Radiative heat transfer solver with fluid motion

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Abstract:
Work is work for some, but for some it is play.

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Contents

1 Definitions

1.1 Independent variables

We refer to the following independent variables:

- Position in the cartesian space $\{x, y, z\}$ is denoted with $\mathbf{x}$ and each component having units $[cm]$.

- Direction, $\{\varphi, \theta\}$, is denoted with $\mathbf{\Omega}$ which takes on the form

$$\mathbf{\Omega} = \begin{bmatrix} \Omega_x \\ \Omega_y \\ \Omega_z \end{bmatrix} \text{ and/or } \mathbf{\Omega} = \begin{bmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{bmatrix},$$

  where φ is the azimuthal-angle and θ is the polar-angle, both in spherical coordinates. Commonly, $\cos\theta$, is denoted with μ. The general dimension of angular phase space is $[steridian]$.

- Photon frequency, ν in $[Hertz]$ or $[s^{-1}]$.

- Time, t in $[s]$.

1.2 Dependent variables

We use the following basic dependent variables:

- The foundation of the dependent unknowns is the **radiation angular intensity**, $I(\mathbf{x}, \mathbf{\Omega}, \nu, t)$ with units $[Joule/cm^2{-}s{-}steradian{-}Hz]$. We often use the corresponding angle-integral of this quantity, $\phi(\mathbf{x}, \nu, t)$, and define it as

$$\phi(\mathbf{x}, \nu, t) = \mathcal{E}c = \int_{4\pi} I(\mathbf{x}, \mathbf{\Omega}, \nu, t)\ d\mathbf{\Omega} \tag{1.1}$$

  with units $[Joule/cm^2{-}s{-}Hz]$. Where c is the speed of light.

- The **radiation energy density**, $\mathcal{E}$, is

$$\mathcal{E}(\mathbf{x}, \nu, t) = \frac{\phi}{c} = \frac{1}{c}\int_{4\pi} I(\mathbf{x}, \mathbf{\Omega}, \nu, t)\ d\mathbf{\Omega} \tag{1.2}$$

  with units $[Joule/cm^3{-}Hz]$.

- The **radiation energy flux**, $\boldsymbol{\mathcal{F}}$, is

$$\boldsymbol{\mathcal{F}}(\mathbf{x}, \nu, t) = \int_{4\pi} \mathbf{\Omega}\ I(\mathbf{x}, \mathbf{\Omega}, \nu, t) d\mathbf{\Omega} \tag{1.3}$$

- **Radiation pressure**, $\boldsymbol{\mathcal{P}}$, is

$$\boldsymbol{\mathcal{P}}(\mathbf{x}, \nu, t) = \frac{1}{c}\int_{4\pi} \mathbf{\Omega}\otimes\mathbf{\Omega} I(\mathbf{x}, \mathbf{\Omega}, \nu, t) d\mathbf{\Omega} \tag{1.4}$$

  and is a tensor.

1.3 Blackbody radiation

A blackbody radiation source, $B(\nu, T)$, is properly described by **Planck's law**,

$$B(\nu, T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{k_B T}} - 1} \tag{1.5}$$

with units $[Joule/cm^2{-}s{-}steridian - Hz]$ where h is Planck's constant and k_B is the Boltzmann constant.

If we integrate the blackbody source over all angle-space and frequencies then we get the mean radiation intensity from a blackbody at temperature T as

$$\begin{aligned} \int_0^\infty \int_{4\pi} B(\nu, T)\ d\mathbf{\Omega} d\nu &= \int_0^\infty \int_{4\pi} \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{k_B T}} - 1}\ d\mathbf{\Omega} d\nu \\ &= 4\pi \int_0^\infty \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{k_B T}} - 1}\ d\nu \\ &= acT^4, \end{aligned} \tag{1.6}$$

with units $[Joule/cm^2{-}s{-}steridian]$ and where a is the **blackbody radiation constant** given by

$$a = \frac{8\pi^5 k_B^4}{15h^3c^3}. \tag{1.7}$$

In both cases this unfortunately is only the intensity. Following Kirchoff's law, which states that the emission and absorption of radiation must be equal in equilibrium, we can determine the **blackbody emission rate**, S_{bb}, from the absorption rate as

$$S_{bb}(\nu, T) = \rho\kappa(\nu)B(\nu, T), \tag{1.8}$$

with units $[Joule/cm^3{-}s{-}steridian{-}Hz]$ where ρ is the material density $[g/cm^3]$ and κ is the opacity $[cm^2/g]$. The combination $\rho\kappa$ is also equal to the macroscopic absorption cross section σ_a, therefore $\rho\kappa(\nu) = \sigma_a$. Data for the opacity of a material is normally available in the form of either the **Rosseland opacity**, κ_{Rs}, or the **Planck opacity**, κ_{Pl}.

2 Conservation equations

2.1 Conservation equation - Radiative transfer

The basic statement of conservation, is

$$\begin{aligned}\frac{1}{c}\frac{\partial I(\mathbf{x},\boldsymbol{\Omega},\nu,t)}{\partial t} &= -\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I(\mathbf{x},\boldsymbol{\Omega},\nu,t) - \sigma_t(\mathbf{x},\nu)I(\mathbf{x},\boldsymbol{\Omega},\nu,t)\\ &+ \int_0^\infty \int_{4\pi} \frac{\nu}{\nu'}\sigma_s(\mathbf{x},\nu'{\to}\nu,\boldsymbol{\Omega}'{\cdot}\boldsymbol{\Omega})I(\mathbf{x},\boldsymbol{\Omega}',\nu',t)d\nu' d\boldsymbol{\Omega}'\\ &+ \sigma_a(\mathbf{x},\nu)B(\nu,T(\mathbf{x},t)) + S\end{aligned} \tag{2.1}$$

where S is any other sources/sinks of radiation intensity.

2.2 Radiative transfer assuming isotropic Thompson scattering

Assuming Thomson-scattering[1] is the only form of scattering, gives

$$\begin{aligned}\frac{1}{c}\frac{\partial I(\mathbf{x},\boldsymbol{\Omega},\nu,t)}{\partial t} &= -\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I(\mathbf{x},\boldsymbol{\Omega},\nu,t) - \sigma_t(\mathbf{x},\nu)I(\mathbf{x},\boldsymbol{\Omega},\nu,t)\\ &+ \frac{\sigma_s(\mathbf{x},\nu)}{4\pi}c\mathcal{E}(\mathbf{x},\nu) + \sigma_a(\mathbf{x},\nu)B(\nu,T(\mathbf{x},t)) + S\end{aligned} \tag{2.2}$$

where S is any other sources/sinks of radiation intensity.

