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Title: Opacity Treatments for Thermal Radiative Transport

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Opacity Treatments for Thermal Radiative Transport

25th International Conference on Transport Theory

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Computational Physics and Methods (CCS-2)
Los Alamos National Laboratory

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Overview

- Multigroup thermal radiation transport requires an averaging choice (weight function) for the opacity in each energy group.
- Classic choices are accurate in a specific solution regime:
  - Planck average (correct in emission-dominated limit)
  - Rosseland average (correct in equilibrium-diffusion limit)
- For problems such as ICF, where x-ray burn-through timings are critical, we prefer using Rosseland.
- But we'd like to use Planck where appropriate, such as emission from a hot interior boundary (*e.g.*, hohlraum).
- There are several methods that attempt to satisfy both of these limits, each in a certain sense.
- We'll review several approaches and compare results.

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Primary goal

- Accurate results for a minimum (or at least affordable) number of groups.

Outline

Background

For simplicity, assume coherent isotropic scattering and LTE emission. Then the radiation intensity $I(\mathbf{x}, t, \nu, \mathbf{\Omega})$ satisfies

$$\frac{1}{c}\partial_t I + \mathbf{\Omega} \cdot \nabla I + \sigma_t I = \sigma_a B + \frac{c}{4\pi}\sigma_s E_\nu \,,$$

where $cE_\nu = \int_{4\pi} I d\Omega$, $B = B(\nu, T_e)$, $\sigma_*(\mathbf{x}, t, \nu)$. Integrate over $\nu_g < \nu < \nu_{g+1}$ (group-g):

$$\frac{1}{c}\partial_t I_g + \mathbf{\Omega} \cdot \nabla I_g + \langle \sigma_t I \rangle_g = \langle \sigma_a B \rangle_g + \frac{c}{4\pi} \langle \sigma_s E_\nu \rangle_g \,.$$

Typically written in the form:

$$\frac{1}{c}\partial_t I_g + \mathbf{\Omega} \cdot \nabla I_g + \sigma_{t,g} I_g = \sigma_{a,g} B_g + \frac{c}{4\pi}\sigma_{s,g} E_g \,.$$

How do we specify the group-averaged opacities $\sigma_{t,g}$, $\sigma_{a,g}$ and $\sigma_{s,g}$?

Some options for the opacity averages

Exact removal

$$\sigma^{I}_{t,g}(\boldsymbol{\Omega}) = \langle \sigma_t I \rangle_g / \langle I \rangle_g$$
$\implies$ Too difficult

Planck average

$$\sigma^{P}_{a,g} = \langle \sigma_a B \rangle_g / \langle B \rangle_g$$
$\implies$ LTE emission is exact

Rosseland average

$$\sigma^{R}_{t,g} = \langle B_T \rangle_g / \langle \sigma_t^{-1} B_T \rangle_g$$
$\implies$ Equi-diff exact

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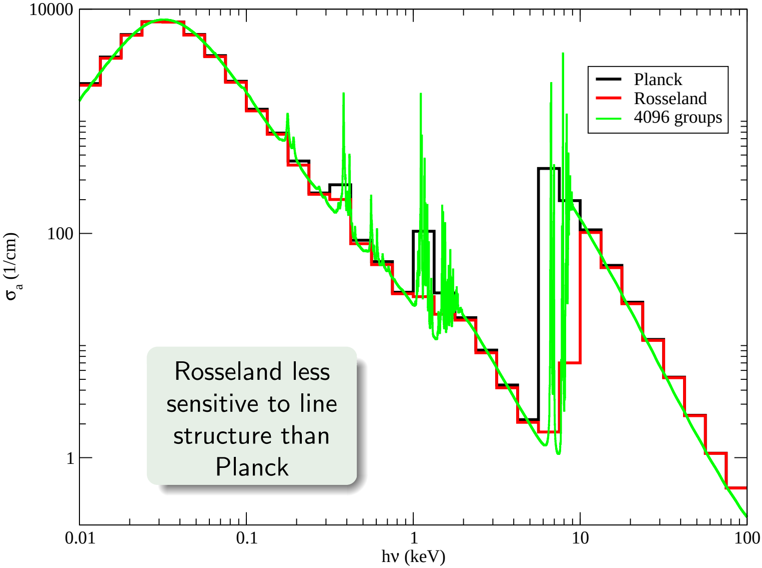
$\implies$ Equi-diff exact

