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Verification (mostly) for High Energy Density Radiation Transport: 5 Case Studies

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Verification (mostly) for High Energy Density Radiation Transport: 5 Case Studies

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Outline

- HEDP issues
- Case 1: Marshak studies
- Case 2: Star-in-space problem
- Case 3: Radiating shock problem
- Case 4: Crooked pipe problem
- Case 5: Angles, angles, angles

High-energy-density physics characteristics

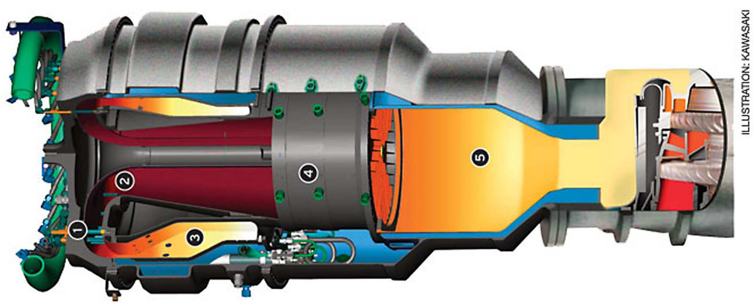
- Definition $p > 1\,\mathrm{Mbar}$ or $e > 1\mathrm{Mbar}\,\mathrm{cm}^3\,\mathrm{g}^{-1}$

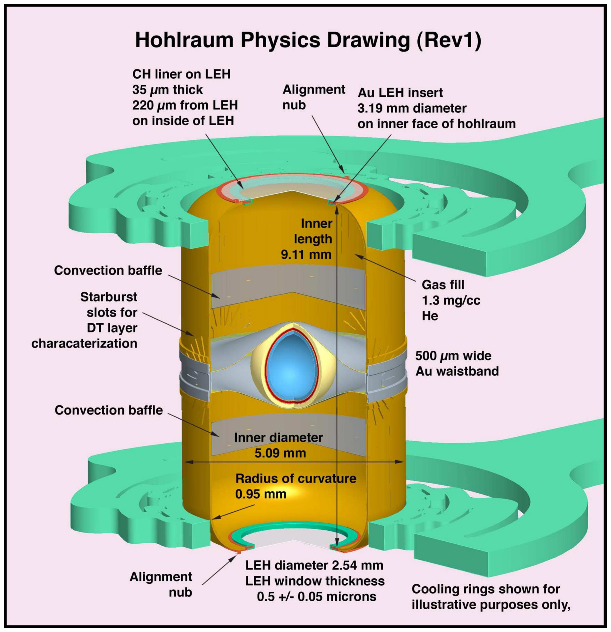
- This is realized in large laboratory machines such as high-power lasers and pulsed-power machines, stars and nuclear explosions

- When p and e are high, so is the temperature, and the radiation $\propto T^4$ becomes a dominant effect

- Large-scale simulations of such experiments have to include radiation transport and have acceptable engineering accuracy

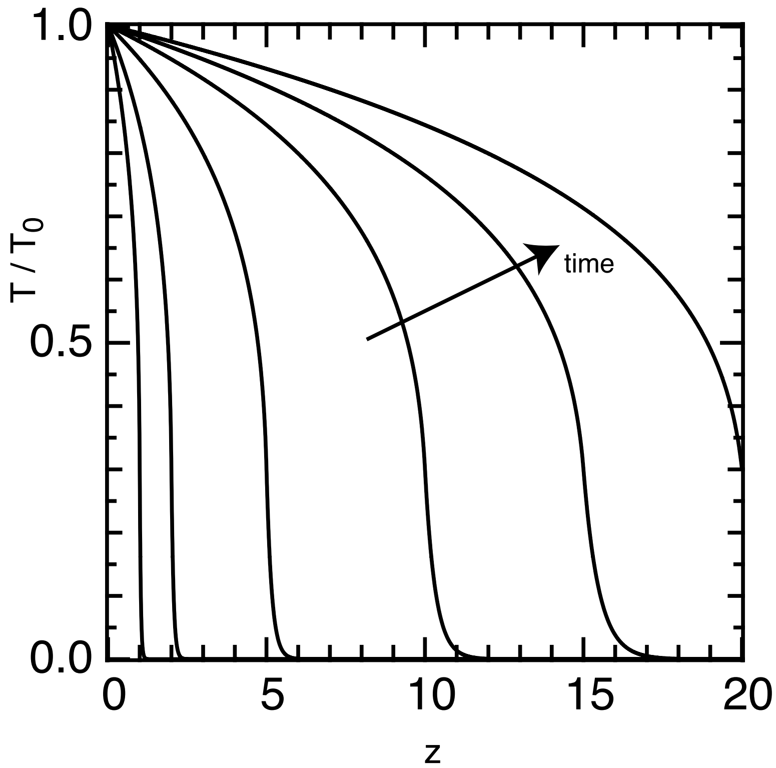
Complexity





Realistic complexity leads to $>10^6$-zone simulations, and accurate radiation transport adds an additional factor $\approx 10^2$–10^4 for unknown intensities per zone. This means 10^4–10^6 cpu-sec per cycle on a 3 GFlop/cpu class machine

Case 1: The Marshak wave



- Hot radiation falls on an initially cold material and heats its surface
- The opacity of cold material is very large, but that of the hot material is much less
- The result is a "bleaching" wave that progresses into the material
- The blow-off of heated material drives a shock wave, *etc., etc.*
- Diffusion may be OK, but in some regimes transport corrections and time-of-flight are important

1-D diffusion and related methods

- The gray radiation moment equations in slab geometry look like this—

$$\frac{\partial E}{\partial t} + \frac{\partial F}{\partial z} = k(4\pi B - cE) \qquad \text{and} \qquad \frac{1}{3c}\frac{\partial F}{\partial t} + \frac{D}{3}\frac{\partial f cE}{\partial z} = -kF$$

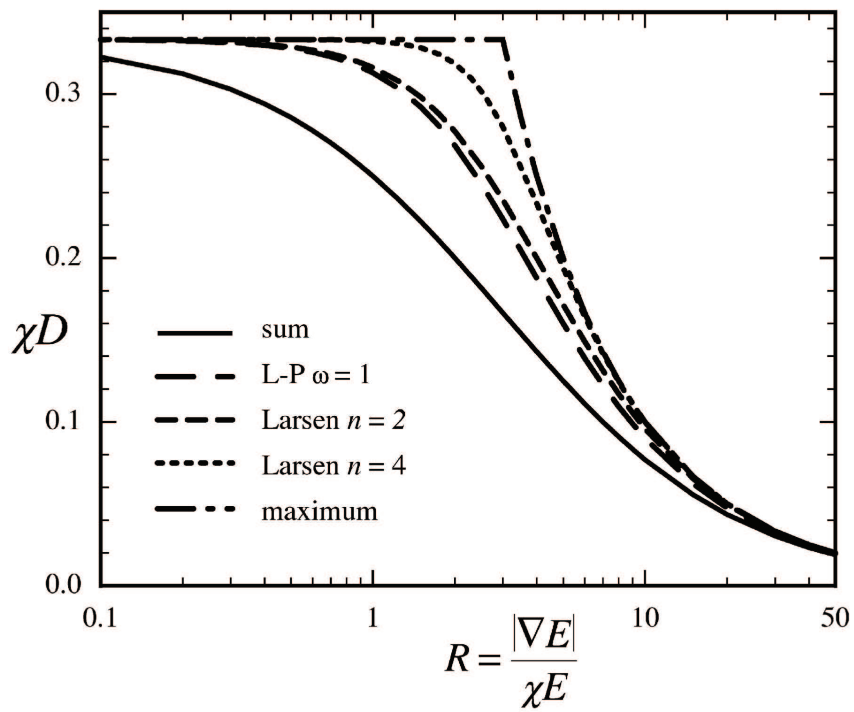
- The P_1 model is to omit the red 3 and the blue D and the green f