Using energy instead of frequency, $\nu \to E$:

$$\begin{aligned}\frac{1}{c}\frac{\partial I(\mathbf{x},\boldsymbol{\Omega},E,t)}{\partial t} &= -\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I(\mathbf{x},\boldsymbol{\Omega},E,t) - \sigma_t(\mathbf{x},E)I(\mathbf{x},\boldsymbol{\Omega},E,t)\\ &+ \frac{\sigma_s(\mathbf{x},E)}{4\pi}c\mathcal{E}(\mathbf{x},E) + \sigma_a(\mathbf{x},E)B(E,T(\mathbf{x},t)) + S\end{aligned} \tag{2.3}$$

where S is any other sources/sinks of radiation intensity.

2.3 Radiative transfer with material motion corrections

Applying relativistic corrections for a material in motion, we can derive

$$\begin{aligned}\frac{1}{c}\frac{\partial I(\mathbf{x},\boldsymbol{\Omega},E,t)}{\partial t} &= -\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I(\mathbf{x},\boldsymbol{\Omega},E,t) - \left(\frac{E_0}{E}\right)\sigma_t(\mathbf{x},E_0)I(\mathbf{x},\boldsymbol{\Omega},E,t)\\ &+ \left(\frac{E}{E_0}\right)^2 \frac{\sigma_s(\mathbf{x},E)}{4\pi}\int_{4\pi}\left(\frac{E_0}{E'}\right)I(\mathbf{x},\boldsymbol{\Omega}',E',t)d\boldsymbol{\Omega}' + \left(\frac{E}{E_0}\right)^2\sigma_a(\mathbf{x},E_0)B(E_0,T(\mathbf{x},t)) + S,\end{aligned} \tag{2.4}$$

where

$$E_0 = E\gamma\left(1-\boldsymbol{\Omega}\cdot\frac{\mathbf{u}}{c}\right) \tag{2.5}$$

$$\gamma = \left[1-\left(\frac{||\mathbf{u}||}{c}\right)^2\right]^{-\frac{1}{2}} \tag{2.6}$$

$$\frac{E_0}{E'} = \gamma\left(1-\boldsymbol{\Omega}'\cdot\frac{\mathbf{u}}{c}\right) \tag{2.7}$$

$$E' = E\frac{1-\boldsymbol{\Omega}\cdot\frac{\mathbf{u}}{c}}{1-\boldsymbol{\Omega}'\cdot\frac{\mathbf{u}}{c}} \tag{2.8}$$

[1] Thomson scattering is the elastic scattering of electromagnetic radiation by a free charged particle. The particle's kinetic energy- as well as the photon's frequency, does not change in such a scattering. The scattering is also isotropic.

2.4 Radiative transfer with material velocity dependencies expanded to $\mathcal{O}(v/c)$

$$
\begin{aligned}
&\frac{1}{c}\frac{\partial I(\mathbf{x},\boldsymbol{\Omega},E,t)}{\partial t}+\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}I(\mathbf{x},\boldsymbol{\Omega},E,t)+\sigma_t(\mathbf{x},E)I(\mathbf{x},\boldsymbol{\Omega},E,t)\\
=&\frac{\sigma_s(\mathbf{x},E)}{4\pi}\phi(E)+\sigma_a(\mathbf{x},E)B(E,T(\mathbf{x},t))\\
&+\left[\left(\sigma_t+E\frac{\partial\sigma_a}{\partial E}\right)I+\frac{\sigma_s}{4\pi}\left(2\phi-E\frac{\partial\phi}{\partial E}\right)+2\sigma_a B(E,T)-B(E,T)\frac{\partial\sigma_a}{\partial E}-\sigma_a E\frac{\partial B(E,T)}{\partial E}\right]\boldsymbol{\Omega}\cdot\frac{\mathbf{u}}{c}\\
&-\frac{\sigma_s}{4\pi}\left(\boldsymbol{\mathcal{F}}-E\frac{\partial\boldsymbol{\mathcal{F}}}{\partial E}\right)\cdot\frac{\mathbf{u}}{c}
\end{aligned}
\tag{2.9}
$$

Radiation energy equation:
Obtained by integrating the transport equation over energy and angle

$$
\begin{aligned}
\frac{\partial\mathcal{E}(\mathbf{x},t)}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}(\mathbf{x},t)=&\int_0^\infty\sigma_a(\mathbf{x},E)\big(4\pi B(E,T)-\phi(\mathbf{x},E,t)\big)dE\\
&+\int_0^\infty\left(\sigma_a+E\frac{\partial\sigma_a}{\partial E}-\sigma_s(E)\right)\boldsymbol{\mathcal{F}}\cdot\frac{\mathbf{u}}{c}dE
\end{aligned}
\tag{2.10}
$$

Radiation momentum equation:
Obtained by first multiplying by $\frac{1}{c}\boldsymbol{\Omega}$, then integrating over all directions and energies,

$$
\begin{aligned}
\frac{1}{c^2}\frac{\partial\boldsymbol{\mathcal{F}}}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{P}}=&-\int_0^\infty\frac{\sigma_t}{c}\boldsymbol{\mathcal{F}}dE\\
&+\int_0^\infty\big(\sigma_s\phi+\sigma_a 4\pi B(E,T)\big)\frac{\mathbf{u}}{c^2}dE\\
&+\int_0^\infty\left(\sigma_a+E\frac{\partial\sigma_a}{\partial E}+\sigma_s\right)\boldsymbol{\mathcal{P}}\cdot\frac{\mathbf{u}}{c}dE
\end{aligned}
\tag{2.11}
$$

2.5 Grey Radiative Transfer

$$
\begin{aligned}
&\frac{1}{c}\frac{\partial I(\mathbf{x},\boldsymbol{\Omega},t)}{\partial t}+\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}I(\mathbf{x},\boldsymbol{\Omega},t)+\sigma_t(\mathbf{x})I(\mathbf{x},\boldsymbol{\Omega},t)\\
=&\frac{\sigma_s}{4\pi}\phi+\frac{\sigma_a}{4\pi}acT^4\\
&+\left[\sigma_t I+\frac{\sigma_s}{4\pi}2\phi+2\sigma_a\frac{1}{4\pi}acT^4-\sigma_a E\frac{\partial B(E,T)}{\partial E}\right]\boldsymbol{\Omega}\cdot\frac{\mathbf{u}}{c}\\
&-\frac{\sigma_s}{4\pi}\boldsymbol{\mathcal{F}}\cdot\frac{\mathbf{u}}{c}
\end{aligned}
\tag{2.12}
$$

