(\rho X_k)_t + \nabla \cdot \rho u X_k = \rho \dot{\omega}_k$$

Conservation of momentum

$$(\rho u)_t + \nabla \cdot (\rho u u + p) = \rho \vec{g}$$

Conservation of energy

$$(\rho E)_t + \nabla \cdot (\rho u E + u p) = \nabla \cdot \kappa \nabla T - \rho Q(\dot{\omega}_k)$$

Equation of State

Timmes equation of state provides:

$$e(\rho, T, X_k) = e_{ele} + e_{rad} + e_{ion} \qquad p(\rho, T, X_k) = p_{ele} + p_{rad} + p_{ion}$$

$$e_{ele} = \text{fermi} \qquad p_{ele} = \text{fermi}$$
$$e_{rad} = aT^4/\rho \qquad p_{rad} = aT^4/3$$
$$e_{ion} = \frac{3kT}{2m_p}\sum_m X_k/A_m \qquad p_{ion} = \frac{\rho kT}{m_p}\sum_m X_k/A_m$$

$$h = e + p/\rho$$

The low-Mach number formalism actually uses

$$h(p, T, X_k) = h(\rho(p, T, X_k), T, X_k).$$

Low Mach Number formulation

Methodology developed for combustion with ideal gas EOS

- Introduced by Rehm and Baum (1978)
- Analysis by Majda and Sethian (1985).

Expand u, ρ, T, X_k, and p, in Mach number, $M = u/c$

$$p(\vec{x}, t) = p_0 + Mp_1 + M^2 p_2$$

Asymptotic analysis shows

$$p(\vec{x}, t) = p_0(t) + \pi(\vec{x}, t) + O(M^3), \text{where } \frac{\pi}{p_0} \sim O(M^2)$$

- $p_0(t)$ does not affect local dynamics
- $\pi(\vec{x}, t)$ does not affect thermodynamics.

Low Mach Number formulation

$$
\begin{aligned}
\rho_t + \nabla \cdot \rho u &= 0 \\
(\rho X_k)_t + \nabla \cdot \rho u X_k &= \rho \dot{\omega}_k \\
(\rho u)_t + \nabla \cdot (\rho u u) &= -\nabla \pi + \rho \vec{g} \\
(\rho h)_t + \nabla \cdot (\rho u h) &= \nabla \cdot \kappa \nabla T - \rho Q(\dot{\omega}_k)
\end{aligned}
$$

Velocity constraint: Differentiate EOS along particle paths

$$
\rho \frac{Dp}{Dt} = 0 = \rho \frac{\partial p}{\partial \rho} \frac{D\rho}{Dt} + \rho \frac{\partial p}{\partial T} \frac{DT}{Dt} + \rho \sum_k \frac{\partial p}{\partial X_k} \frac{DX_k}{Dt}
$$

to obtain

$$
\nabla \cdot u = \frac{1}{\rho^2 \frac{\partial p}{\partial \rho}} \left(\rho \frac{\partial p}{\partial T} \frac{DT}{Dt} + \rho \sum_m \frac{\partial p}{\partial X_k} \dot{\omega}_k \right) \equiv S
$$

Fractional Step Approach

1. Advance velocity from $\vec{U}^n$ to $\vec{U}^{n+1,*}$ using explicit advection terms and a lagged pressure gradient.

2. Update the species, enthalpy and temperature

3. Use the updated values to compute S^{n+1}

4. Decompose $\vec{U}^{n+1,*}$ to extract the component satisfying the divergence constraint.

We currently use Strang splitting to advance the species, enthalpy and temperature.

Strang Splitting

Species/enthalpy advance

$$
\begin{aligned}
(\rho X_k)_t + \nabla \cdot \rho u X_k &= \rho \dot{\omega}_k \\
(\rho h)_t + \nabla \cdot (\rho u h) &= \nabla \cdot \kappa \nabla T - \rho Q(\dot{\omega}_k)
\end{aligned}
$$

Stiff kinetics relative to fluid dynamical time scales

Operator split approach

- Chemistry $\Rightarrow \Delta t/2$
- Advection – Diffusion $\Rightarrow \Delta t$
  - BDS unsplit Godunov
  - Crank-Nicolson Diffusion
- Chemistry $\Rightarrow \Delta t/2$

Properties of the methodology

- Formulation conserves species, mass and energy.
- Overall operator-split projection formulation is 2nd-order accurate in space and time.
- Second-order Godunov treatment of advection
- Embedded in parallel adaptive projection framework
  - Structured adaptive mesh refinement
  - Refinement in space and time
  - Parallelization using BoxLib framework
    - Large-grained data distribution
    - Dynamic load balancing