- Diffusion is to omit the $\partial F/\partial t$ term entirely and the green f; flux-limited diffusion includes an appropriate D

- The $P_{1/3}$ model of Olson, Auer and Hall omits the D and the f but includes the red 3

- The VEF method omits the red 3 and the D but includes a suitable f, perhaps self-consistently calculated

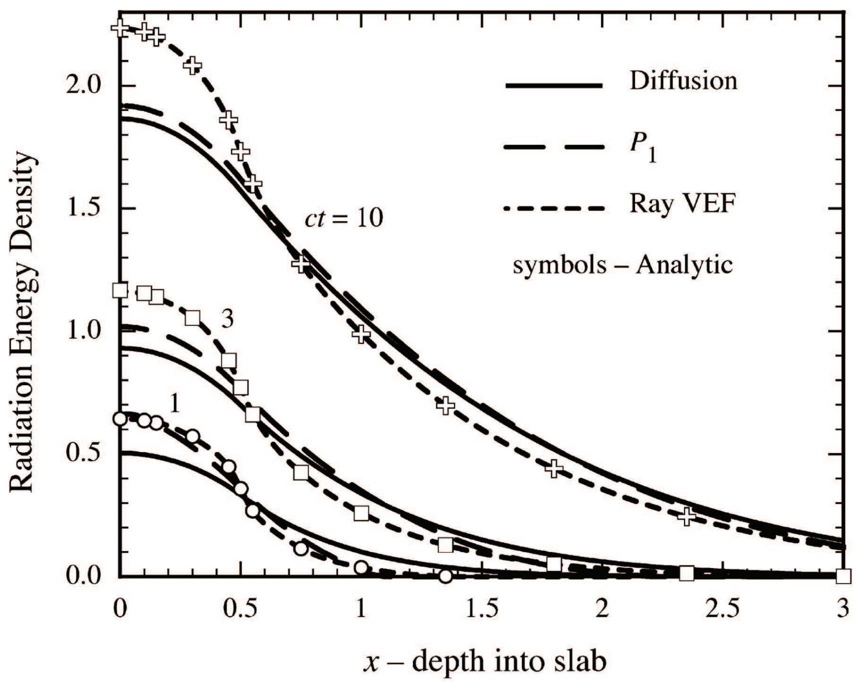
There is a range of flux-limiter functions



(Olson, Auer and Hall, JQSRT, 64, 619 [2000])

- The traditional ones are Wilson's "max" and "sum" Ds
- The Levermore-Pomraning D comes from Chapman-Enskog theory
- The Larsen functions are other *ad hoc* interpolations between the large and small R limits
- Larsen $n = 2$ is a good fit to Levermore-Pomraning and cheaper
- The original "max" and "sum" versions now seem to be outliers

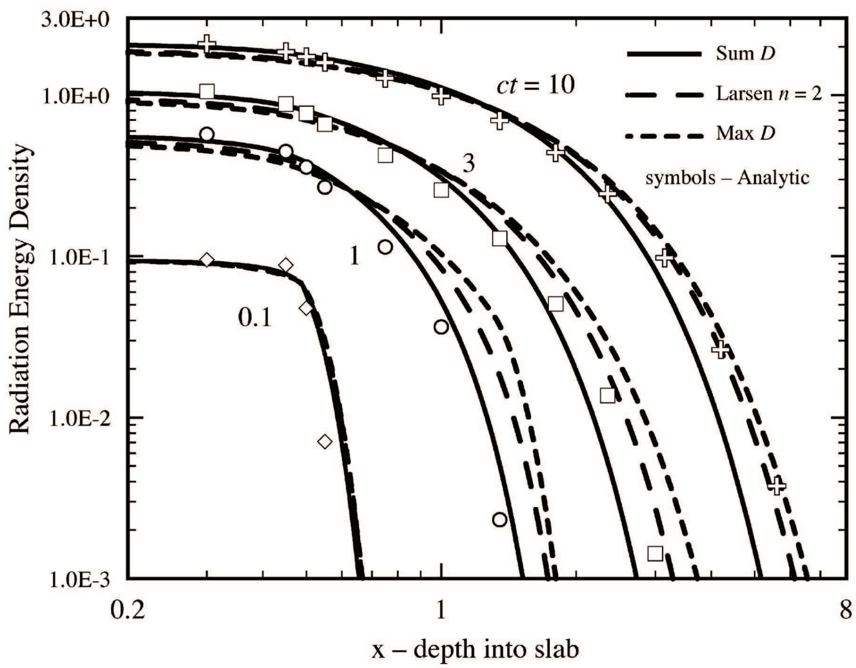
Benchmark results for the Su-Olson linear Marshak problem



- This case has a constant opacity k, but $e \propto T^4$, which makes the problem linear; an analytic solution exists
- VEF is accurate here, but P-1 and diffusion have problems at small τ
- Diffusion (not FLD) has a racing-ahead problem

(Olson, Auer and Hall, JQSRT, 64, 619 [2000])

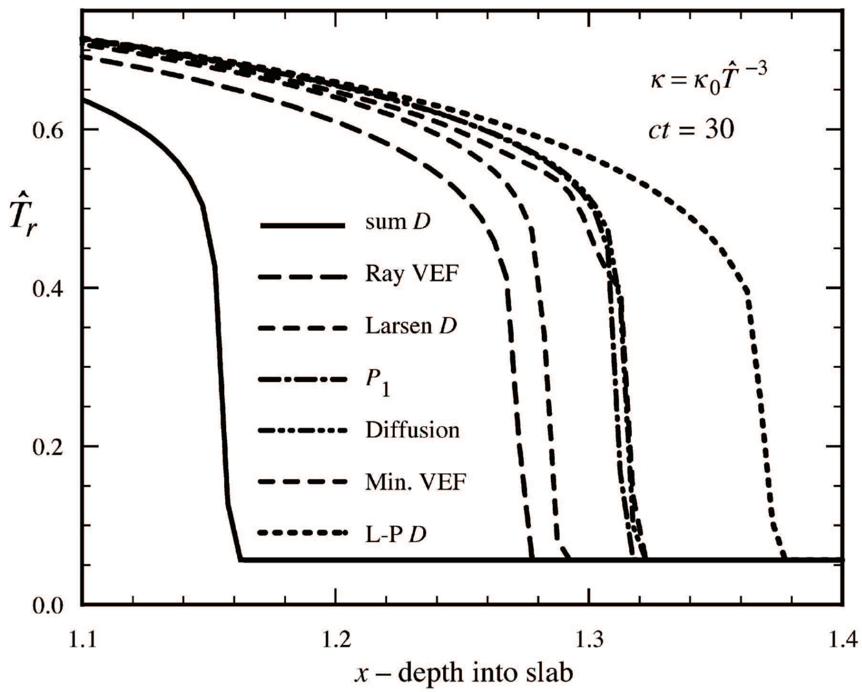
Su-Olson results with flux limiters



- At early time the radiation is free-streaming and any D does OK
- At middle time ($ct \approx$ mean free path) the flux limiter makes a difference and first "sum" is best and then later "max" and Larsen $n = 2$ are best

(Olson, Auer and Hall, JQSRT, 64, 619 [2000])

Olson-Auer-Hall Marshak wave with variable opacity



(Olson, Auer and Hall, JQSRT, 64, 619 [2000])

- The Su-Olson Marshak wave with constant opacity lack the "bleaching" effect of the real wave
- That is partially rectified by assuming an opacity $\propto 1/T^3$
- This figure shows how the wave propagation looks with a selection of flux limiters and Eddington factors
- The right answer (Ray VEF) is the second slowest wave, next to "sum", which is much too slow
- The consensus of most of the other methods is too fast, with the one closest to the truth being Larsen's $n = 2$ FL

Marshak wave summary

- No diffusion-like method is perfect
- The "max" and "sum" flux limiters are the poorest
- The *ad hoc* Eddington-factor methods are poor
- The Levermore-Pomraning ($\varpi \neq 1$) method is poor, but the variation with $\varpi = 1$ is fairly good, on a par with Larsen's $n = 2$ method
- P_1 and $P_{1/3}$ are good, but not better than Larsen $n = 2$ for the variable-opacity case
- The self-consistent VEF method is accurate, as it should be
- Implicit Monte Carlo does a good job on this problem, especially in the difference formulation; see Granlibakken 2004, paper by Szöke, Brooks, McKinley and Daffin

Case 2: Star-in-space problem

- This problem is extremely simple: an opaque sphere radiates isotropically into a surrounding vacuum
- This arises, as the name implies, in extended stellar atmospheres
- It also occurs in ICF hohlraum problems, where the source and receiver are reversed
- “Toto, we’re not in diffusion any more”
- This problem elicits a variety of responses from the algorithms, almost all bad

What goes wrong?