Radiation energy equation:
Obtained by integrating Eq. (2.12) over energy and angle

$$
\frac{\partial\mathcal{E}(\mathbf{x},t)}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{F}}(\mathbf{x},t)=\sigma_a c\big(aT^4-\mathcal{E}\big)+\big(\sigma_a-\sigma_s\big)\boldsymbol{\mathcal{F}}\cdot\frac{\mathbf{u}}{c}
\tag{2.13}
$$

Radiation momentum equation:
Obtained by first multiplying Eq. (2.12) by $\frac{1}{c}\boldsymbol{\Omega}$, then integrating over all directions and energies,

$$
\frac{1}{c^2}\frac{\partial\boldsymbol{\mathcal{F}}}{\partial t}+\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{P}}=-\frac{\sigma_t}{c}\boldsymbol{\mathcal{F}}+\big(\sigma_s c\mathcal{E}+\sigma_a acT^4\big)\frac{\mathbf{u}}{c^2}+\sigma_t\boldsymbol{\mathcal{P}}\cdot\frac{\mathbf{u}}{c}
\tag{2.14}
$$

2.6 Grey Diffusion Approximation

Approximating the angular dependence of $I(\mathbf{\Omega})$ with a P_1 spherical harmonic expansion, such that the entries of $\boldsymbol{\mathcal{P}}$ are given by

$$(\boldsymbol{\mathcal{P}})_{i,j} = \frac{1}{3}\mathcal{E}\delta_{i,j}, \tag{2.15}$$

the radiation energy equation is unaffected but the radiation momentum equation changes. We repeat the radiation energy equation below, and the altered radiation moment equations:

$$\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{F}}(\mathbf{x}, t) = \sigma_a c\big(aT^4 - \mathcal{E}\big) + \big(\sigma_a - \sigma_s\big)\boldsymbol{\mathcal{F}} \cdot \frac{\mathbf{u}}{c}, \tag{2.16}$$

$$\frac{1}{3}\boldsymbol{\nabla}\mathcal{E} = -\frac{\sigma_t}{c}\boldsymbol{\mathcal{F}} + \big(\sigma_s c\mathcal{E} + \sigma_a acT^4\big)\frac{\mathbf{u}}{c^2} + \sigma_t \frac{1}{3}\mathcal{E}\frac{\mathbf{u}}{c}. \tag{2.17}$$

Useful transformations:

$$\mathcal{E}_0 = \mathcal{E} - \frac{2}{c^2}\boldsymbol{\mathcal{F}} \cdot \mathbf{u} \tag{2.18a}$$

$$\mathcal{E} = \mathcal{E}_0 + \frac{2}{c^2}\boldsymbol{\mathcal{F}}_0 \cdot \mathbf{u} \tag{2.18b}$$

$$\boldsymbol{\mathcal{F}}_0 = \boldsymbol{\mathcal{F}} - \big(\mathcal{E}\mathbf{u} + \boldsymbol{\mathcal{P}} \cdot \mathbf{u}\big) \tag{2.18c}$$

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_0 + \big(\mathcal{E}_0\mathbf{u} + \boldsymbol{\mathcal{P}}_0 \cdot \mathbf{u}\big) \tag{2.18d}$$

$$\boldsymbol{\mathcal{P}}_0 = \boldsymbol{\mathcal{P}} - \frac{2}{c^2}\mathbf{u} \otimes \boldsymbol{\mathcal{F}} \tag{2.18e}$$

$$\boldsymbol{\mathcal{P}} = \boldsymbol{\mathcal{P}}_0 + \frac{2}{c^2}\mathbf{u} \otimes \boldsymbol{\mathcal{F}}_0 \tag{2.18f}$$

With the P_1 approximation

$$\boldsymbol{\mathcal{F}}_0 = \boldsymbol{\mathcal{F}} - \frac{4}{3}\mathcal{E}\mathbf{u} \tag{2.18g}$$

$$\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{F}}_0 + \frac{4}{3}\mathcal{E}\mathbf{u} \tag{2.18h}$$

Applying these transformations the radiation energy- and moment equation can be expressed as

$$\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{F}}(\mathbf{x}, t) = \sigma_a c\big(aT^4 - \mathcal{E}_0\big) - \sigma_t\boldsymbol{\mathcal{F}} \cdot \frac{\mathbf{u}}{c}, \tag{2.19}$$

$$\frac{1}{3}\boldsymbol{\nabla}\mathcal{E} = -\frac{\sigma_t}{c}\boldsymbol{\mathcal{F}}_0 + \sigma_a c\big(aT^4 - \mathcal{E}\big)\frac{\mathbf{u}}{c^2}. \tag{2.20}$$

Several simplifications to these equations are made. Firstly arriving at the expression for the radiation energy equation,

$$\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{F}}(\mathbf{x}, t) = \sigma_a c\big(aT^4 - \mathcal{E}\big) - \sigma_t\boldsymbol{\mathcal{F}}_0 \cdot \frac{\mathbf{u}}{c}, \tag{2.21}$$

then the radiation momentum equation,

$$\frac{1}{3}\boldsymbol{\nabla}\mathcal{E} = -\frac{\sigma_t}{c}\boldsymbol{\mathcal{F}}_0 \tag{2.22}$$

from which we can get expression for $\boldsymbol{\mathcal{F}}_0$ and $\boldsymbol{\mathcal{F}}$ in terms of $\mathcal{E}$ as

$$\boldsymbol{\mathcal{F}}_0 = -\frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E} \tag{2.23}$$

and

$$\begin{aligned} \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} &= -\frac{\sigma_t}{c}\left(\boldsymbol{\mathcal{F}} - \frac{4}{3}\mathcal{E}\mathbf{u}\right) \\ \therefore \boldsymbol{\mathcal{F}} &= -\frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E} + \frac{4}{3}\mathcal{E}\mathbf{u}. \end{aligned} \tag{2.24}$$