Applications

Computational studies

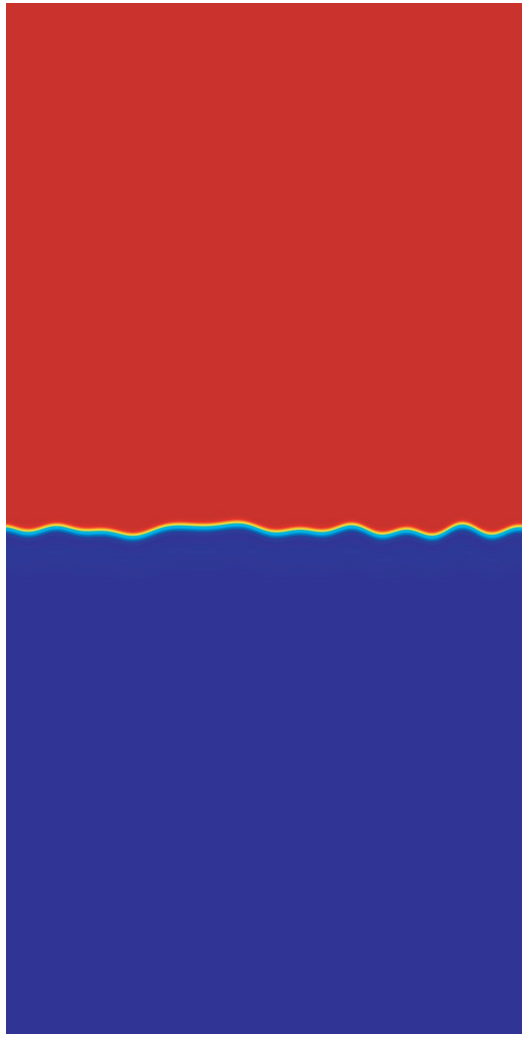
- Validation against compressible code (FLASH)
- Landau-Darrieus instabilities
- Rayleigh Taylor instabilities

Rayleigh Taylor instabilities

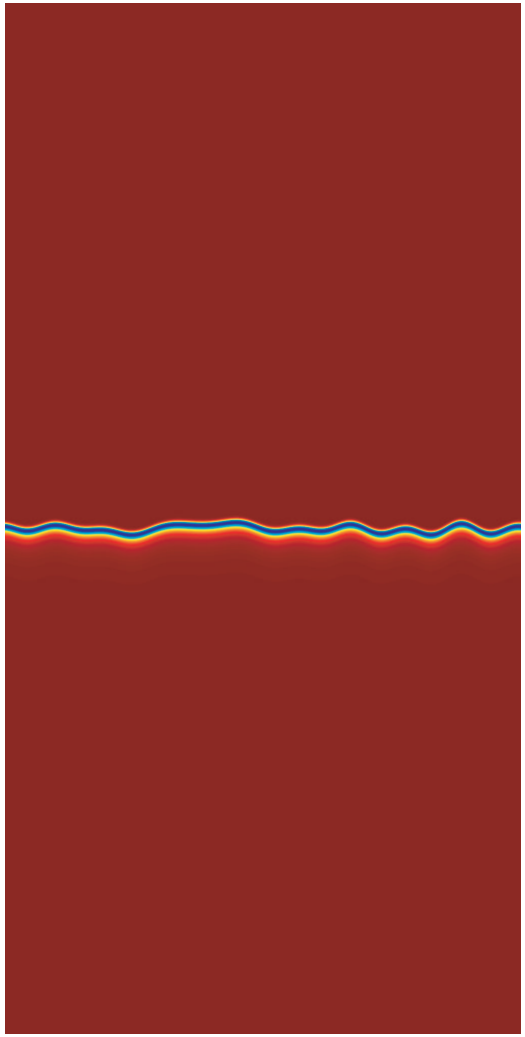
- Carbon, oxygen and magnesium flame
- Inflow, $\rho^{12}\mathrm{C} = 5 \times 10^6$, $\rho^{16}\mathrm{O} = 5 \times 10^6$, $T = 1 \times 10^7$
- 163.84 cm x 327.68 cm, 2D domain
- Effective resolution 1024 x 2048
- Initialize with randomly perturbed laminar flame solution