Alternatives

- **Multiband**: Strives to resolve opacity variation. May use either Planck or Rosseland as a weighting, within each group.
- **Solution adaptive**: Dynamic choice based on local solution conditions (Sampson 1965, Ludwig 1992, Clouet 2000). Rough idea: Detect optically-thick regions and use Rosseland; transition to Planck in thinner regions.
- **Artificial scattering**: Use Planck emission, but add scattering to ensure Rosseland limit is also satisfied (Pomraning 1971).
- **Reconstruction**: Use Rosseland and Planck values to reconstruct new values that satisfy Rosseland and/or Planck in a certain sense (*e.g.*, over expanded group ranges).

Example of iron spectrum and group averages

$T_e = 1$ keV, $\rho = 1$ g/cc, 32 groups



Rosseland less sensitive to line structure than Planck

Outline

A P_N approach to artificial scattering

- Write the first two angular moment equations as:

$$\partial_t E_g + \nabla \cdot \mathbf{F}_g = \sigma_{a,g}^{P} \left(4\pi B_g - cE_g\right) ,$$
$$\frac{1}{c}\partial_t \mathbf{F}_g + c\nabla \cdot \mathbf{P}_g = -\sigma_{t,g}^{R} \mathbf{F}_g .$$

- Using different opacity averages is common for nonequilibrium diffusion.
- Desirable properties:
  - Emission is exact, $\sigma_{a,g}^{P} B_g$.
  - In optically-thick regions, $\mathbf{F}_g \approx -\left(c/3\sigma_{t,g}^{R}\right) \nabla E_g$.
  - The higher-order moment equations, using Rosseland or Planck, don't change these properties.

For the grey case, Pomraning derived a family of methods that yield the moment equations above[a]

[a] JQSRT, vol. 11, pp. 597–615 (1971)

Artificial Scattering

Based on Pomraning's 1971 "effective scattering" approach

- Add a term proportional to $\sigma^P_{t,g} - \sigma^R_{t,g}$:

$$\frac{1}{c}\partial_t I_g + \mathbf{\Omega} \cdot \nabla I_g + \sigma^P_{t,g} I_g = \sigma^P_{a,g} B_g + \frac{c}{4\pi}\sigma_{s,g} E_g + \left(\sigma^P_{t,g} - \sigma^R_{t,g}\right) S_g \, .$$

  and select S_g to satisfy the moment equations on the previous slide.

- Isotropic:
  - $S_g = I_g - \frac{c}{4\pi} E_g$.
  - Most accurate in Pomraning's numerical results (grey cases).
  - But may result in negative total scattering.
- Linear: $S_g = \frac{3}{4\pi}\mathbf{\Omega} \cdot \mathbf{F}_g$.
- Mixed: Use isotropic approach, unless the total scattering is negative, in which case use linear.
  - Approach taken in this study.
- Any of these choices satisfy the equilibrium-diffusion limit.

Outline

Reconstruction of $\sigma_{a,g}$

- Given: $\sigma^P_{a,g}$, $\sigma^R_{a,g}$, ... for each group-g.
- Use these integral moments to *reconstruct* the underlying function $\sigma_a(\nu)$.
- Unlike artificial scattering, a pre-processing step.
- Some options:

1. Finite element: Reconstruct a function $\sigma_a(\nu)$ for each $\nu \in [\nu_g, \nu_{g+1}]$ that satisfies moments ("modal" approach):
   - Example: $\sigma_a(\nu) = C/\nu^p$. Select C and p to satisfy both Planck and Rosseland.
   - Not robust when line structure is present.
   - Our current multigroup implementations require modification.
   - Leave for future work.
2. Double interval: For each odd-g, find reconstructed values $\sigma_{a,g}$ and $\sigma_{a,g+1}$ so that both the Planck and Rosseland averages are satisfied over the double interval $[\nu_g, \nu_{g+2}]$ (Lowrie & Haut 2014; related to Cullen & Pomraning 1980).
3. Weighted Planck. Described next.