- Here are the spherical geometry, steady-state, moment equations in vacuum:

$$\frac{dF}{dr} + \frac{2}{r}F = 0 \qquad \text{and} \qquad \frac{dP}{dr} + \frac{3P - E}{r} = 0$$

- The first equation says $F \propto 1/r^2$, which is correct

- The problem is the second equation, and in any variation of diffusion P is replaced by $E/3$, which implies $E = \mathrm{constant}$, a very bad answer

- Not only that, but all P_n methods give the same result, $E = \mathrm{constant}$, if the sphere radiates isotropically

- Characteristic ray methods will be exact in this case, if the rays properly sample the radiating disk

What about the VEF method(s)?

- With an Eddington factor χ, the 1st moment equation becomes

$$\frac{dP}{dr} + \frac{3P - E}{r} = \frac{d\chi E}{dr} + \frac{(3\chi - 1)E}{r} = \frac{1}{q}\frac{dq\chi E}{dr} = 0$$

- and q is Auer's sphericality function defined by

$$\ln q = \int \left(3 - \frac{1}{\chi}\right)\frac{dr}{r}$$

- So the solution is $E \propto 1/(q\chi)$, and the rabbit in the hat is χ, the Eddington factor

The exact Eddington factor

- The half-angle subtended by the sphere of radius R at a radius $r > R$ is $\cos^{-1}\mu$, where $\mu = \sqrt{1 - R^2/r^2}$
- The moments then become $cE = 2\pi I_0(1 - \mu)$, $F = \pi I_0(1 - \mu^2)$ and $cP = 2\pi I_0(1 - \mu^3)/3$
- The Eddington factor is $\chi = (1 + \mu + \mu^2)/3$
- With this χ, q turns out to be $q \propto 1/(1 - \mu^3)$, so $E \propto (1 - \mu)$, the right answer

Streaming solutions with Eddington factor formulae

- There are several prescriptions for χ as a function of $f = F/cE$: Minerbo's, Levermore's, Kershaw's, and the exact relation based on $\chi = (1+\mu+\mu^2)/3$ and $f = (1+\mu)/2$

- From $q\chi E =$ constant and $r^2 F =$ constant we infer

$$\frac{qR^2}{r^2} = \frac{2\chi(.5)f}{\chi(f)}$$

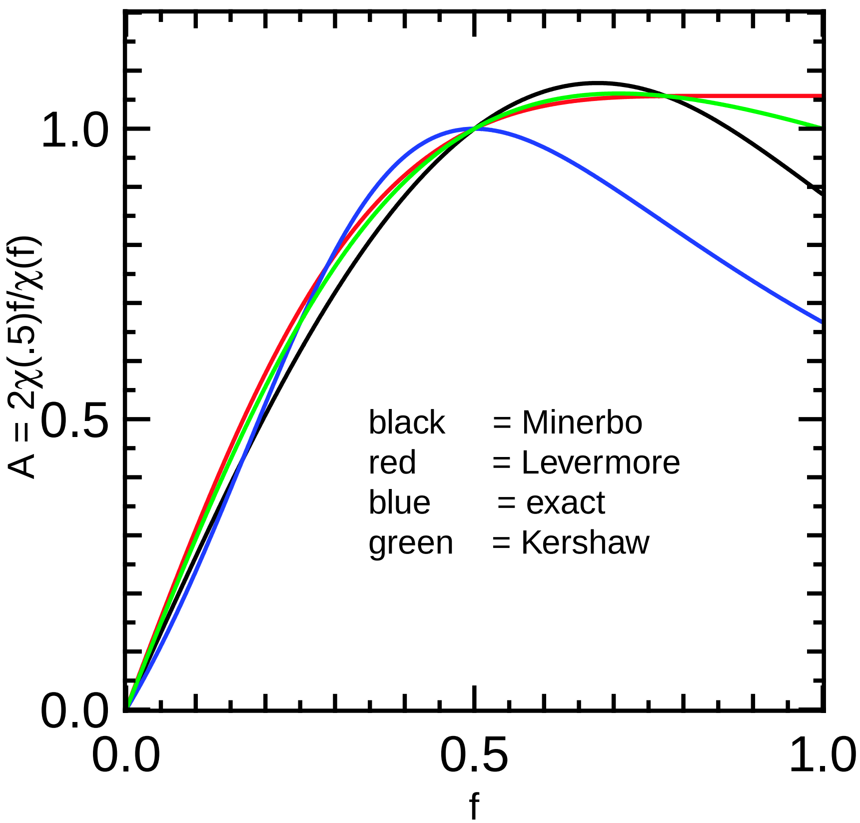
  taking $q = 1$ and $f = 1/2$ at $r = R$

- $A \equiv qR^2/r^2$ obeys the differential equation

$$\frac{d\ln A}{d\ln r} = 1 - \frac{1}{\chi(f)}$$

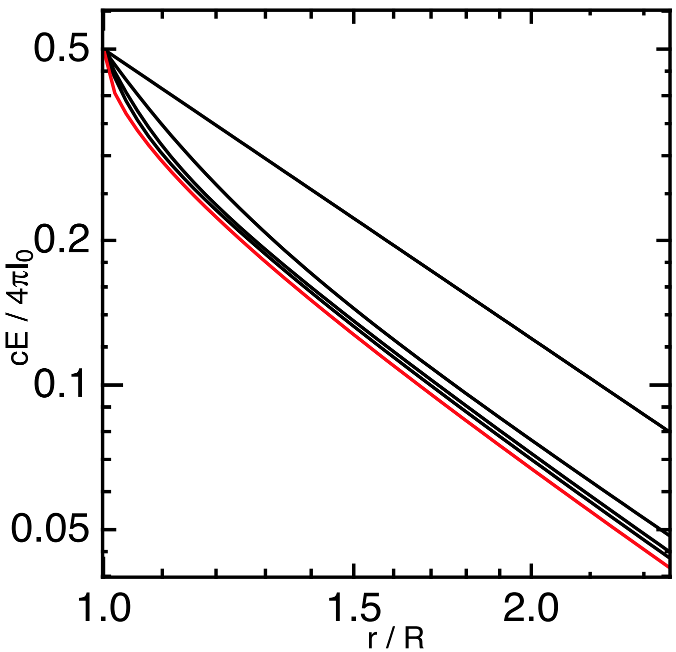
- This means that A decreases with r and therefore $f/\chi(f)$ must decrease with f, if f is to be physically reasonable

None of the common Eddington factor prescriptions obey reasonableness



- The surface of the sphere, $r = R$, corresponds to $f = 1/2$, where $A = 1$
- A must decrease as r increases, which leads to solutions with f decreasing from 1/2 for Minerbo's, Levermore's and Kershaw's functions; the regime $f \to 1$ for large r can't be reached
- The one that works is "exact", namely $\chi = (1 - 2f + 4f^2)/3$
- This function is unphysical in another sense, since it is not monotonic with f, and has a minimum value = 1/4 at $f = 1/4$

The S_n methods are much better



- In S_n you solve these equations

$$\frac{\mu_i}{r^2}\frac{d(r^2 I_i)}{dr} + \frac{2}{r w_i}\left[\alpha_{i+1/2} I_{i+1/2} - \alpha_{i-1/2} I_{i-1/2}\right] = 0$$