Simulation results

Temperature



Carbon Abundance



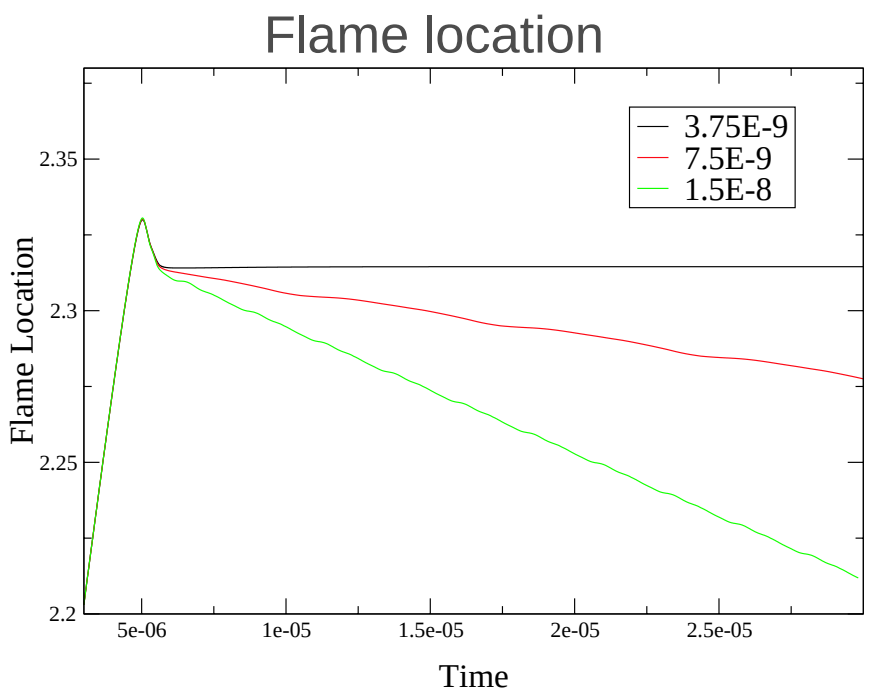
Energy

Splitting

Observations:

- Stiffness of reaction terms requires implicit integration
- Strang splitting limits accuracy to second-order
- Splitting errors lead to additional timestep restrictions

In 1-d flame problem, at fixed Δx, flame speed is very sensitive to Δt.



Improving the numerics

Potential options to couple advection, diffusion and reaction

- Fully implicit MOL approaches
  - BDF or IRK integration methodology
  - Fully coupled nonlinear solve
- Weak (lagged) coupling of operators
  - Boris and Oran
  - Sun
  - Iterated operator splitting methods
  - Approximate factorization
  - Difficult to make higher-order
- Spectral deferred corrections
  - Introduced by Dutt, Greengard and Rokhlin for ODE
  - Minion – SISDC
  - Bourlioux, Layton, Minion – MISDC
  - Layton, Minion – Conservative MISDC

Spectral deferred correction

Given an ODE $u_t = f(t, u)$ on an interval $[a, b]$. We can write the solution of the ODE as an integral

$$u(t) = u_a + \int_a^t f(\tau, u)\, d\tau$$

Suppose we have an approximate solution $\hat{u}(t)$. Define the residual

$$E(t, \hat{u}) = u_a + \int_a^t f(\tau, \hat{u})\, d\tau - \hat{u}(t)$$

Then, the error $\delta(t) \equiv u(t) - \hat{u}$ satisfies

$$\delta(t) = u(t) - \hat{u(t)} = (u_a + \int_a^t f(\tau, u)\, d\tau) - (u_a + \int_a^t f(\tau, \hat{u})\, d\tau - E(t, \hat{u}))$$

$$\delta(t) = \int_a^t (f(\tau, \hat{u} + \delta) - f(\tau, \hat{u}))d\tau + E(t, \hat{u})$$

Spectral deferred correction (p2)

Idea of SDC is to compute an initial $\hat{u}$ at M Gauss points, t^m.

Recall

$$\delta(t) = \int_a^t (f(\tau, \hat{u} + \delta) - f(\tau, \hat{u}))d\tau + E(t, \hat{u})$$

where $E(t, \hat{u}) = u_a + \int_a^t f(\tau, \hat{u})\, d\tau - \hat{u}(t)$
If we evaluate $E(t, \hat{u})$ at t^m by spectral quadrature, then we can use a lower order approximation to the integral to improve the accuracy of $\hat{u}$

$$\hat{u}^{new} = \hat{u}^{old} + \delta$$

Observe that we can rewrite the δ equation in terms of $\hat{u}$ at t^{m+1}:

$$\begin{aligned}\hat{u}^{new,m+1} = \hat{u}^{new,m} \quad & +\Delta t(f(t^{m+1}, \hat{u}^{new,m+1}) - f(t^{m+1}, \hat{u}^{old,m+1})) \\ & + \int_{t^m}^{t^{m+1}} f(\tau, \hat{u}^{old})\, d\tau\end{aligned}$$

SDC for Advection/Diffusion/Reaction

SDC is iteratively improving a higher-order polynomial approximation to the solution over a time interval

MISDC for advection/diffusion/reaction:

- Treat each term separately using a simple OS approach
- Explicit advection, implicit diffusion, implicit reactions
- Use different time steps for each process
- Iterate procedure with SDC interpolating polynomial
  - Interpolating polynomial couples the processes

We want to use the deferred correction ideas to couple advection, reaction and diffusion

- Use different representations for each physical process
- Reuse existing components of the methodology
- Integrate reactions using VODE – Think of VODE as "exact"