Weighted Planck

- Scale all Planck opacities by α, to give the grey Rosseland:

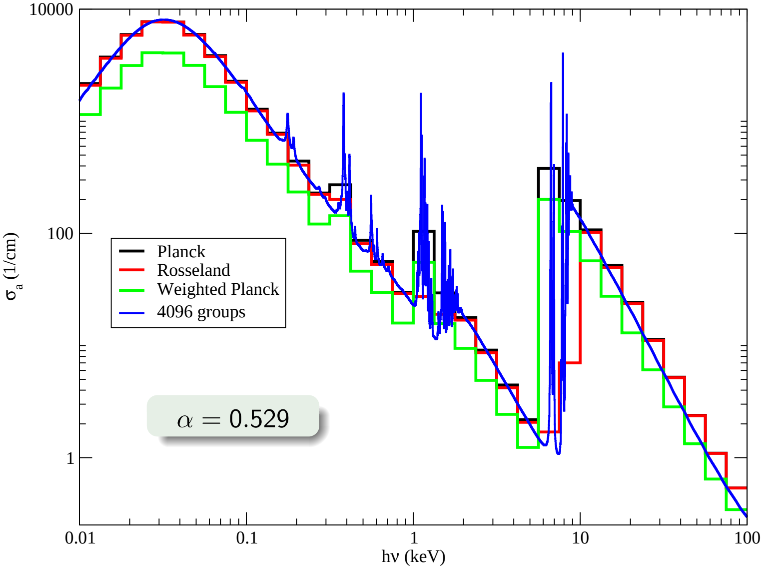
$$\sum_g \left(\alpha\sigma^P_{a,g} + \sigma_{s,g}\right)^{-1} (dB/dT)_g = \sum_g \left(\sigma^R_{t,g}\right)^{-1} (dB/dT)_g \ .$$

- Set $\sigma_{a,g} = \alpha\sigma^P_{a,g}$; scattering unchanged.
- Borrowed from idea used for neutron transport.[1]
- Typically, $0 < \alpha \leq 1$.
- Requires nonlinear solve for α, but there's only one root.

[1] Saller, Larsen, Downar, "An Asymptotic Scaling Factor for Multigroup Cross Sections," *ANS Mathematics & Computation Conference*, Nashville, TN (2015).