These expressions for $\boldsymbol{\mathcal{F}}_0$ and $\boldsymbol{\mathcal{F}}$ are both then inserted into the radiation energy equation as follows

$$
\begin{aligned}
&\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{F}}(\mathbf{x}, t) = \sigma_a c\big(aT^4 - \mathcal{E}\big) - \sigma_t \boldsymbol{\mathcal{F}}_0 \cdot \frac{\mathbf{u}}{c} \\
\rightarrow\ &\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla}\cdot\bigg(- \frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E} + \frac{4}{3}\mathcal{E}\mathbf{u}\bigg) = \sigma_a c\big(aT^4 - \mathcal{E}\big) - \sigma_t\bigg(- \frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E}\bigg) \cdot \frac{\mathbf{u}}{c} \\
\rightarrow\ &\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla}\cdot\bigg(- \frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E}\bigg) + \frac{4}{3}\boldsymbol{\nabla}\cdot(\mathcal{E}\mathbf{u}) = \sigma_a c\big(aT^4 - \mathcal{E}\big) + \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}.
\end{aligned}
\tag{2.25}
$$

Arriving at a **diffusion form** of the **radiation energy equation**,

$$
\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla}\cdot\bigg(- \frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E}\bigg) + \frac{4}{3}\boldsymbol{\nabla}\cdot(\mathcal{E}\mathbf{u}) = \sigma_a c\big(aT^4 - \mathcal{E}\big) + \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}. \tag{2.26}
$$

2.7 Conservation equation for fluid flow

The governing equations we consider here are the Euler equations defined as

$$
\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0 \tag{2.27}
$$

$$
\frac{\partial (\rho \mathbf{u})}{\partial t} + \boldsymbol{\nabla} \cdot \{\rho \mathbf{u} \otimes \mathbf{u}\} + \boldsymbol{\nabla} p = \mathbf{f}, \tag{2.28}
$$

$$
\frac{\partial E}{\partial t} + \boldsymbol{\nabla} \cdot [(E + p)\mathbf{u}] = q \tag{2.29}
$$

where ρ is the fluid density, $\mathbf{u} = [u_x, u_y, u_z] = [u, v, w]$ is the fluid velocity in cartesian coordinates, p is the fluid pressure, E is the material energy-density comprising kinetic energy-density, $\frac{1}{2}\rho||\mathbf{u}||^2$, and internal energy-density, ρe, such that $E = \frac{1}{2}\rho||\mathbf{u}||^2 + \rho e$, where e is the specific internal energy. The values q and $\mathbf{f}$ are abstractly used here as energy- and moment- sources/sinks, respectively.

The ideal gas law provides the closure relation

$$
p = (\gamma - 1)\rho e \tag{2.30}
$$

where γ is the ratio of the constant-pressure specific heat, c_p, to the constant-volume specific heat, c_v, i.e., $\gamma = \frac{c_p}{c_v}$, and is a material property.

Coupling terms:

$$
\begin{aligned}
\mathbf{f} &= \frac{\sigma_t}{c}\boldsymbol{\mathcal{F}}_0 \\
&= -\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}
\end{aligned}
\tag{2.31}
$$

and

$$
\begin{aligned}
q &= -\bigg(\sigma_a c(aT^4 - \mathcal{E}) - \sigma_t \boldsymbol{\mathcal{F}}_0 \cdot \frac{\mathbf{u}}{c}\bigg) \\
&= \sigma_a c(\mathcal{E} - aT^4) - \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}
\end{aligned}
\tag{2.32}
$$

2.8 The set of Radiation Hydrodynamics Grey Diffusion Equations

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0 \tag{2.33a}$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \boldsymbol{\nabla} \cdot \{\rho \mathbf{u} \otimes \mathbf{u}\} + \boldsymbol{\nabla} p = -\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}, \tag{2.33b}$$

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla} \cdot [(E+p)\mathbf{u}] = \sigma_a c(\mathcal{E} - aT^4) - \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u} \tag{2.33c}$$

$$\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla}\cdot\Big(- \frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E}\Big) + \frac{4}{3}\boldsymbol{\nabla}\big(\mathcal{E}\mathbf{u}\big) = \sigma_a c\big(aT^4 - \mathcal{E}\big) + \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}. \tag{2.33d}$$

where

$$E = \frac{1}{2}\rho||\mathbf{u}||^2 + \rho e, \tag{2.33e}$$

$$p = (\gamma - 1)\rho e, \tag{2.33f}$$

$$T = \frac{1}{C_v} e \tag{2.33g}$$

$$\sigma_t(T) = \sigma_s(T) + \sigma_a(T) \tag{2.33h}$$

$$\sigma_s(T) = \rho\kappa_s(T) \tag{2.33i}$$

$$\sigma_a(T) = \rho\kappa_a(T) \tag{2.33j}$$

3 Notations

First we define the following terms

- The radiation momentum source

$$\mathbf{S}_{rp} = \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \tag{3.1a}$$

- The radiation energy source

$$S_{re} = \sigma_a c\big(aT^4 - \mathcal{E}\big) + \frac{1}{3}\boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u} \tag{3.1b}$$

- The conserved hydrodynamic variables

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho\mathbf{u} \\ E \end{bmatrix} \tag{3.1c}$$

- The hydrodynamic flux

$$\mathcal{F}^H = \begin{bmatrix} \rho u \\ \rho u u + p \\ \rho u v \\ \rho u w \\ (E+p)u \end{bmatrix} \tag{3.1d}$$

- The radiation energy current

$$\mathbf{J} = -\frac{c}{3\sigma_t}\boldsymbol{\nabla}\mathcal{E} \tag{3.1e}$$

Next, we use these terms to define a more condensed version of the RHGD equations.

$$\frac{\partial \mathbf{U}}{\partial t} + \boldsymbol{\nabla} \cdot \mathcal{F}^H(\mathbf{U}) = \begin{bmatrix} 0 \\ -\mathbf{S}_{rp} \\ -S_{re} \end{bmatrix} \tag{3.2}$$

$$\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} + \frac{4}{3}\boldsymbol{\nabla}\cdot\big(\mathcal{E}\mathbf{u}\big) = S_{re}. \tag{3.3}$$

4 Overview of temporal numerical scheme

$$\frac{\partial \mathbf{U}}{\partial t} + \boldsymbol{\nabla} \cdot \mathcal{F}^H(\mathbf{U}) = \begin{bmatrix} 0 \\ -\mathbf{S}_{rp} \\ -S_{re} \end{bmatrix} \tag{4.1a}$$

$$\frac{\partial \mathcal{E}}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} + \frac{4}{3} \boldsymbol{\nabla} \cdot (\mathcal{E}\mathbf{u}) = S_{re}. \tag{4.1b}$$