Linear deferred corrections algorithm

Consider the system $u_t = A(u) + D(u) + R(u)$

Integral form of solution is

$$u^{n+1} = u^n + \int_{t^n}^{t^{n+1}} A(u) + D(u) + R(u)\, d\tau$$

Approximate terms separately:

- A approximated as piecewise constant in time
- D linear in time
- R "exact" integration using VODE

Components of the algorithm

1. Compute an initial solution
2. Construct a representation of the solution
3. Iterative correction to improve the solution

Second-order Godunov

Consider

$$u_t + a u_x = F \quad \text{for} \quad a > 0$$

Second-order Godunov – cell-centered discretization

1. Construct (4th-order) slopes in each cell: δu_j^n
2. Predict time-centered value at cell edge using characteristics

$$u_{j+1/2}^{n+1/2} = u_j^n + 1/2(\Delta t - a\Delta x)\delta u_j^n + 1/2 \Delta t F$$

3. Construct fluxes for conservative difference

$$a u_x = \frac{a u_{j+1/2}^{n+1/2} - a u_{j-1/2}^{n+1/2}}{\Delta x}$$

Initialization of $\hat{u}$

1. Compute $A^{n+1/2}$ with Godunov scheme, using $D(u^n)$ as source
2. Solve for $\tilde{u}^{n+1}$ in order to compute $D(\tilde{u}^{n+1})$:

$$(I - \Delta t D)\tilde{u}^{n+1} = u^n + \Delta t A^{n+1/2}$$

3. Integrate reactions with VODE:

$$u' = R(u) + D(\tilde{u}^{n+1}) + A^{n+1/2} \quad \text{with} \quad u_0 = u^n$$

which in integral form gives

$$\hat{u}^{n+1} = u^n + \int_{t^n}^{t^{n+1}} (R(u) + D(\tilde{u}^{n+1}) + A^{n+1/2})\, d\tau$$

Construct approximation

Construct a polynomial approximation to advection and diffusion during time step

$$A^{n+1/2} + ((t^{n+1} - t)D(u^n) + (t - t^n)D(\hat{u}^{n+1})/\Delta t$$

$$I(t) \equiv \int_{t^n}^{t} A^{n+1/2} + ((t^{n+1} - \tau)D(u^n) + (\tau - t^n)D(\hat{u}^{n+1})/\Delta t \; d\tau$$

From ODE integration define

$$I_R \equiv \int_{t^n}^{t^{n+1}} R(u)d\tau = u^{n+1} - u^n - \Delta t(D(\tilde{u}^{n+1}) + A^{n+1/2})$$

We then approximate

$$\int_{t^n}^{t^{n+1}} A(u) + D(u) + R(u) \; d\tau \approx I(t^{n+1}) + I_R$$

SDC for A/D/R: Iterative correction

1. Update advection $A^{n+1/2,new}$ with Godunov-type scheme, using $D(u^n)$ and I_R as sources for characteristic tracing.
2. Solve for $\tilde{u}^{n+1,new}$ in order to compute $D(\tilde{u}^{n+1,new})$:

$$\begin{aligned}\tilde{u}^{n+1,new} = u^n \quad &+ \quad \Delta t(D(\tilde{u}^{n+1,new}) - D(\hat{u}^{n+1,old})) \\ &+ \quad \Delta t(A^{n+1/2,new} - A^{n+1/2,old}) + I(t^{n+1}) + I_R\end{aligned}$$

3. Integrate reactions with VODE

$$u_t = R(u) + I'(t) + D(\tilde{u}^{n+1,new}) - D(\hat{u}^{n+1,old}) + A^{n+1/2,new} - A^{n+1/2,old}$$

with $u_0 = u^n$

$$\begin{aligned}\hat{u}^{n+1,new} \quad &= \quad u^n + I(t^{n+1}) + \int_{t^n}^{t^{n+1}} R(u)d\tau \\ &+ \quad \Delta t(D(\tilde{u}^{n+1,new}) - D(\hat{u}^{n+1,old}) + A^{n+1/2,new} - A^{n+1/2,old})\end{aligned}$$

Update solution representation

From ODE integration update

$$I_R = \hat{u}^{n+1,new} - u^n - I(t^{n+1}) \quad - \quad \Delta t(D(\tilde{u}^{n+1,new}) - D(\hat{u}^{n+1,old}))$$
$$- \quad \Delta t(A^{n+1/2,new} - A^{n+1/2,old})$$

Update polynomial approximation to effect of advection and diffusion during time step

$$A^{n+1/2,new} + ((t^{n+1} - t)D(u^n) + (t - t^n)D(\hat{u}^{n+1,new}))/\Delta t$$

$$I(t) = \int_{t^n}^{t^{n+1}} A^{n+1/2} + ((t^{n+1} - \tau)D(u^n) + (\tau - t^n)D(\hat{u}^{n+1,new})/\Delta t \; d\tau$$

Iteration improves order of accuracy one order up to accuracy of quadrature rule.

