SDIRK Time Integration and Variable Material Properties for Radiative Transfer

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March 25, 2013

1 Generic SDIRK

Consider a generic Butcher Tableaux:

Stage	c_i	a			
1	c_1	γ	0	$\dots$	0
2	c_2	a_{21}	γ	0	$\vdots$
i	c_i	a_{i1}	a_{i2}	$\ddots$	0
s	c_s	a_{c1}	a_{c2}	$\dots$	γ
		b_1	b_2	$\dots$	b_s

Let ψ be our variable of interest. Then $\psi_{n+1} = \psi(t_n + \Delta t)$ is:

$$\psi_{n+1} = \psi_n + \Delta t \sum_{i=1}^{s} b_i k_i \tag{1}$$

where k_i is defined as:

$$k_i = f\left(t_n + c_i \Delta t\ ,\ \psi_n + \Delta t \sum_{j=1}^{i} c_{ij} k_j \right)$$

and

$$f(t,\psi) = \frac{\partial \psi}{\partial t}$$

Eq. (1) can also be interpreted as meaning:

$$\psi_i = \psi_n + \Delta t \sum_{j=1}^{i} a_{ij} f\left(t_n + \Delta t c_j, \psi_j\right) \tag{2}$$

2 Grey Equations

We know that the 1D, mono-energetic (grey) radiative transfer equations are:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu \frac{\partial}{\partial x} I + \sigma_t I = \frac{\sigma_s}{4\pi}\phi + \frac{\sigma_a}{4\pi} acT^4 + S_I$$

$$C_v \frac{\partial T}{\partial t} = \sigma_a \left(\phi - acT^4\right) + S_T$$

Solving for the time derivatives:

$$\frac{\partial I}{\partial t} = c\left[\frac{\sigma_s}{4\pi}\phi + \frac{\sigma_a}{4\pi}acT^4 - \mu\frac{\partial I}{\partial x} - \sigma_t I + S_I\right]$$

$$\frac{\partial T}{\partial t} = \frac{1}{C_v}\left[\sigma_a\left(\phi - acT^4\right) + S_T\right]$$

Before going any further, we spatially discretize our equations, expanding in an arbitrary order Lagrangian basis. First, transforming to a generic reference element:

$$\begin{aligned} x &= x_i + \frac{\Delta x_i}{2}s \\ s &\in [-1,1] \\ \Delta x_i &= x_{i+1/2} - x_{i-1/2} \\ x_i &= \frac{x_{i+1/2} + x_{i-1/2}}{2} \end{aligned}$$

For generality, let $\widetilde{x}$ and $\widetilde{y}$ be unknowns represented using our finite element representation:

$$\widetilde{x}(s) = \vec{\mathbf{B}}(s)\cdot\vec{\mathbf{x}} = \mathbf{B_1}(s)x_1 + \mathbf{B_2}x_2 + \cdots + \mathbf{B_N}x_N$$

where

$$\vec{\mathbf{B}} = \begin{bmatrix} \mathbf{B_1} \\ \mathbf{B_2} \\ \vdots \\ \mathbf{B_N} \end{bmatrix}$$

and

$$\mathbf{B_i} = \frac{\prod_{k\neq i}(x_k - x)}{\prod_{k\neq i}(x_k - x_i)}$$

Further suppose we wish to take an integral of the form:

$$\int_{-1}^{1}\vec{\mathbf{B}}\widetilde{x}\Delta x_i ds$$

we represent this result as

$$\mathbf{M}\vec{\mathbf{x}}$$

where

$$\mathbf{M}_{ij} = \frac{\Delta x_i}{2}\int_{-1}^{1}\mathbf{B_i}(s)\mathbf{B_j}(s)ds \approx \frac{\Delta x_i}{2}\sum_{q=1}^{N_q} w_q \mathbf{B_i}(s)\Big|_{s=s_q}\mathbf{B_j}(s)\Big|_{s=s_q}$$

Similarly if we want to calculate the integral:

$$\int_{-1}^{1}\vec{\mathbf{B}}\widetilde{x}\widetilde{y}\Delta x_i ds$$

we will denote this result as:

$$\widehat{\mathbf{M}}_x\vec{\mathbf{y}}$$

where

$$\widehat{\mathbf{M}}_{x,ij} = \frac{\Delta x_i}{2} \int_{-1}^{1} x(s)\mathbf{B_i}(s)\mathbf{B_j}(s)ds \approx \frac{\Delta x_i}{2} \sum_{q=1}^{N_q} \left\{ w_q \mathbf{B_i}\Big|_{s=s_q} \mathbf{B_j}\Big|_{s=s_q} \left[\vec{\mathbf{x}} \cdot \vec{\mathbf{B}}(s)\Big|_{s=s_q} \right] \right\}$$