4.1 Predictor phase

$\tau = \frac{1}{\frac{1}{2}\Delta t}$

$$\tau(\mathbf{U}^{n*} - \mathbf{U}^n) + \boldsymbol{\nabla} \cdot \mathcal{F}^H(\mathbf{U}^n) = \mathbf{0} \tag{4.2a}$$

$$\tau(\mathcal{E}^{n*} - \mathcal{E}^n) + \left(\frac{4}{3} \boldsymbol{\nabla} \cdot (\mathcal{E}\mathbf{u})\right)^n = 0 \tag{4.2b}$$

$$\tau(\mathbf{U}^{n+\frac{1}{2}} - \mathbf{U}^{n*})_{0,1} = \begin{bmatrix} 0 \\ -\mathbf{S}_{rp} \end{bmatrix}^n \tag{4.2c}$$

$$\begin{aligned} \sigma_t^{n+\frac{1}{2}} &= \rho^{n+\frac{1}{2}} (\kappa_s(T^n) + \kappa_a(T^n)) \\ \sigma_a^{n+\frac{1}{2}} &= \rho^{n+\frac{1}{2}} \kappa_a(T^n) \end{aligned} \tag{4.2d}$$

$$\tau(\mathbf{U}^{n+\frac{1}{2}} - \mathbf{U}^{n*})_2 = \frac{1}{2} \sigma_a^{n+\frac{1}{2}} c \left(\mathcal{E}^{n+\frac{1}{2}} + \mathcal{E}^n - a\left(T^{4,n+\frac{1}{2}} + T^{4,n}\right)\right) - \left(\frac{1}{3} \boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}\right)^n \tag{4.2e}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2} \boldsymbol{\nabla} \cdot \left(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\right) = \frac{1}{2} \sigma_a^{n+\frac{1}{2}} c \left(a\left(T^{4,n+\frac{1}{2}} + T^{4,n}\right) - \mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^n \right) + \left(\frac{1}{3} \boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}\right)^n \tag{4.2f}$$

$$T^{4,n+\frac{1}{2}} = T^{4,n*} + \frac{4T^{3,n*}}{C_v}(e^{n+\frac{1}{2}} - e^{n*}) \tag{4.2g}$$

4.2 Corrector phase

$\tau = \frac{1}{\Delta t}$

$$\tau(\mathbf{U}^{n+\frac{1}{2}*} - \mathbf{U}^n) + \boldsymbol{\nabla} \cdot \mathcal{F}^H(\mathbf{U}^{n+\frac{1}{2}}) = \mathbf{0} \tag{4.3a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}*} - \mathcal{E}^n) + \left(\frac{4}{3} \boldsymbol{\nabla} \cdot (\mathcal{E}\mathbf{u})\right)^{n+\frac{1}{2}} = 0 \tag{4.3b}$$

$$\tau(\mathbf{U}^{n+1} - \mathbf{U}^{n+\frac{1}{2}*})_{0,1} = \begin{bmatrix} 0 \\ -\mathbf{S}_{rp} \end{bmatrix}^{n+\frac{1}{2}} \tag{4.3c}$$

$$\begin{aligned} \sigma_t^{n+1} &= \rho^{n+1} (\kappa_s(T^{n+\frac{1}{2}}) + \kappa_a(T^{n+\frac{1}{2}})) \\ \sigma_a^{n+1} &= \rho^{n+1} \kappa_a(T^{n+\frac{1}{2}}) \end{aligned} \tag{4.3d}$$

$$\tau(\mathbf{U}^{n+1} - \mathbf{U}^{n+\frac{1}{2}*})_2 = \frac{1}{2} \sigma_a^{n+1} c \left(\mathcal{E}^{n+1} + \mathcal{E}^n - a\left(T^{4,n+1} + T^{4,n}\right)\right) - \left(\frac{1}{3} \boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}\right)^{n+\frac{1}{2}} \tag{4.3e}$$

$$\tau(\mathcal{E}^{n+1} - \mathcal{E}^{n+\frac{1}{2}*}) + \frac{1}{2} \boldsymbol{\nabla} \cdot \left(\mathbf{J}^{n+1} + \mathbf{J}^n\right) = \frac{1}{2} \sigma_a^{n+1} c \left(a\left(T^{4,n+1} + T^{4,n}\right) - \mathcal{E}^{n+1} - \mathcal{E}^n \right) + \left(\frac{1}{3} \boldsymbol{\nabla}\mathcal{E} \cdot \mathbf{u}\right)^{n+\frac{1}{2}} \tag{4.3f}$$

$$T^{4,n+1} = T^{4,n+\frac{1}{2}*} + \frac{4T^{3,n+\frac{1}{2}*}}{C_v}(e^{n+1} - e^{n+\frac{1}{2}*}) \tag{4.3g}$$

5 Finite Volume Spatial Discretization

To apply a finite volume spatial discretization we integrate our time-discretized equations over the volume, V_c, of cell c, and afterwards divide by V_c. This leaves all the terms containing τ unchanged. In this process we develop the following terms:

5.1 Hydrodynamic and Radiation-energy advection

$$\frac{1}{V_c}\int_{V_c} \boldsymbol{\nabla}\cdot\mathcal{F}^H(\mathbf{U})dV = \frac{1}{V_c}\sum_f \mathbf{A}_f\cdot\mathcal{F}^H(\mathbf{U}_f) \tag{5.1}$$

$$\frac{1}{V_c}\int_{V_c} \left(\frac{4}{3}\boldsymbol{\nabla}\cdot(\mathcal{E}\mathbf{u})\right)dV = \frac{1}{V_c}\sum_f \frac{4}{3}\mathbf{A}_f\cdot(\mathcal{E}\mathbf{u})_f \tag{5.2}$$

The face values are reconstructed from gradients in both the predictor and corrector phases. In the corrector-phase the hydrodynamic flux, $\mathcal{F}^H$, is used in its earlier defined form, whilst in the corrector-phase the flux is determined by an approximate Riemann-solver, i.e., the HLLC Riemann solver.