Can retain lagged approximation to I_R

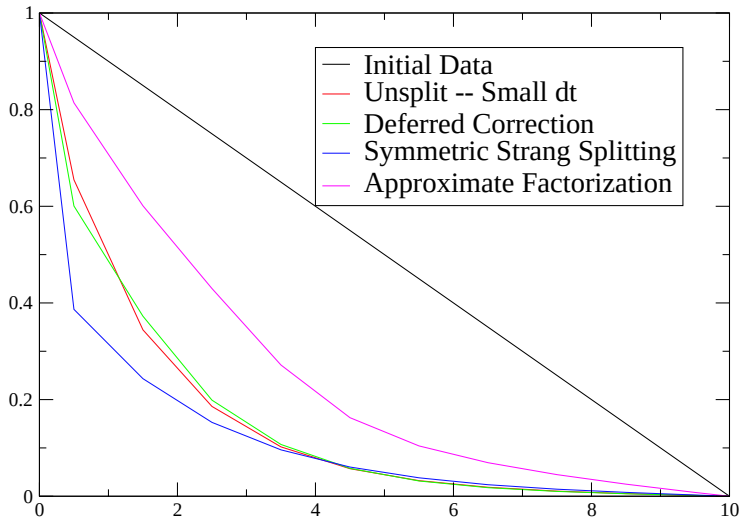
Sample Problem

Consider a simplified advection-diffusion-reaction problem
We define, for $i = 1, ...4$,

$$y_{i\,t} + u y_{i\,x} = D y_{i\,xx} + R_i$$

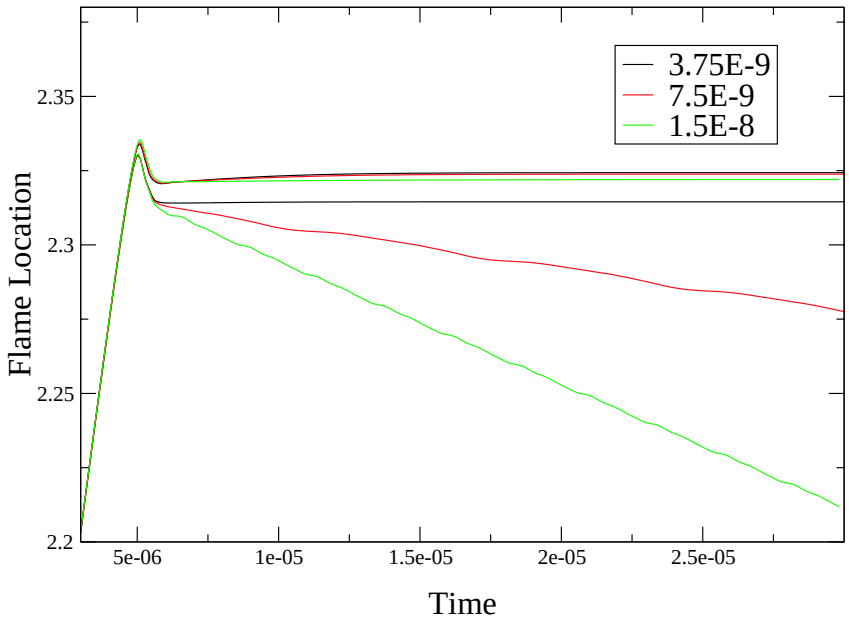
$$\begin{aligned} R_1 &= -k_1 y_1 y_4 - k_2 y_1, \\ R_2 &= k_1 y_1 y_4, \\ R_3 &= k_2 y_1, \\ R_4 &= -k_1 y_1 y_4. \end{aligned}$$