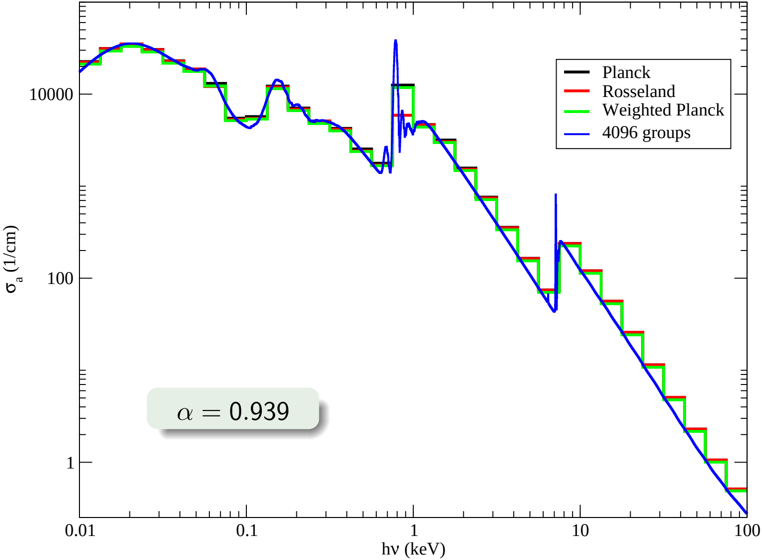
Weighted Planck spectrum: $T_e = 1$ keV

$\rho = 1$ g/cc, 32 groups



Weighted Planck spectrum: $T_e = 0.1$ keV

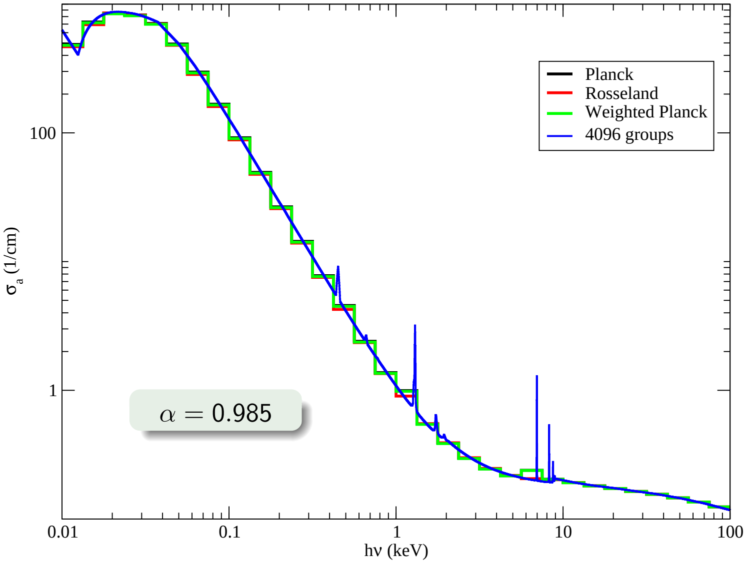
$\rho = 1$ g/cc, 32 groups



$\alpha = 0.939$

Weighted Planck spectrum: $T_e = 10$ keV

$\rho = 1$ g/cc, 32 groups



$\alpha = 0.985$

Pomraning '71 vs. Weighted Planck

Summary

Value	Pomraning '71	Weighted Planck
Emission	$\sigma_{a,g}^{P} B_g$	$\alpha \sigma_{a,g}^{P} B_g$
$\mathbf{F}_g^{(1)}$	$-\frac{c}{3\sigma_{t,g}^{R}} \nabla B_g^{(0)}$	$-\frac{c}{3(\alpha\sigma_{a,g}^{P}+\sigma_{s,g})} \nabla B_g^{(0)}$
$\mathbf{F}^{(1)}$	$-\frac{c}{3\sigma_t^{R}} \nabla B^{(0)}$	$-\frac{c}{3\sigma_t^{R}} \nabla B^{(0)}$
Scattering	$\frac{c}{4\pi}\sigma_{s,g} E_g + \left(\sigma_{t,g}^{P} - \sigma_{t,g}^{R}\right) S_g$	$\frac{c}{4\pi}\sigma_{s,g} E_g$

Comments

- Red indicates exact value.
- $\mathbf{F}_g^{(1)}$ is the $O(\varepsilon^1)$-value of the radiative flux from the equilibrium-diffusion limit analysis.
- $\mathbf{F}^{(1)} = \sum_g \mathbf{F}_g^{(1)}$.
- For smooth opacities, $(1-\alpha) \propto \max_g \left(\sigma_{t,g}^{P} - \sigma_{t,g}^{R}\right)$.

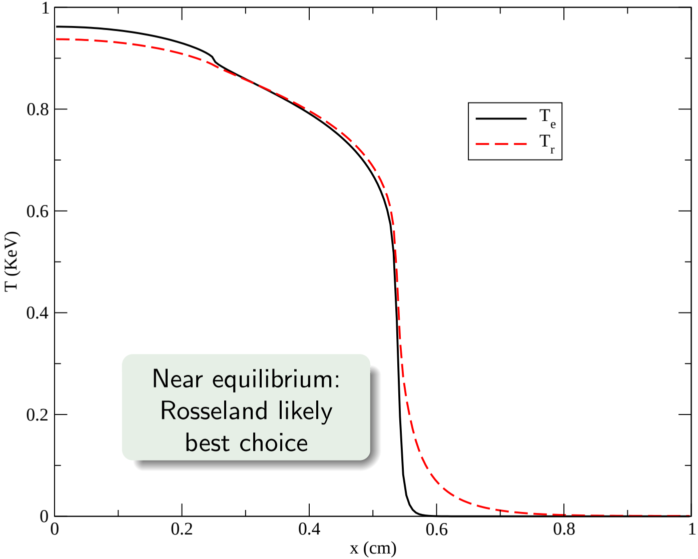
Outline

Model Problems

- 3 problems; extensions to Su & Olson (1997), but no analytic solutions.
- 1-D slab, $0 \leq x \leq 1$. Reflection $x = 0$; vacuum $x = 1$.
- Constant volumetric material source S_v applied over $0 \leq x \leq 0.25$.
- Initial condition: $T_r = 0$ and $T_e = \begin{cases} 10\,\text{eV} & 0 \leq x \leq 0.25, \\ 0.001\,\text{eV} & 0.25 < x \leq 1. \end{cases}$
- Increasing S_v drives the source region more out of equilibrium.
  - Expect Planck accurate for emission-dominated problems.
  - $T_{e,\max}$ is a good metric.
- Unless optically thin, a Marshak wave propagates from the source region.
  - Expect Rosseland accurate for optically-thick problems.
  - Wave location a good metric.
- All results computed with Capsaicin (S_{12}); opacities from TOPS.