Predictor phase:
For the predictor phase we have the following:

$$\boldsymbol{\nabla}\cdot\mathcal{F}^H(\mathbf{U}^n) \mapsto \frac{1}{V_c}\sum_f \mathbf{A}_f\cdot\mathcal{F}^H(\mathbf{U}_f^n) \tag{5.3}$$

$$\left(\frac{4}{3}\boldsymbol{\nabla}\cdot(\mathcal{E}\mathbf{u})\right)^n \mapsto \frac{1}{V_c}\sum_f \frac{4}{3}\mathbf{A}_f\cdot(\mathcal{E}\mathbf{u})_f^n \tag{5.4}$$

$$\mathbf{U}_f^n = \mathbf{U}_c^n + (\mathbf{x}_f - \mathbf{x}_c)\cdot\{\boldsymbol{\nabla}\mathbf{U}\}_c^n \tag{5.5}$$

$$\mathcal{E}_f^n = \mathcal{E}_c^n + (\mathbf{x}_f - \mathbf{x}_c)\cdot\{\boldsymbol{\nabla}\mathcal{E}\}_c^n \tag{5.6}$$

Corrector phase:
For the corrector phase we have the following:

$$\boldsymbol{\nabla}\cdot\mathcal{F}^H(\mathbf{U}^{n+\frac{1}{2}}) \mapsto \frac{1}{V_c}\sum_f \mathbf{A}_f\cdot\mathbf{F}^{*hllc}(\mathbf{U}_f^{n+\frac{1}{2}}) \tag{5.7}$$

$$\left(\frac{4}{3}\boldsymbol{\nabla}\cdot(\mathcal{E}\mathbf{u})\right)^{n+\frac{1}{2}} \mapsto \frac{1}{V_c}\sum_f \frac{4}{3}\mathbf{A}_f\cdot(\mathcal{E}\mathbf{u})_{upw}^{n+\frac{1}{2}} \tag{5.8}$$

where

$$\mathbf{U}_f^{n+\frac{1}{2}} = \mathbf{U}_c^{n+\frac{1}{2}} + (\mathbf{x}_f - \mathbf{x}_c)\cdot\{\boldsymbol{\nabla}\mathbf{U}\}_c^{n+\frac{1}{2}} \tag{5.9}$$

$$(\mathcal{E}\mathbf{u})_{upw}^{n+\frac{1}{2}} = \begin{cases} (\mathcal{E}\mathbf{u})_{c,f}^{n+1}, & \text{if } \mathbf{u}_{c,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f > 0 \text{ and } \mathbf{u}_{cn,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f > 0 \quad \rightarrow|\rightarrow \\ (\mathcal{E}\mathbf{u})_{cn,f}^{n+1}, & \text{if } \mathbf{u}_{c,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f < 0 \text{ and } \mathbf{u}_{cn,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f < 0 \quad \leftarrow|\leftarrow \\ (\mathcal{E}\mathbf{u})_{cn,f}^{n+1} + (\mathcal{E}\mathbf{u})_{c,f}^{n+1}, & \text{if } \mathbf{u}_{c,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f > 0 \text{ and } \mathbf{u}_{cn,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f < 0 \quad \rightarrow|\leftarrow \\ 0, & \text{if } \mathbf{u}_{c,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f < 0 \text{ and } \mathbf{u}_{cn,f}^{n+\frac{1}{2}}\cdot\mathbf{n}_f > 0 \quad \leftarrow|\rightarrow \end{cases} \tag{5.10}$$

$$\mathcal{E}_{c,f}^{n+\frac{1}{2}} = \mathcal{E}_c^{n+\frac{1}{2}} + (\mathbf{x}_f - \mathbf{x}_c)\cdot\{\boldsymbol{\nabla}\mathcal{E}\}_c^{n+\frac{1}{2}} \tag{5.11}$$

5.2 Density and momentum updates

We apply the same process as before:

$$-\frac{1}{V_c}\int_{V_c} \mathbf{S}_{rp} dV = -\frac{1}{V_c}\sum_f \frac{1}{3}\mathbf{A}_f \mathcal{E}_f, \tag{5.12}$$

however, here we want $\mathcal{E}_f$ to satisfy the following relationship

$$\frac{D_c}{||\mathbf{x}_{cf}||}(\mathcal{E}_f - \mathcal{E}_c) = \frac{D_{cn}}{||\mathbf{x}_{fcn}||}(\mathcal{E}_{cn} - \mathcal{E}_f) \tag{5.13}$$

where

$$D_c = -\frac{c}{3\sigma_{t,c}} \tag{5.14}$$

and where $\mathbf{x}_{cf}$ is the vector from cell c's centroid to the face centroid, $\mathbf{x}_{fcn}$ is the vector from the face centroid to cell cn's centroid (where cell cn is the neighbor to c at face f). The norm $||\cdot||$ refers to the L_2 norm.

Solving the above relationship for $\mathcal{E}_f$ we first set

$$k_c = \frac{D_c}{||\mathbf{x}_{cf}||}, \qquad k_n = \frac{D_{cn}}{||\mathbf{x}_{fcn}||}$$

then get

$$\begin{aligned} k_c\mathcal{E}_f - k_c\mathcal{E}_c &= k_n\mathcal{E}_{cn} - k_n\mathcal{E}_f \\ \rightarrow \quad (k_c + k_n)\mathcal{E}_f &= k_n\mathcal{E}_{cn} + k_c\mathcal{E}_c \\ \therefore \mathcal{E}_f &= \frac{k_n\mathcal{E}_{cn} + k_c\mathcal{E}_c}{k_c + k_n}. \end{aligned} \tag{5.15}$$

Predictor phase:

$$-\mathbf{S}_{rp}^n \mapsto -\frac{1}{V_c}\sum_f \frac{1}{3}\mathbf{A}_f \mathcal{E}_f^n \tag{5.16}$$

Corrector phase:

$$-\mathbf{S}_{rp}^{n+\frac{1}{2}} \mapsto -\frac{1}{V_c}\sum_f \frac{1}{3}\mathbf{A}_f \mathcal{E}_f^{n+\frac{1}{2}} \tag{5.17}$$

5.3 Energy equations

Only two terms require special consideration here, the current and the kinetic energy terms,

$$\begin{aligned} \frac{1}{V_c}\int_{V_c} \boldsymbol{\nabla}\cdot\mathbf{J}\ dV &= \frac{1}{V_c}\sum_f \mathbf{A}_f\cdot\mathbf{J}_f \\ \frac{1}{V_c}\int_{V_c} \frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\ dV &= \frac{1}{V_c}\sum_f \frac{1}{3}\mathbf{A}_f\cdot(\mathcal{E}\mathbf{u})_f. \end{aligned} \tag{5.18}$$

Therefore

$$\boldsymbol{\nabla}\cdot\mathbf{J}^n \mapsto \frac{1}{V_c}\sum_f \mathbf{A}_f\cdot\mathbf{J}_f^n \tag{5.19}$$