- The I_i are zone-centered in μ and the $I_{i+1/2}$ are edge-centered; the αs are helper quantities derived from the quadrature set

- With diamond-difference in angle $I_i = (I_{i-1/2} + I_{i+1/2})/2$

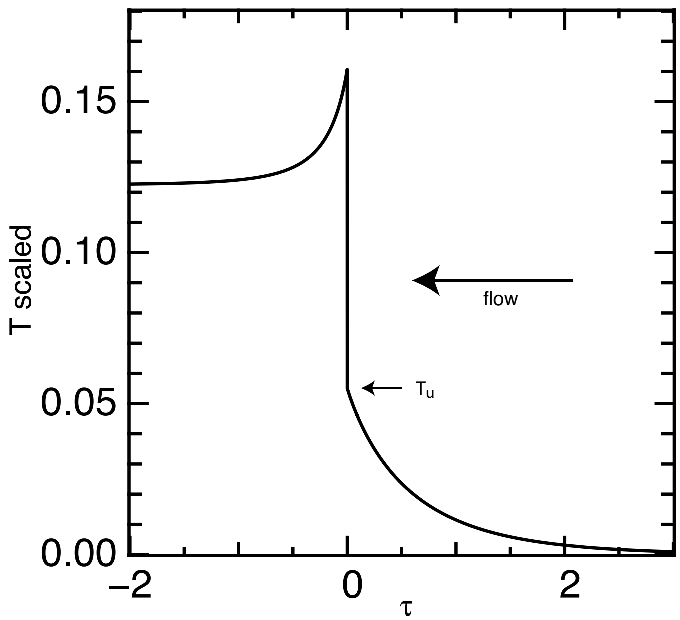
- The figure compares the S_2, S_4, S_6 and S_8 results with the exact answer (red)

- S_2 is off by a factor 2, a lot better than P_1, and S_8 is off by only 5%; the asymptotic behavior is $\propto 1/r^2$ for all n

Star-in-space summary

- Some methods give $E \sim$ constant instead of declining roughly as $1/r^2$: any kind of diffusion, P_n of any order
- The characteristic-ray method (tangent rays) is exact
- *Ad hoc* Eddington-factor closures behave unphysically for this problem
- The S_n results are good: S_2 is up to a factor 2 off, but for larger n the error declines to a few percent

Case 3: The radiating shock problem



- In a strong enough shock wave the radiation from shocked material preheats the material ahead of the shock
- This makes the peak temperature higher, but then there is a sharp cooling spike in which T comes down to the fi nal value
- The question is, what is the ratio f_s of the precursor temperature T_u to the fi nal downstream temperature?
- This depends on a radiation-strength parameter, $Q \equiv 2\sigma_B u_s^5/\pi R^4 \rho_0$
- There is disagreement on whether f_s gradually approaches 1 as $Q \to \infty$, or whether $f_s = 1$ above a critical Q, or some other behavior

The fbw model

- The idealized model is ideal-gas ($\gamma = 4/3$, $p = \rho R T$), constant gray opacity, steady flow in slab geometry

- We non-dimensionalize using ρ_0, u_s and R as units; radiation quantities are in units of $\rho_0 u_s^3/2$

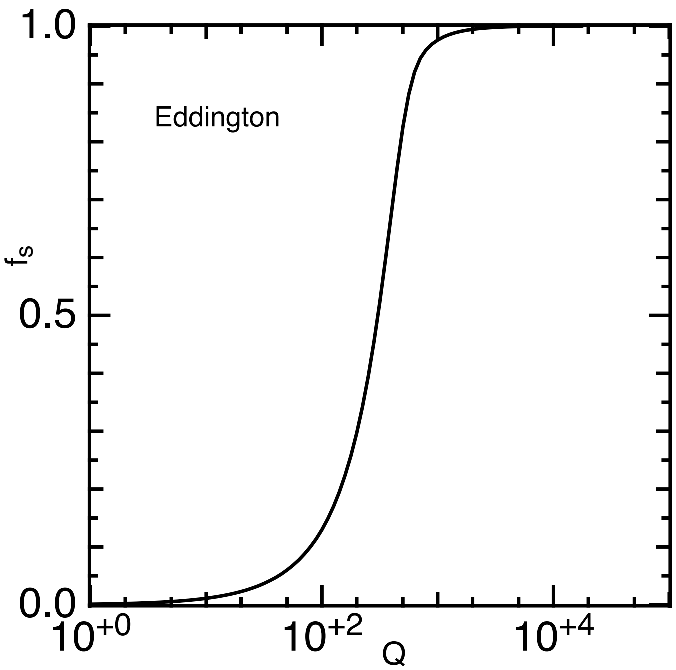
- The normalized specific volume is $\eta \equiv \rho_0/\rho$

- The steady flow equations give the non-dimensional temperature and flux

$$T = \eta(1-\eta) \qquad \text{and} \qquad F = (1-\eta)\left(\frac{\eta}{\eta_f} - 1\right)$$

- Here η_f is the final downstream volume, $\eta_f = (\gamma - 1)/(\gamma + 1)$

The non-equilibrium diffusion approach



- In the Eddington approximation the radiation moment equations are (with $B = Q[\eta(1-\eta)]^4$)

$$\frac{dF}{d\tau} = 4\pi(B - J) \qquad \text{and} \qquad \frac{4\pi}{3}\frac{dJ}{d\tau} = -F$$

- Substituting for F as a function of η and dividing the equations gives a single ODE for J *vs.* η

- I match integrations from far upsteam and downstream at the shock, where η satisfi es the jump condition $\Delta F = 0$ and J is continuous

- The results for various Qs are shown in the plot

- There is no shock that is exactly critical ($f_s = 1$), but f_s turns the corner sharply near $Q = 800$

- This is consistent with Zel'dovich's statements

What about exact transport?

- The VEF radiation moment equations are

$$\frac{dF}{d\tau} = 4\pi(B - J) \qquad \text{and} \qquad \frac{4\pi}{3}\frac{d f_E J}{d\tau} = -F$$

- The Eddington factor f_E has to be found self-consistently by solving the transfer equation

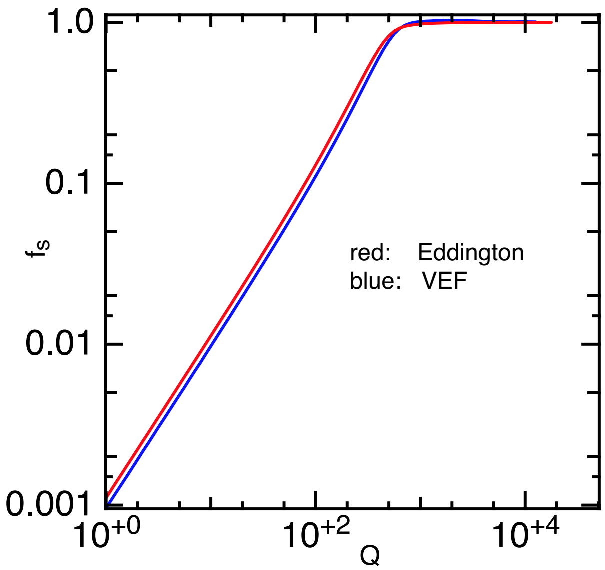
- For this I used two methods: (1) Feautrier solutions using 4-point Gaussian quadrature in each of 5 divisions of each hemisphere; (2) applying the exponential-integral kernels to the cubic spline interpolant of Planck function *vs.* τ