Sample Results for Model Problem, Iron, Small S_ν

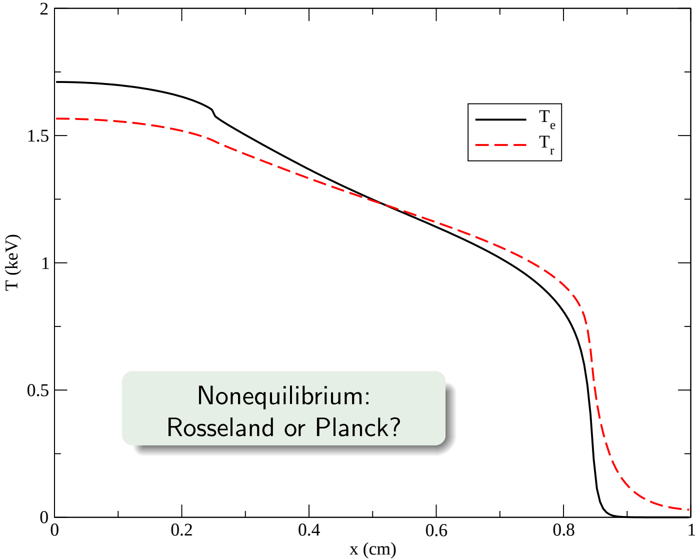
$S_\nu = 0.1$ jerks/cm^3/ns, $t = 2$ ns, 2048 groups



Near equilibrium: Rosseland likely best choice

Sample Results for Model Problem, Iron, Large S_ν

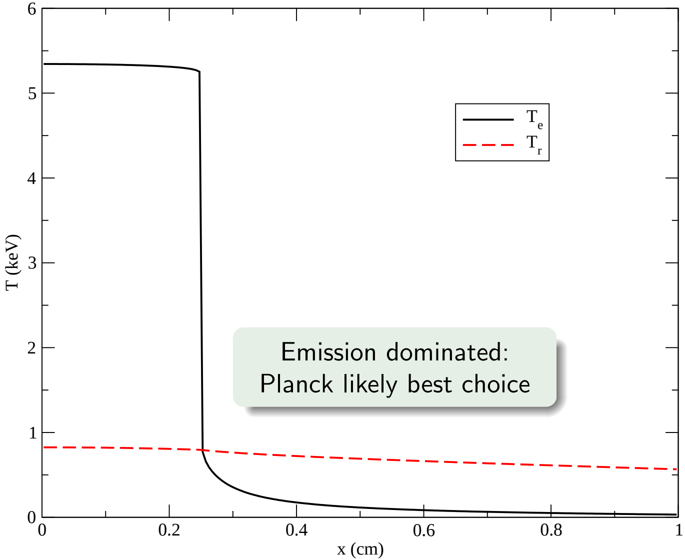
$S_\nu = 1$ jerks/cm^3/ns, $t = 0.6$ ns, 2048 groups



Nonequilibrium:
Rosseland or Planck?