Effect of coupling



Model problem

$D = 10,\ k_1 = 20,\ k_2 = 4$



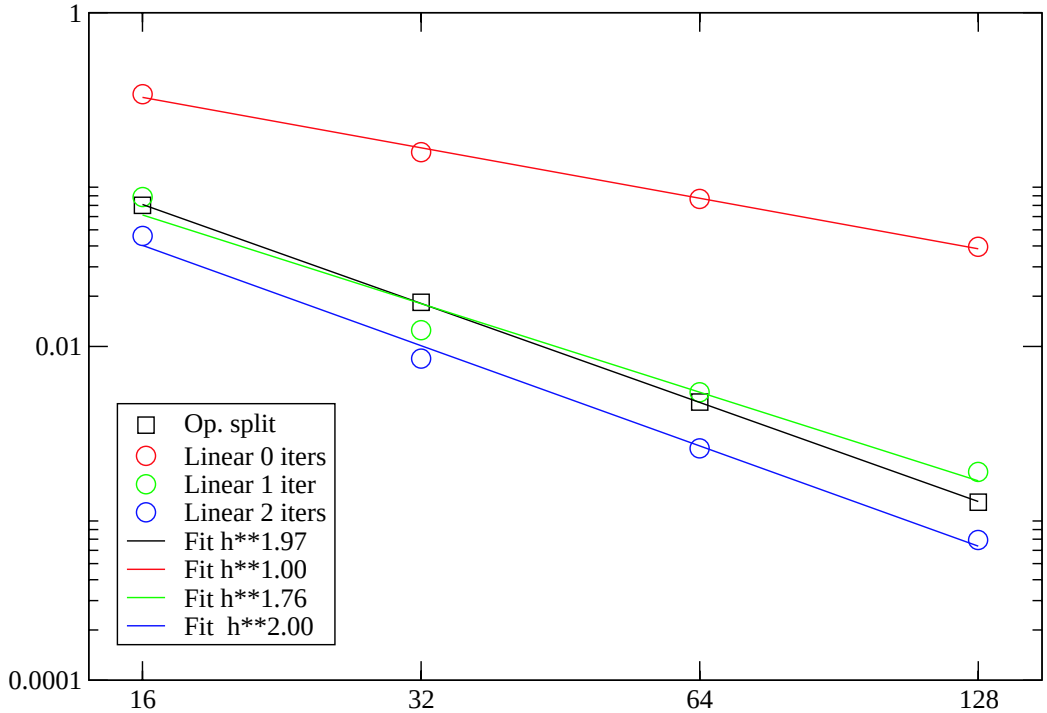
Flame location

Model Problem Convergent Results

We initialize the problem on a $[0, 1]$ domain with $y_1 = .5(1 + \sin(2\pi x))$, $y_2 = y_3 = 0$, and $y_4 = .5(1 + \sin(2\pi(x - .1)))$ with $D = 1$, $k_1 = 20$, $k_2 = 4$

The calculations are run to $t = 0.0625$ with $\Delta t = 0.5\Delta x$ (recalling $u = 1$).

Below we present a combined norm of the errors of y_i, with the error defined as the difference from the "exact" solution (that generated with $nx = 2048.$).



Log-Log Plot of Errors from Schemes

Higher-order Extensions

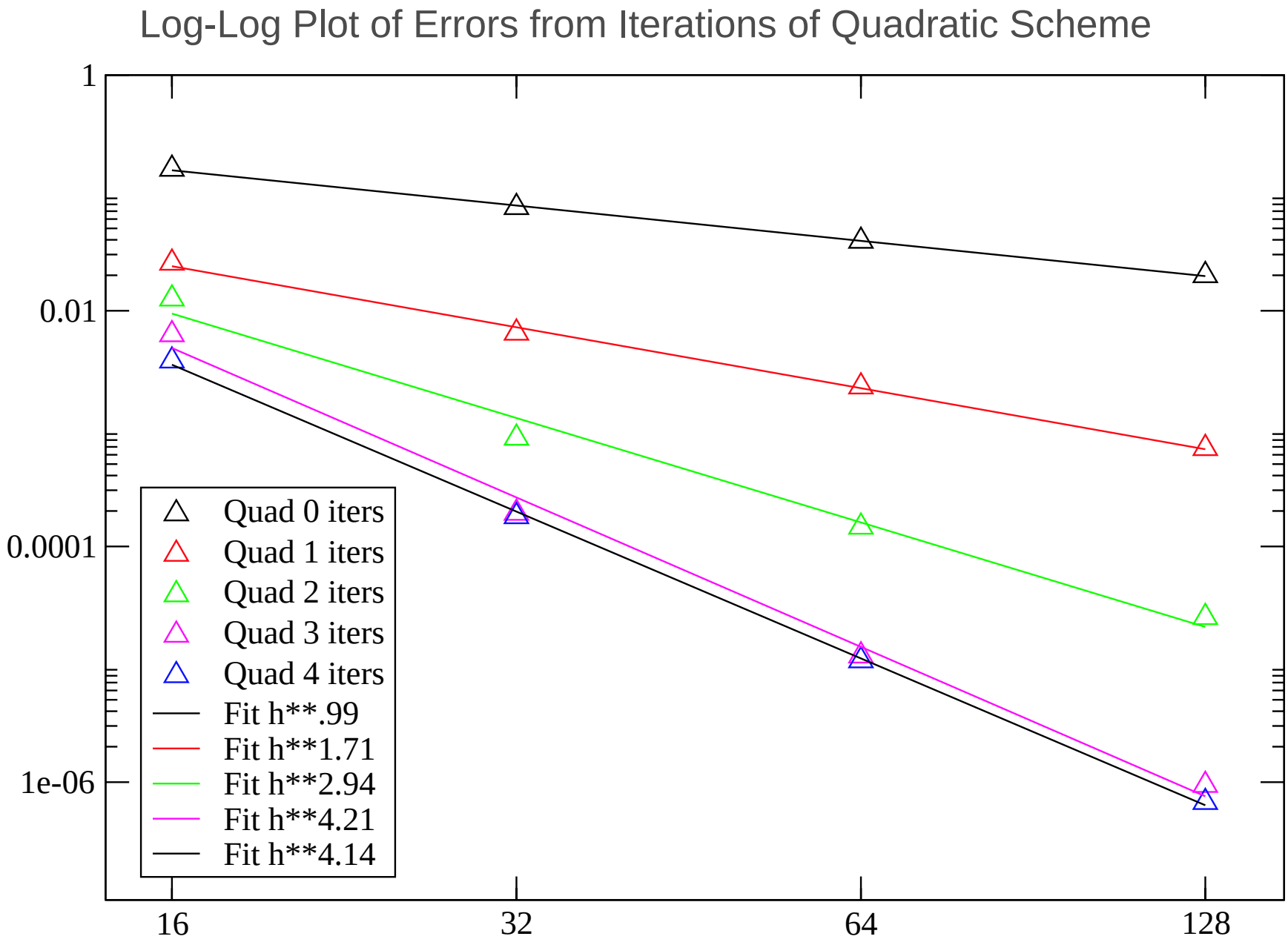
Higher-order temporal integration (4th order)