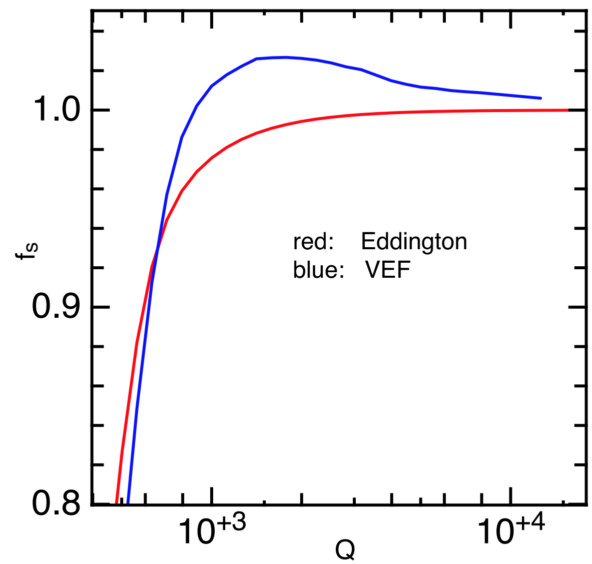
- After each RT solution the Eddington factor was re-computed and a relaxation was applied before the next solution of the steady flow equations

- The combined equations give $K \equiv f_E J$ *vs.* η, and another integration yields τ

- The convergence was found to be good for low and moderate Q, and less good for large Q

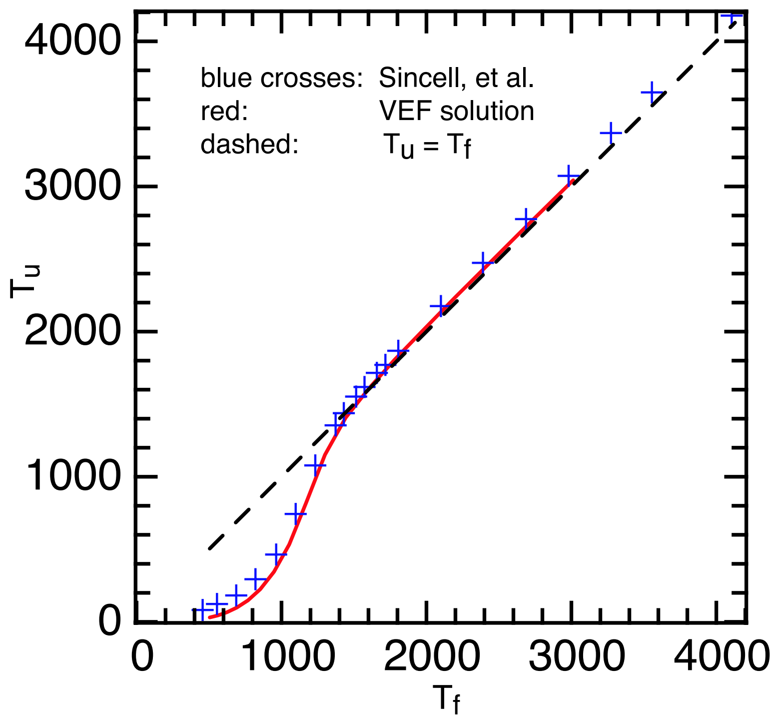
The VEF results imply that there is a critical shock, and $f_s \to 1$ from above as $Q \to \infty$





The accurate VEF solutions show a modest 14% shift in Q for a given f_s, but also pass through $f_s = 1$ at $Q \approx 880$. The VEF f_s results for $Q > 2000$ have a ± 0.001 uncertainty due to imperfect convergence.

Comparison with Sincell, *et al.*

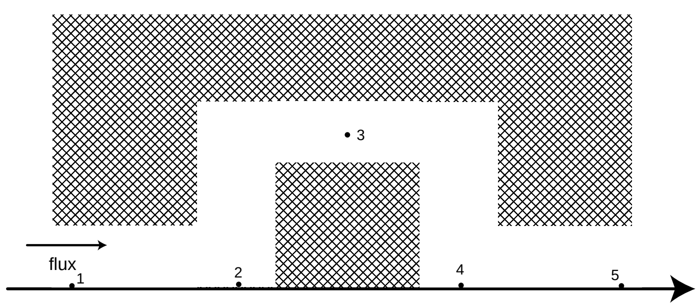


- Sincell, Gehmeyr and Mihalas (Shock Waves, **9**, 391 [1999]) studied radiating shocks with the adaptive Titan code, which also uses the VEF method
- The data for ambient density, molecular weight and gas law ($\gamma = 5/3$) were specified, and the velocity of the piston driving the shock took various values
- The figure shows the pre-shock temperature $T_u = f_s T_f$ *vs.* the final temperature T_f
- The Sincell, *et al.*, results agree fairly well with the present VEF method
- Both Sincell, *et al.*, and the present study show f_s crossing $f_s = 1$ and then tending asymptotically toward that relation

Radiating-shock summary

- The difference between diffusion and transport is significant: the Eddington factor has strong spatial variation
- There is a qualitative difference between Eddington and VEF results for the shock precursor temperature —
  - For Eddington the precursor temperature rises monotonically as a fraction of the final temperature as shock strength increases,
  - But for VEF the shock becomes critical (fraction 100%) at a certain strength
- Some of the computational aspects of this problem are quite difficult, suggesting that it could be a good benchmark

Case 4: The crooked pipe



- Isotropic radiation is incident from the left, beginning at $t = 0$, at the opening in a pipe that has a fat center section containing an obstructing plug

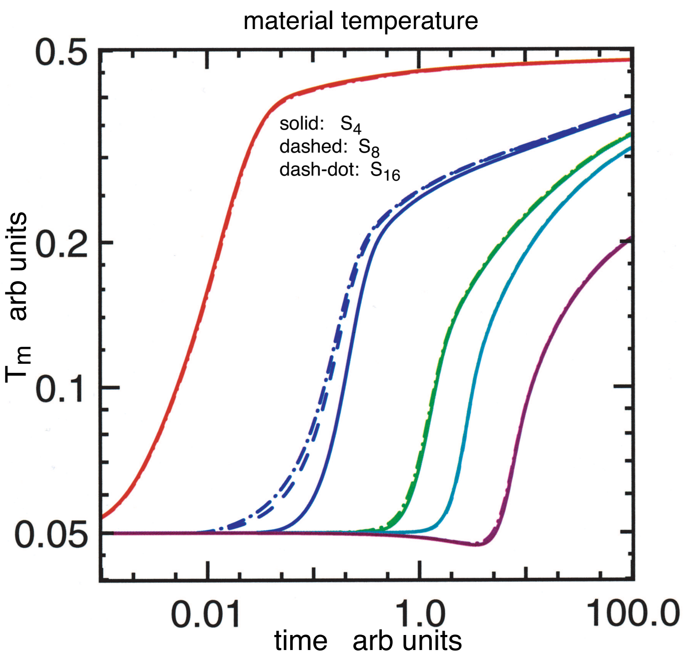
- The pipe material is assumed to be very opaque, with a diffusely reflection surface $(\text{albedo} = 1)$

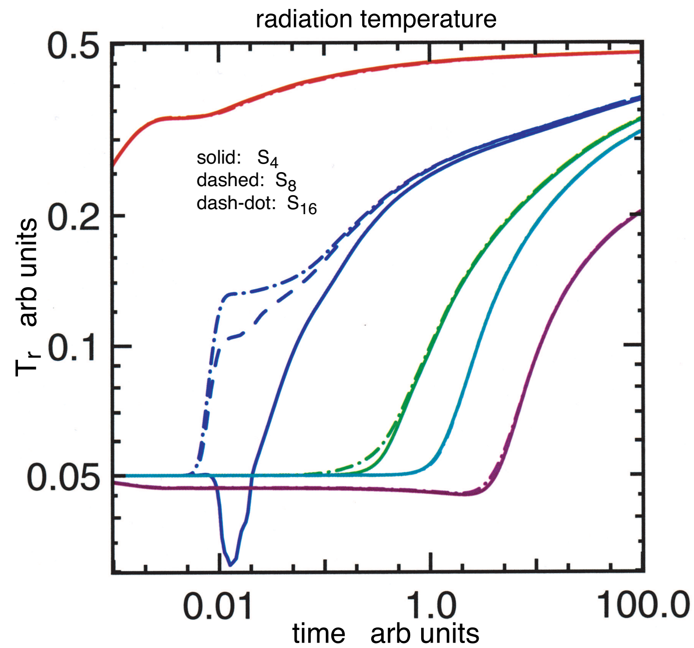
- The object is to find the time dependence of the radiation energy density at various places along the pipe