For $\mathbf{J}_f$ we have

$$\mathbf{J}_f = -\frac{c}{3\sigma_{tf}}\left(\boldsymbol{\nabla}\mathcal{E}\right)_f \tag{5.20}$$

Now define

$$\begin{aligned} \sigma_{tf} &= \frac{1}{2}\sigma_{t,c} + \frac{1}{2}\sigma_{t,cn} \\ D_f &= -\frac{c}{3\sigma_{tf}} \end{aligned} \tag{5.21}$$

To get

$$\mathbf{J}_f = D_f\big(\mathcal{E}_{cn} - \mathcal{E}_c\big)\frac{\mathbf{x}_{cn} - \mathbf{x}_c}{||\mathbf{x}_{cn} - \mathbf{x}_c||^2} \tag{5.22}$$

Define

$$\mathbf{k}_f = D_f\frac{\mathbf{x}_{cn} - \mathbf{x}_c}{||\mathbf{x}_{cn} - \mathbf{x}_c||^2} \tag{5.23}$$

from which we get

$$\mathbf{J}_f = \mathbf{k}_f\big(\mathcal{E}_{cn} - \mathcal{E}_c\big) \tag{5.24}$$

For the kinetic energy terms we use the reconstructed values as in the Hydrodynamic and radiation-energy advection portion.

$$\left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \mapsto \frac{1}{V_c}\sum_f \frac{1}{3}\mathbf{A}_f\cdot(\mathcal{E}_f^n\mathbf{u}_f^n) \tag{5.25}$$

5.4 Predictor phase

$$\tau(E^{n+\frac{1}{2}} - E^{n*}) = \frac{1}{2}\sigma_a^{n+\frac{1}{2}}c\Big(\mathcal{E}^{n+\frac{1}{2}} + \mathcal{E}^n - a\big(T^{4,n+\frac{1}{2}} + T^{4,n}\big)\Big) - \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.26a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = \frac{1}{2}\sigma_a^{n+\frac{1}{2}}c\Big(a\big(T^{4,n+\frac{1}{2}} + T^{4,n}\big) - \mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^n\Big) + \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.26b}$$

$$T^{4,n+\frac{1}{2}} = T^{4,n*} + \frac{4T^{3,n*}}{C_v}(e^{n+\frac{1}{2}} - e^{n*}) \tag{5.26c}$$

Define:

$$\begin{aligned} k_1 &= \frac{1}{2}\sigma_a^{n+\frac{1}{2}}c \\ k_2 &= \frac{4T^{3,n*}}{C_v} \end{aligned} \tag{5.27}$$

$$\tau(E^{n+\frac{1}{2}} - E^{n*}) = k_1\Big(\mathcal{E}^{n+\frac{1}{2}} + \mathcal{E}^n - a\big(T^{4,n+\frac{1}{2}} + T^{4,n}\big)\Big) - \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.28a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = k_1\Big(a\big(T^{4,n+\frac{1}{2}} + T^{4,n}\big) - \mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^n\Big) + \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.28b}$$

$$T^{4,n+\frac{1}{2}} = T^{4,n*} + k_2(e^{n+\frac{1}{2}} - e^{n*}) \tag{5.28c}$$

$$\tau(E^{n+\frac{1}{2}} - E^{n*}) = k_1\mathcal{E}^{n+\frac{1}{2}} + k_1\mathcal{E}^n - k_1 aT^{4,n+\frac{1}{2}} - k_1 aT^{4,n} - \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.29a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = k_1 aT^{4,n+\frac{1}{2}} + k_1 aT^{4,n} - k_1\mathcal{E}^{n+\frac{1}{2}} - k_1\mathcal{E}^n + \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.29b}$$

$$T^{4,n+\frac{1}{2}} = T^{4,n*} + k_2(e^{n+\frac{1}{2}} - e^{n*}) \tag{5.29c}$$

$$\tau(E^{n+\frac{1}{2}} - E^{n*}) = k_1\mathcal{E}^{n+\frac{1}{2}} + k_1\mathcal{E}^n - k_1a\big(T^{4,n*} + k_2(e^{n+\frac{1}{2}} - e^{n*})\big) - k_1aT^{4,n} - \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.30a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = k_1a\big(T^{4,n*} + k_2(e^{n+\frac{1}{2}} - e^{n*})\big) + k_1aT^{4,n} - k_1\mathcal{E}^{n+\frac{1}{2}} - k_1\mathcal{E}^n + \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.30b}$$

$$\tau(E^{n+\frac{1}{2}} - E^{n*}) = k_1\mathcal{E}^{n+\frac{1}{2}} + k_1\mathcal{E}^n - k_1aT^{4,n*} - k_1ak_2e^{n+\frac{1}{2}} + k_1ae^{n*} - k_1aT^{4,n} - \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.31a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = k_1aT^{4,n*} + k_1ak_2e^{n+\frac{1}{2}} - k_1ae^{n*} + k_1aT^{4,n} - k_1\mathcal{E}^{n+\frac{1}{2}} - k_1\mathcal{E}^n + \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \tag{5.31b}$$

Define:

$$\begin{aligned} k_3 &= k_1\mathcal{E}^n - k_1aT^{4,n*} + k_1ae^{n*} - k_1aT^{4,n} - \left(\frac{1}{3}\boldsymbol{\nabla}\mathcal{E}\cdot\mathbf{u}\right)^n \\ k_4 &= -k_1ak_2 \end{aligned} \tag{5.32}$$

$$\tau(E^{n+\frac{1}{2}} - E^{n*}) = k_1\mathcal{E}^{n+\frac{1}{2}} + k_3 + k_4e^{n+\frac{1}{2}} \tag{5.33a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = -k_1\mathcal{E}^{n+\frac{1}{2}} - k_3 - k_4e^{n+\frac{1}{2}} \tag{5.33b}$$