- Divide interval $[0, \Delta t]$ into two subintervals
- Compute initial solution from two steps of basic algorithm
- Construct quadratic approximation to advection and diffusion on the interval by evaluation operators at t^n, $t^{n+1/2}$ and t^{n+1} and define $I^Q(t)$ to be the integral of that quadratic
- From ODE solve define I_{R_1} and I_{R_2} representing the effective of chemistry over the two subintervals.
- Perform iterative correction as before

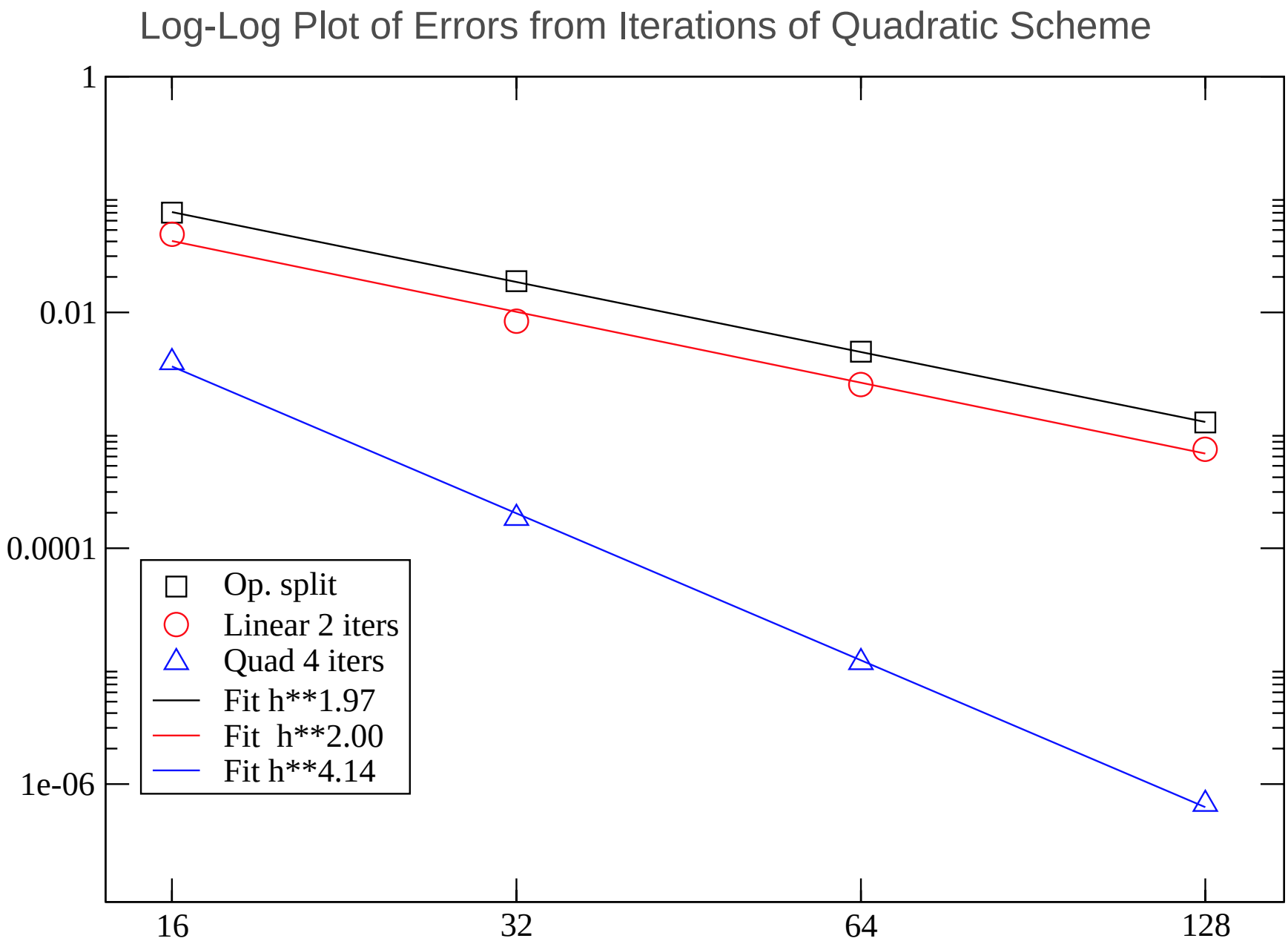
Higher-order in space

- Use higher-order approximations in constructing quadratic approximation
  - PPM for the advection terms
  - Higher-order centered difference for diffusion
- Solve correction equations with lower-order operators
  - Second-order Godunov for the advection terms
  - Second-order centered difference for diffusion