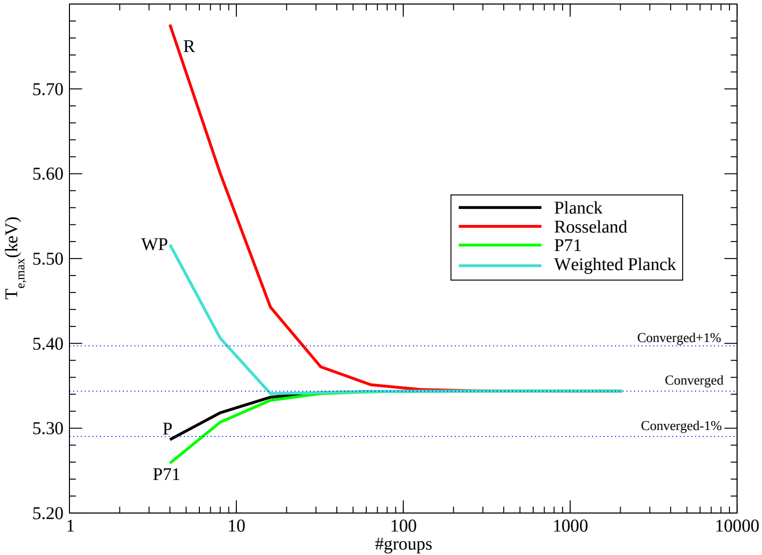
Model Problem with Helium, Large S_v

$S_v = 1$ jerks/cm^3/ns, $t = 0.6$ ns, 2048 groups



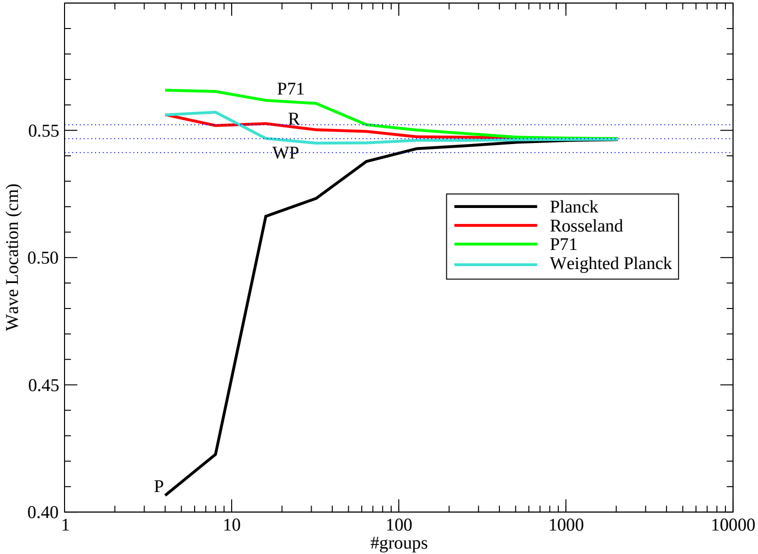
Convergence of $T_{e,\max}$

Emission-dominated problem (Helium, $S_v = 1$ jerks/cm^3/ns)



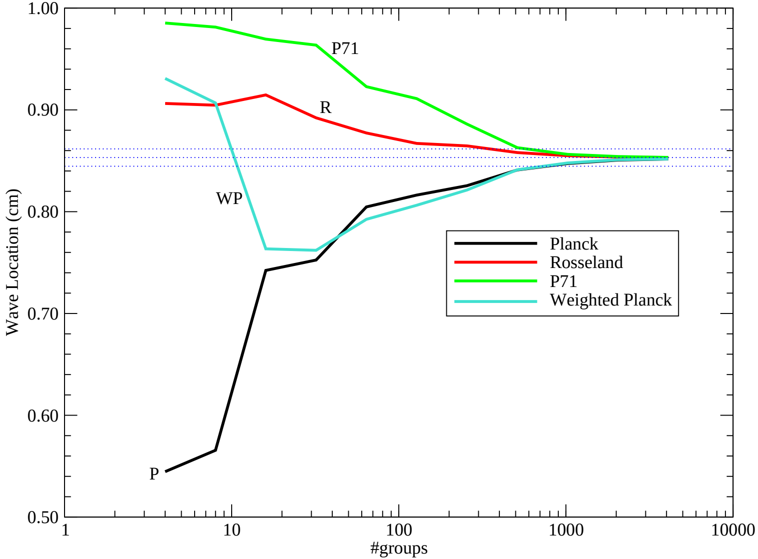
Convergence of Marshak Wave Position

Near-equilibrium problem (Iron, $S_v = 0.1$ jerks/cm^3/ns)