Note:

$$E^{n+\frac{1}{2}} = (\frac{1}{2}\rho||\mathbf{u}||^2)^{n+\frac{1}{2}} + \rho^{n+\frac{1}{2}}e^{n+\frac{1}{2}} \tag{5.34}$$

$$\tau((\frac{1}{2}\rho||\mathbf{u}||^2)^{n+\frac{1}{2}} + \rho^{n+\frac{1}{2}}e^{n+\frac{1}{2}} - E^{n*}) = k_1\mathcal{E}^{n+\frac{1}{2}} + k_3 + k_4e^{n+\frac{1}{2}} \tag{5.35a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = -k_1\mathcal{E}^{n+\frac{1}{2}} - k_3 - k_4e^{n+\frac{1}{2}} \tag{5.35b}$$

$$\tau(\frac{1}{2}\rho||\mathbf{u}||^2)^{n+\frac{1}{2}} + \tau\rho^{n+\frac{1}{2}}e^{n+\frac{1}{2}} - \tau E^{n*} = k_1\mathcal{E}^{n+\frac{1}{2}} + k_3 + k_4e^{n+\frac{1}{2}} \tag{5.36a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = -k_1\mathcal{E}^{n+\frac{1}{2}} - k_3 - k_4e^{n+\frac{1}{2}} \tag{5.36b}$$

$$\big(\tau\rho^{n+\frac{1}{2}} - k_4\big)e^{n+\frac{1}{2}} = k_1\mathcal{E}^{n+\frac{1}{2}} + k_3 - \tau(\frac{1}{2}\rho||\mathbf{u}||^2)^{n+\frac{1}{2}} + \tau E^{n*} \tag{5.37a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\boldsymbol{\cdot}\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = -k_1\mathcal{E}^{n+\frac{1}{2}} - k_3 - k_4 e^{n+\frac{1}{2}} \tag{5.37b}$$

Define:

$$\begin{aligned} k_5 &= \frac{k_1}{\tau\rho^{n+\frac{1}{2}}} \\ k_6 &= \frac{k_3 - \tau(\frac{1}{2}\rho||\mathbf{u}||^2)^{n+\frac{1}{2}} + \tau E^{n*}}{\tau\rho^{n+\frac{1}{2}}} \end{aligned} \tag{5.38}$$

$$e^{n+\frac{1}{2}} = k_5\mathcal{E}^{n+\frac{1}{2}} + k_6 \tag{5.39a}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\boldsymbol{\cdot}\big(\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^n\big) = -k_1\mathcal{E}^{n+\frac{1}{2}} - k_3 - k_4 e^{n+\frac{1}{2}} \tag{5.39b}$$

$$\tau(\mathcal{E}^{n+\frac{1}{2}} - \mathcal{E}^{n*}) + \frac{1}{2}\boldsymbol{\nabla}\cdot\mathbf{J}^{n+\frac{1}{2}} + \frac{1}{2}\boldsymbol{\nabla}\cdot\mathbf{J}^n = -k_1\mathcal{E}^{n+\frac{1}{2}} - k_3 - k_4k_5\mathcal{E}^{n+\frac{1}{2}} - k_4k_6 \tag{5.40a}$$

$$\big(\tau + k_1 + k_4k_5\big)\mathcal{E}^{n+\frac{1}{2}} + \frac{1}{2}\boldsymbol{\nabla}\cdot\mathbf{J}^{n+\frac{1}{2}} = -k_3 - k_4k_6 + \tau\mathcal{E}^{n*} - \frac{1}{2}\boldsymbol{\nabla}\cdot\mathbf{J}^n \tag{5.41a}$$

Recall:

$$\boldsymbol{\nabla}\cdot\mathbf{J} \mapsto \frac{1}{V_c}\sum_f \mathbf{A}_f\cdot\mathbf{J}_f \tag{5.42}$$

and

$$\mathbf{J}_f = \mathbf{k}_f\big(\mathcal{E}_{cn} - \mathcal{E}_c\big) \tag{5.43}$$

$$\big(\tau + k_1 + k_4k_5\big)\mathcal{E}^{n+\frac{1}{2}} + \frac{1}{2V_c}\sum_f \mathbf{A}_f\cdot\mathbf{k}_f^{n+\frac{1}{2}}(\mathcal{E}_{cn}^{n+\frac{1}{2}} - \mathcal{E}_c^{n+\frac{1}{2}}) = -k_3 - k_4k_6 + \tau\mathcal{E}^{n*} - \frac{1}{2V_c}\sum_f \mathbf{A}_f\cdot\mathbf{k}_f^n(\mathcal{E}_{cn}^n - \mathcal{E}_c^n) \tag{5.44a}$$

A Angular integration identities

Identity A-1

$$\int_{4\pi} d\mathbf{\Omega} = 4\pi.$$

Identity A-2

$$\int_{4\pi} \mathbf{\Omega} \; d\mathbf{\Omega} = 0.$$

Identity A-3 Given the known three component vector, $\mathbf{v}$,

$$\int_{4\pi} \mathbf{\Omega} \cdot \mathbf{v} \; d\mathbf{\Omega} = 0.$$

Identity A-4 Given the known three component vector, $\mathbf{v}$,

$$\int_{4\pi} \mathbf{\Omega} \cdot \boldsymbol{\nabla}(\mathbf{\Omega} \cdot \mathbf{v}) \; d\mathbf{\Omega} = \frac{4\pi}{3} \boldsymbol{\nabla} \cdot \mathbf{v}.$$

Identity A-5 Given the scalar, a,

$$\int_{4\pi} \mathbf{\Omega} \Big(\mathbf{\Omega} \cdot \boldsymbol{\nabla} a \Big) \; d\mathbf{\Omega} = \frac{4\pi}{3} \boldsymbol{\nabla} a.$$

Identity A-6 Given the known three component vector, $\mathbf{v}$,

$$\int_{4\pi} \mathbf{\Omega} \Big(\mathbf{\Omega} \cdot \mathbf{v} \Big) \; d\mathbf{\Omega} = \frac{4\pi}{3} \mathbf{v}.$$

Identity A-7 Given the known three component vector, $\mathbf{v}$,

$$\int_{4\pi} \mathbf{\Omega} \Big(\mathbf{\Omega} \cdot \boldsymbol{\nabla}(\mathbf{\Omega} \cdot \mathbf{v}) \Big) \; d\mathbf{\Omega} = 0.$$

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B Roderigues's formula

Roderigues' formula for the rotation of a vector $\mathbf{v}$ about a unit vector $\mathbf{a}$ with right-hand rule

$$\mathbf{v}_{rotated} = \cos\theta\mathbf{v} + (\mathbf{a}\cdot\mathbf{v})(1-\cos\theta)\mathbf{a} + \sin\theta(\mathbf{a}\times\mathbf{v}) \tag{B.1}$$

In matrix form

$$\mathbf{v}_{rotated} = A\mathbf{v} \tag{B.2}$$

where

$$A = \begin{bmatrix} 0 & -a_z & a_y \\ a_z & 0 & -a_x \\ -a_y & a_x & 0 \end{bmatrix} \tag{B.3}$$

and

$$R = I + \sin\theta A + (1-\cos\theta)A^2 \tag{B.4}$$