- It is known that diffusion and transport give quite different results for this problem

- The precise definition of the problem is in Graziani, F. and LeBlanc, J., UCRL-MI-143393 (2000)

Crooked-pipe results with S_4, S_8 and S_{16} (Paul Nowak)





The curves show temperatures at the 5 fiducial locations. The greatest sensitivity is at the first right-angle bend, where S_4 has a hard time getting the radiation arrival right

Crooked-pipe summary

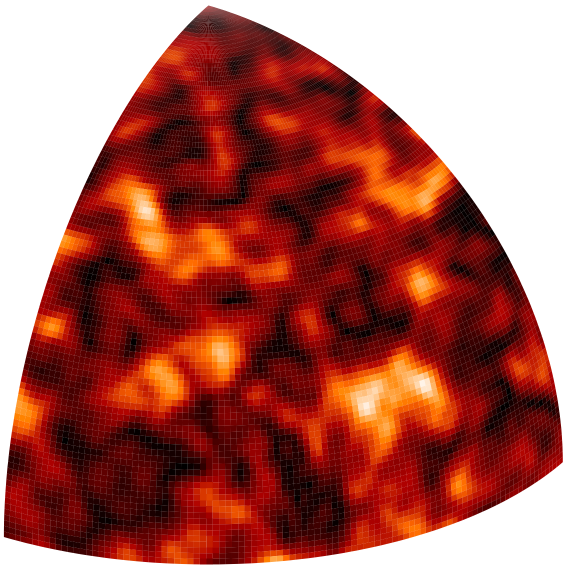
- I am not going to say any more about this problem
- Nick Gentile has published a description of his Implicit Monte Carlo Diffusion method, and a hybrid IMD/IMC method, including studies of the crooked-pipe problem, in Gentile, N. A., *J. Comp. Phys.*, **172**, 543–571 (2001)
- In Nick's following talk he will describe all this
- Paul Nowak has studied this problem with 2-D S_n, and Nick will describe some of these results also
- The short version is that IMD/IMC and S_n both perform well

Case 5: Angle, angles, angles

"The three most important things about radiation transport in 2-D and 3-D are angles, angles and angles"

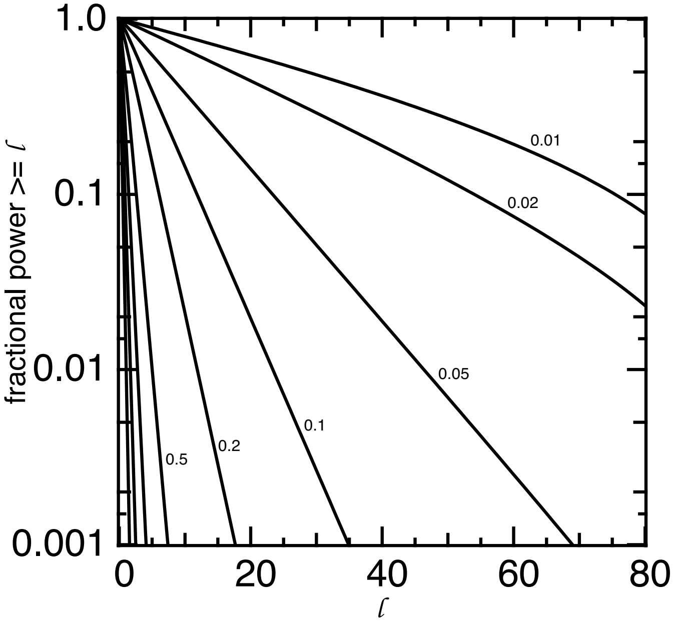
- Most of our S_n transport calculations are not converged in angles, and doubling the angle set halves the error, which is none too small
- Double angles means double running time, which is already (for S_8, 50 groups, 10^6 zones) $\gtrsim 10$ cpu-hours per cycle in 3-D
- This provides a major incentive for keeping the geometry simple: 2-D, or 3-D with only large, well-defined structures

How many angles are needed?



- In 1-D slab problems a few angles suffice
- In 2-D problems with smooth source distributions or short mean free paths something like S_4 or S_8 might be OK
- But it can get much worse
- The picture shows a realization of the angular distribution of the intensity at a point in an infinite 3-D medium with a broad-band random Gaussian emissivity with $|\mathbf{k}| \leq 1.73$ and $\kappa\rho = 0.035$ (I assumed a $1/k$ power spectrum)
- You can see that S_8 has no hope of describing this radiation field

You can estimate the necessary angle resolution from $|\mathbf{k}|$ and $\kappa\rho$



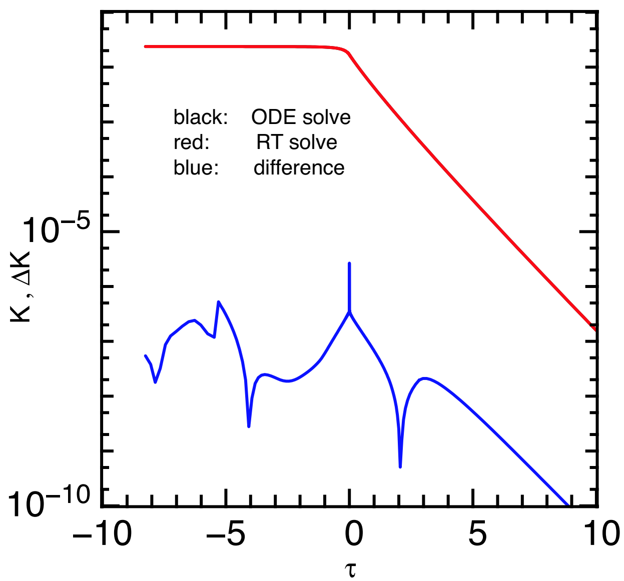
- We consider a single Fourier mode for the emissivity in an infinite medium and construct the spherical harmonic expansion of the intensity
- The plot is the fraction of the total power in harmonics above ℓ. The parameter on the curves is $\kappa\rho/k$
- A rule of thumb is that to see at least 90% of the power you need ℓs up to at least $k/(\kappa\rho) = k\lambda_p$, where λ_p is the radiation mean free path
- The $\ell_{\max}$ equivalent to S_n order N is around $\ell_{\max} = N$ (it varies because the quadrature set may not be exact for the maximal number of polynomials)

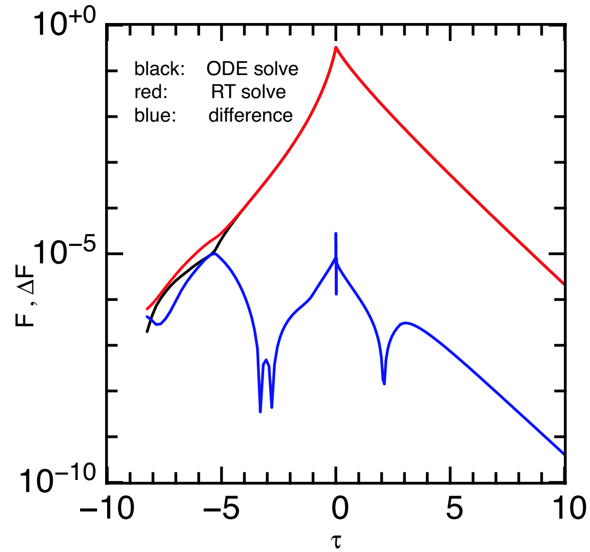
Angles summary

- The S_n order is a major cost factor in transport calculations; the time increases with $N(N+2)$
- It is easy to construct a problem that would need $N \gtrapprox 100$ for an accurate solution; the solar chromosphere is of this sort
- So far, the best method of treating such problems is, “Don’t do that”
- The Reed-Hill-Mordant benchmark is one case where S_8 is noticeably not good enough compared with S_{24}