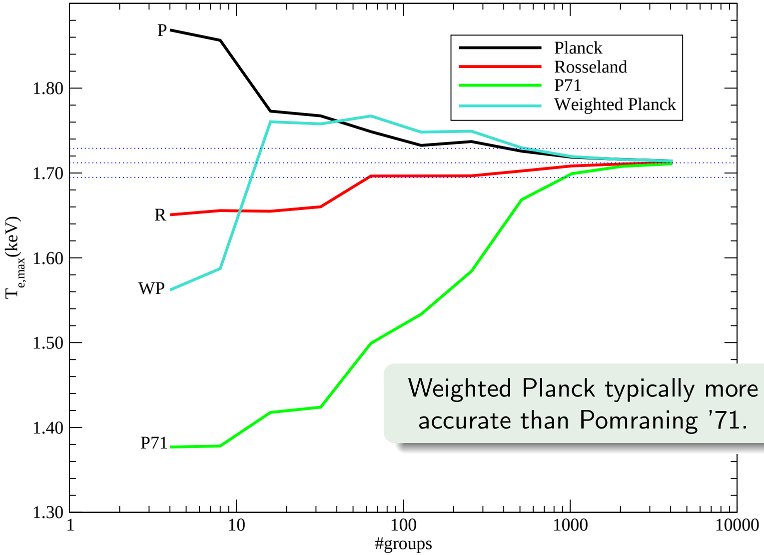
Convergence of Marshak Wave Position

Nonequilibrium problem (Iron, $S_v = 1$ jerks/cm^3/ns)



Convergence of Maximum Temperature

Nonequilibrium problem (Iron, $S_v = 1$ jerks/cm^3/ns)



Weighted Planck typically more accurate than Pomraning '71.

Weighted Planck with cutoff

- High-energy groups are not optically-thick, so they should not be weighted:

$$\sigma_{a,g} = \alpha_g \sigma_{a,g}^P$$

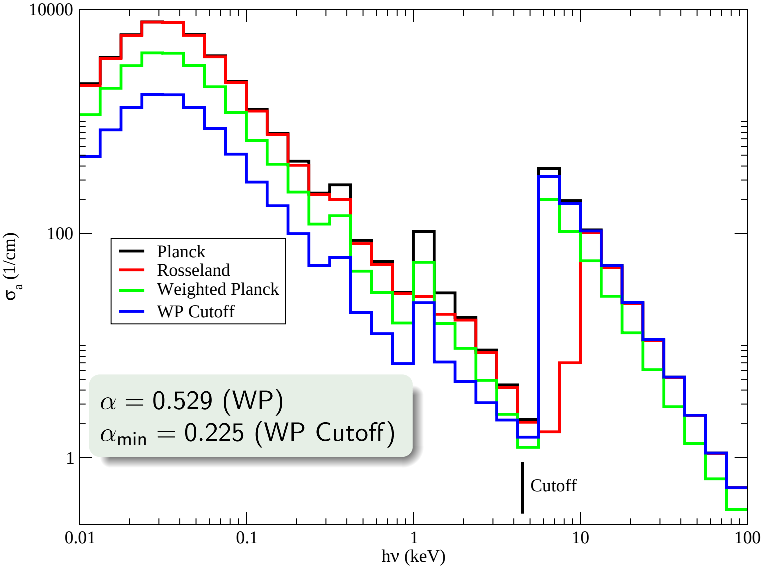
where $\alpha_g = 1$ for large photon energies,

$$\alpha_g = 1 + \frac{\beta}{1 + (\nu_g/\nu_C)^\gamma} .$$

- β is a constant, to be determined so that grey Rosseland value is attained.
- ν_C is the cutoff frequency.
- γ is selected so that α_g transitions from $\alpha = 1$ to $\alpha = \alpha_{\text{min}}$ over ≈ 4 groups.
- Apply only for 16 or more groups.

WP with spectrum cutoff: $T_e = 1$ keV

$\rho = 1$ g/cc, 32 groups, $h\nu_C = 4.5\,T_e$

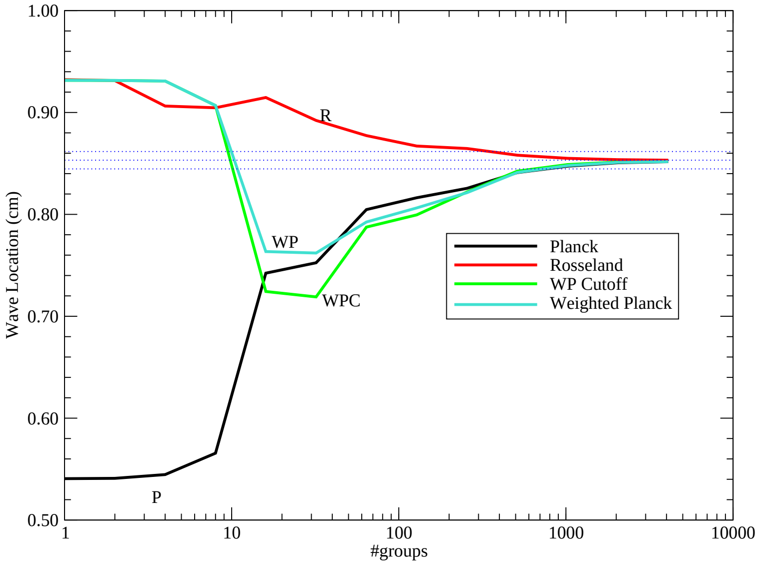


$\alpha = 0.529$ (WP)