Convergence of quadratic iterations

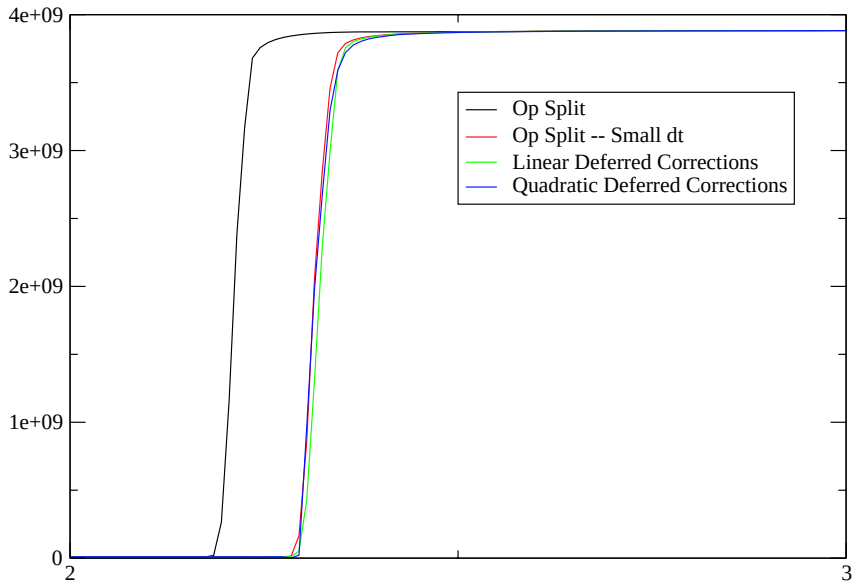


Comparison of schemes



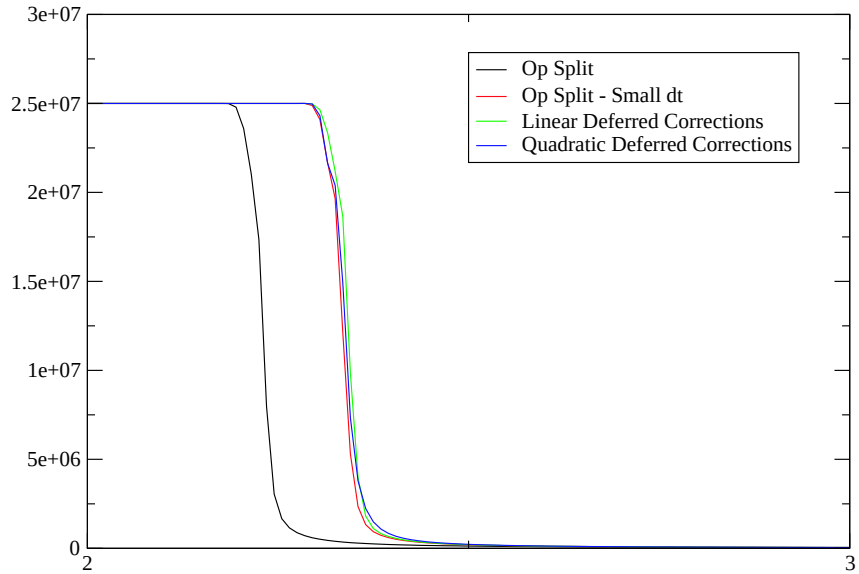
1-D Supernovae flames

Temperature



$\Delta x = .01$

Carbon Abundance



$\Delta x = .01$

Summary and Remarks / Future work

- Low Mach number methodology for modeling nuclear flames in Type Ia supernovae
  - Eliminates acoustic waves
  - Projection based fractional step algorithm
  - Parallel, adaptive implementation
- Spectral deferred corrections
  - Couples processes
  - Extensible to higher-order

Remarks

- Integrate deferred corrections into multi-dimensional code
- Extend ideas to treat the entire system
- SDC is not L-stable
  - Limits to time step if not advection dominated
  - Explore alternative ansatz for solution structure
- Many variations on this theme are possible