Backup Slides

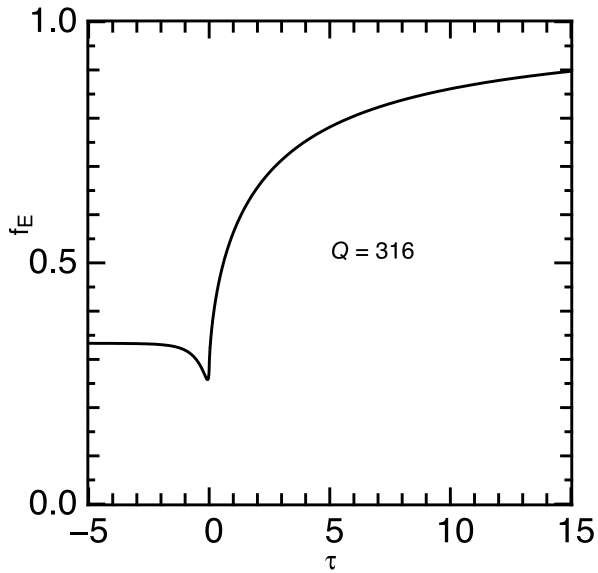
Consistency

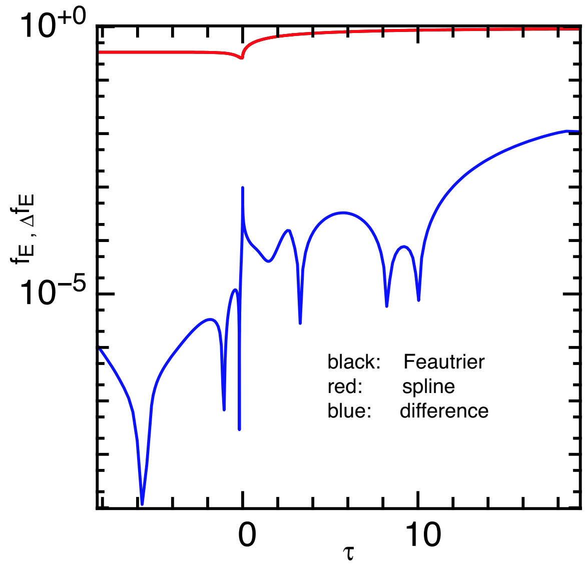




A measure of both f_E convergence and ODE and transfer accuracy is whether the radiation moments from the ODE agree with those from the transfer solution. Here ($Q = 316$) K is very good, and F is good except in the downstream region where it is very small and the ODE is very stiff

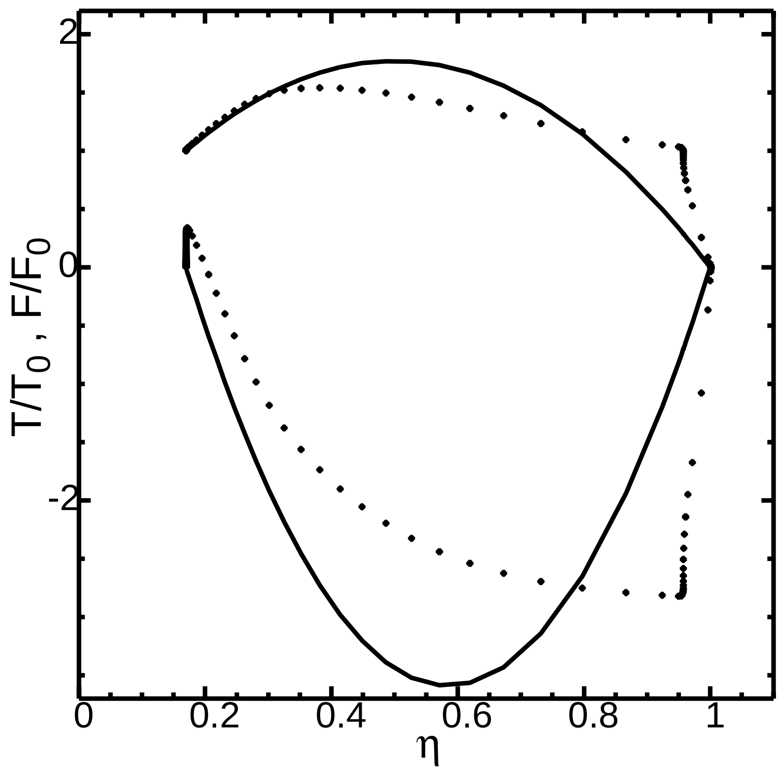
Eddington factor check





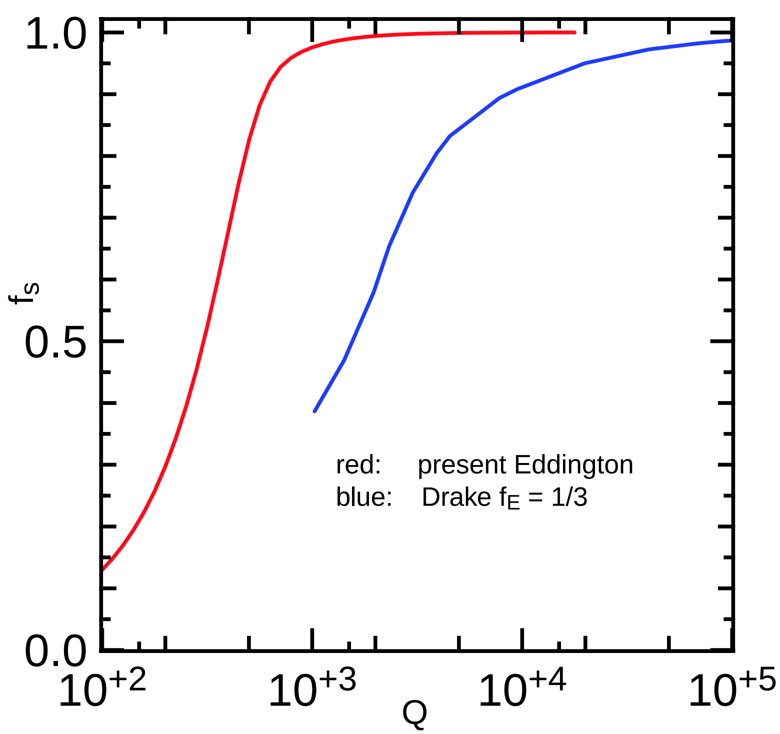
For a given relation of τ to η, there are two quite different ways of solving the radiative transfer: Feautrier finite difference method, and spline E_n-function quadrature. The left plot shows the non-trivial behavior of f_E in close-up, and the right plot compares the two methods

Some aspects of the Sincell, *et al.,* calculations are puzzling



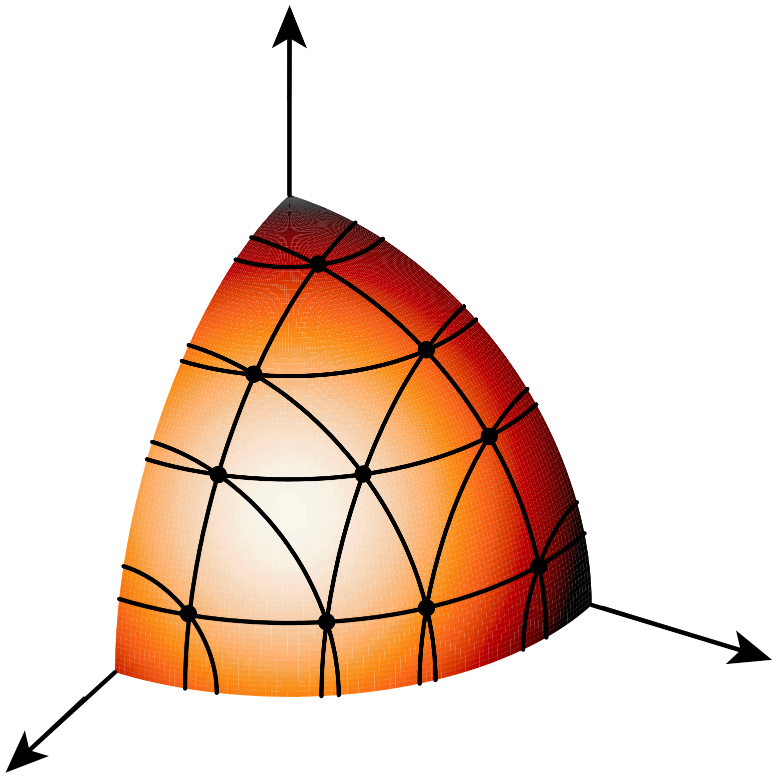
- The figure shows the profiles (dots) through a 16 $\mathrm{km\,s^{-1}}$ shock of the temperature (upper) and the negative flux (lower)
- The curves are the relations given earlier, based on the conservation laws
- Why the calculated points do not follow the conservation relations is mysterious
- The range $1/2 \leq \eta \leq 3/4$ lies within the shock proper, where pseudoviscosity might alter the conservation laws