$\alpha_{\text{min}} = 0.225$ (WP Cutoff)

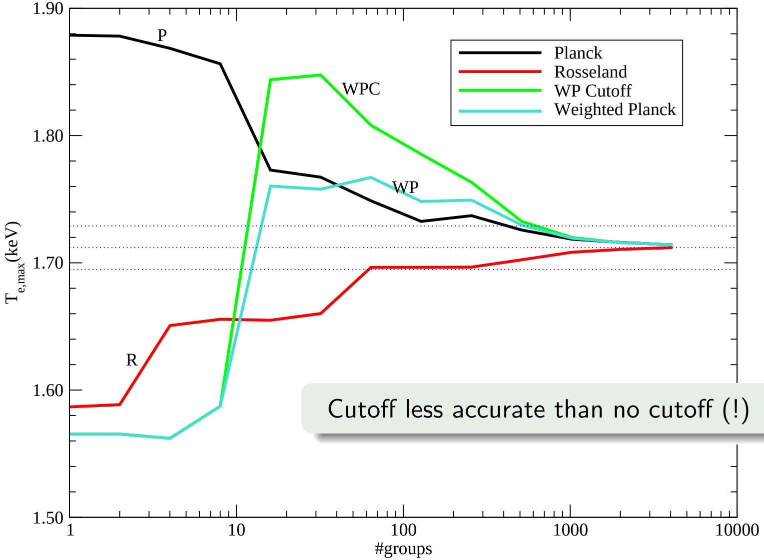
Cutoff: Convergence of Marshak Wave Position

Nonequilibrium problem (Iron, $S_v = 1$ jerks/cm^3/ns)



Cutoff: Convergence of Maximum Temperature

Nonequilibrium problem (Iron, $S_v = 1$ jerks/cm^3/ns)



Cutoff less accurate than no cutoff (!)

Summary and Future Work

Summary

- It's straightforward to devise a group treatment that's accurate in both the equilibrium-diffusion and emission-dominated limits.
- Unfortunately, the method may be inaccurate away from these limits.
- A promising approach is Weighted Planck, but more work is needed.
- The assumption "use Planck when thin" needs revisiting.

Future work

- Comparisons for a wider range of problems.
- Error bounds.
- Combine Weighted Planck with multiband.

Questions?

Acknowledgments

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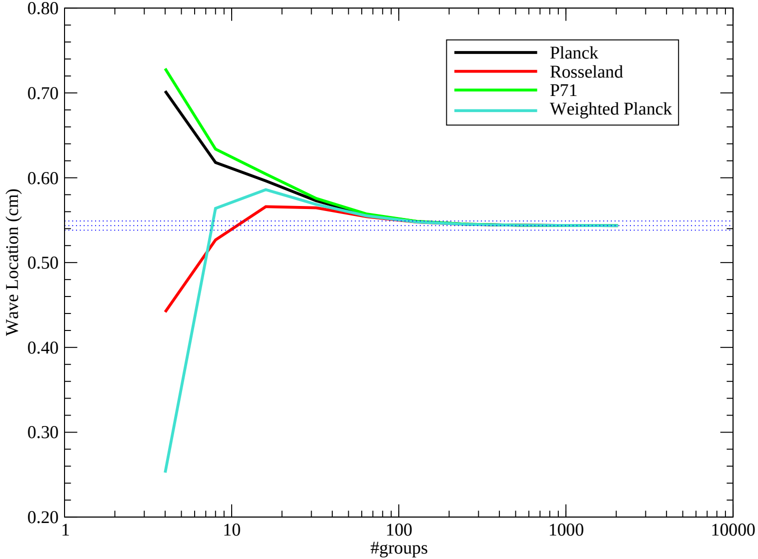
EXTRAS

Convergence of Marshak Wave Position

Emission-dominated problem (Helium, $S_v = 1$ jerks/cm^3/ns)



Convergence of $T_{e,\max}$

Near-equilibrium problem (Iron, $S_v = 0.1$ jerks/cm^3/ns)