Comparison with Drake



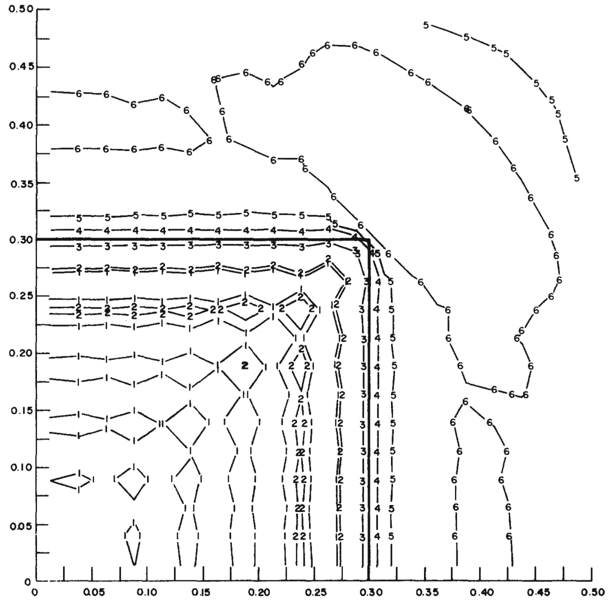
- In a recent preprint Paul Drake reviews the question of whether or not f_s attains unity at any finite Q
- The $f_E \neq 1/3$ and $f_E = 1/3$ cases differ, but numerical results are provided for $f_E = 1/3$, as shown in the figure
- Why Drake's results and the present results differ so much is not understood at present

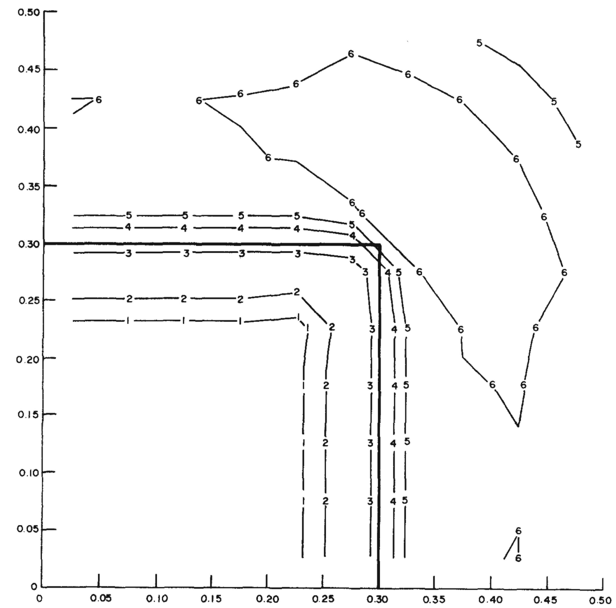
Angle sets in S_n



- There is nothing comparable to Gaussian quadrature for integrations over the unit sphere; that leaves some scope for invention of angle quadrature sets
- Carlson and Lathrop invented the sets most frequently used; the Level-Symmetric set for order $N = 8$ is shown in the picture
- In general, the rays form a triangle picture in each octant, and there are $N/2$ rows in the triangle
- That makes $N(N+2)/8$ angles per octant or $N(N+2)$ in the full sphere

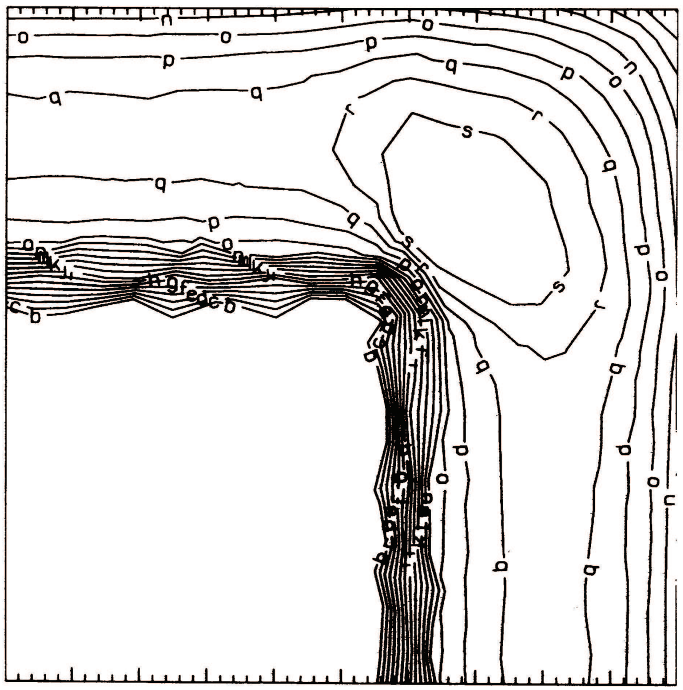
The Reed-Hill-Mordant S_n benchmark

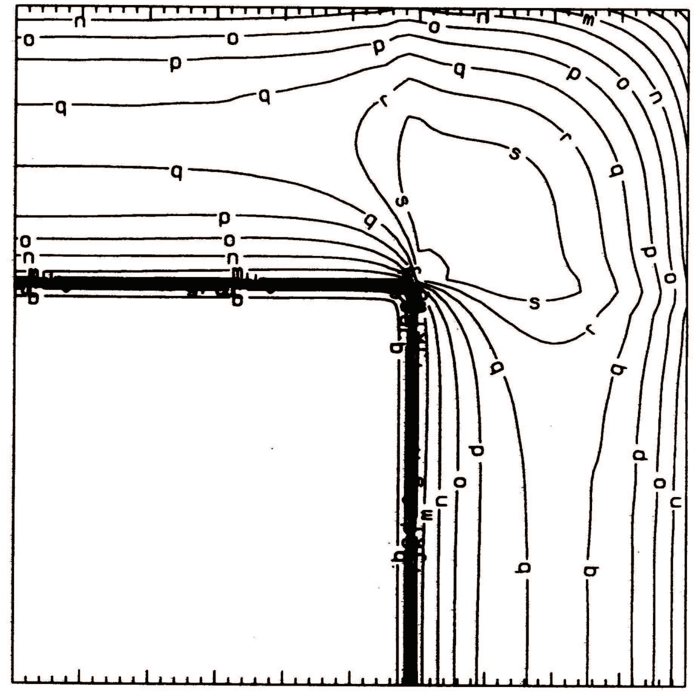




This is an X-Y geometry problem with a glowing translucent square rod that has a cold opaque rod down the middle of it. The left figure shows S_8 calculations by Mordant (1981) with a 20×20 mesh, the right with 10×10

The Dykema, *et al.*, calculations of the Reed-Hill-Mordant problem show the effect of more zones and S_{24}





Both calculations are S_{24}; the left has a distorted 20×20 mesh, the right has 60×60. The difference in angular resolution for S_8 vs. S_{24} is $26°$ vs. $9°$