Our fundamental unknowns will be expressed as:

$$\begin{aligned} I(s) &= \vec{\mathbf{B}}(s) \cdot \vec{\mathbf{I}} \\ T(s) &= \vec{\mathbf{B}}(s) \cdot \vec{\mathbf{T}} \end{aligned}$$

where:

$$\begin{aligned} \vec{\mathbf{T}} &= \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_N \end{bmatrix} \\ \vec{\mathbf{I}} &= \begin{bmatrix} I_1 \\ I_2 \\ \vdots \\ I_N \end{bmatrix} \end{aligned}$$

Material properties will be interpolated in space from their values at the finite element interpolation points. For example:

$$\begin{aligned} \frac{\sigma_a}{C_v}(s) &= \sum_{j=1}^{N} \mathbf{B_j}(s) \frac{\sigma_a}{C_v}\Big|_{T=T_j} = \vec{\mathbf{B}} \cdot \frac{\vec{\sigma_\mathbf{a}}}{\mathbf{C_v}} \\ \sigma_t(s) &= \sum_{j=1}^{N} \sigma_t(T_j)\mathbf{B_j}(s) = \vec{\mathbf{B}} \cdot \vec{\sigma}_t \end{aligned}$$

The Planck function, $B(T)$ will be similarly expanded:

$$B(s) = \vec{\mathbf{B}}(s) \cdot \widehat{\mathbf{B}}$$

where for the grey case:

$$\widehat{\mathbf{B}} = \frac{1}{4\pi} \begin{bmatrix} acT_1^4 \\ \vdots \\ acT_j^4 \\ \vdots \\ acT_N^4 \end{bmatrix}$$

Since the Planck function is a highly nonlinear function of T, we elect to linearize it about an arbitrary temperature, T^*:

$$B(T) \approx B(T^*) + \frac{\partial}{\partial T}\left[B(T^*)\right](T - T^*)$$

for the grey case:

$$acT^4 \approx \left[ac(T^*)^4 + 4ac(T^*)^3(T - T^*)\right]$$

Expressing in vector/matrix form:

$$\widehat{\mathbf{B}} = \vec{\mathbf{B}}^* + \widehat{\mathbf{D}}^* \left(\vec{\mathbf{T}} - \vec{\mathbf{T}}^* \right) \tag{3}$$

where:

$$\vec{\mathbf{B}}^* = \begin{bmatrix} \vdots \\ B(T_j^*) \\ \vdots \end{bmatrix}$$

and $\widehat{\mathbf{D}}^*$ is a $N \times N$ diagonal matrix with non zero elements, d_{jj}:

$$d_{jj} = \left. \frac{\partial B}{\partial T} \right|_{T=T_j^*}$$

Since the sources are slightly prickly, that is we don't necessarily want to express S_I and S_T as polynomials in the basis functions, we definte the following vectors:

$$\begin{aligned} \vec{S}_{I,j} &= \int_{-1}^{1} \mathbf{B_j} S_I(s)\ ds \\ \vec{S}_{T,j} &= \int_{-1}^{1} \mathbf{B_j} S_T(s)\ ds \end{aligned}$$

Having defined all this notation, we give the spatially discretized equations for cell i:

$$\frac{\partial}{\partial t} \left[\mathbf{M}\vec{\mathbf{I}} \right] = c \left[\frac{1}{4\pi} \widehat{\mathbf{M}}_{\sigma_s} \vec{\phi} + \widehat{\mathbf{M}}_{\sigma_a} \left(\vec{\mathbf{B}}^* + \widehat{\mathbf{D}}^* \left(\vec{\mathbf{T}} - \vec{\mathbf{T}}^* \right) \right) - \widehat{\mathbf{M}}_{\sigma_t} \vec{\mathbf{I}} - \widehat{\mathbf{L}\vec{\mathbf{I}}} + \vec{S}_I \right] \tag{4}$$

$$\frac{\partial}{\partial t} \left[\widehat{\mathbf{M}}_{C_v^*} \vec{\mathbf{T}} \right] = \widehat{\mathbf{M}}_{\sigma_a} \left(\vec{\phi} - 4\pi \vec{\mathbf{B}}^* - 4\pi \mathbf{D}^* \left(\vec{\mathbf{T}} - \vec{\mathbf{T}}^* \right) \right) + \vec{S}_T \tag{5}$$

where $\widehat{\mathbf{L}\vec{\mathbf{I}}}$ is defined as:

$$\begin{aligned} \widehat{\mathbf{L}\vec{\mathbf{I}}} &= \mathbf{L}\vec{\mathbf{I}} + \vec{\mathbf{L}} I_{in} + \hat{\mathbf{L}}\vec{\mathbf{I}} && (6) \\ \mathbf{L}_{ij} &= -\mu \int_{-1}^{1} \frac{\partial B_i(s)}{\partial s} B_j(s) ds && (7) \\ \vec{\mathbf{L}}_i &= \begin{cases} \text{if } \mu > 0 & \vec{\mathbf{L}}_i = -\mu \mathbf{B_i}(-1) \\ \text{else} & \vec{\mathbf{L}}_i = \mu \mathbf{B_i}(1) \end{cases} && (8) \\ \hat{\mathbf{L}}_{ij} &= \begin{cases} \text{if } \mu > 0 & \hat{\mathbf{L}}_{ij} = \mu \mathbf{B_i}(1) \mathbf{B_j}(1) \\ \text{else} & \hat{\mathbf{L}}_{ij} = -\mu \mathbf{B_i}(-1) \mathbf{B_j}(-1) \end{cases} && (9) \\ & && (10) \end{aligned}$$

Solving for k_I and k_T we have:

$$k_I = c\mathbf{M}^{-1} \left[\frac{1}{4\pi} \widehat{\mathbf{M}}_{\sigma_s} \vec{\phi} + \widehat{\mathbf{M}} \sigma_a \left(\vec{\mathbf{B}}^* + \widehat{\mathbf{D}}^* \left(\vec{\mathbf{T}} - \vec{\mathbf{T}}^* \right) \right) - \widehat{\mathbf{M}}_{\sigma_t} \vec{\mathbf{I}} - \widehat{\mathbf{L}\vec{\mathbf{I}}} + \vec{S}_I \right] \tag{11}$$

$$k_T = \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a} \left(\vec{\phi} - 4\pi \vec{\mathbf{B}}^* - 4\pi \mathbf{D}^* \left(\vec{\mathbf{T}} - \vec{\mathbf{T}}^* \right) \right) + \vec{S}_T \right] \tag{12}$$

2.1 First RK step

We know look at Eq. (2) for step 1 of an arbitrary, diagonally implicit RK scheme:

$$\vec{\mathbf{I}}_1 = \vec{\mathbf{I}}_n + c\Delta t a_{11}\mathbf{M}^{-1}\left[\frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a,*}\left(\vec{\mathbf{B}}^* + \widehat{\mathbf{D}}^*\left(\vec{\mathbf{T}}_1 - \vec{\mathbf{T}}^*\right)\right) - \widehat{\mathbf{M}}_{\sigma_t,*}\vec{\mathbf{I}}_1 - \widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \vec{S}_I\right] \quad (13)$$

$$\vec{\mathbf{T}}_1 = \vec{\mathbf{T}}_n + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^* - 4\pi\mathbf{D}^*\left(\vec{\mathbf{T}}_1 - \vec{\mathbf{T}}^*\right)\right) + \vec{S}_T\right] \quad (14)$$

We now use Eq. (14) to eliminate the unknown temperature, $\vec{\mathbf{T}}_1$ from Eq. (13). Solving Eq. (14) for $\vec{\mathbf{T}}_1$:

$$\vec{\mathbf{T}}_1 + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\vec{\mathbf{T}}_1 = \vec{\mathbf{T}}_n + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a*}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^* + 4\pi\mathbf{D}^*\vec{\mathbf{T}}^*\right) + \vec{S}_T\right]$$

$$\begin{aligned}\vec{\mathbf{T}}_1 = \left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^* + 4\pi\mathbf{D}^*\vec{\mathbf{T}}^*\right) + \vec{S}_T\right]\right]\ldots \\ + \left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}^* - \vec{\mathbf{T}}^*\right]\end{aligned}$$

$$\begin{aligned}\vec{\mathbf{T}}_1 = \left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a*}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right]\right]\ldots \\ + \left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]\vec{\mathbf{T}}^*\ldots \\ - \left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\vec{\mathbf{T}}^*\end{aligned}$$

$$\vec{\mathbf{T}}_1 = \vec{\mathbf{T}}^* + \left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a*}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right]\right] \quad (15)$$

Inserting Eq. (15) into Eq. (13):

$$\begin{aligned}\vec{\mathbf{I}}_1 = \vec{\mathbf{I}}_n + c\Delta t a_{11}\mathbf{M}^{-1}\left[\frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^* - \widehat{\mathbf{M}}_{\sigma_t,*}\vec{\mathbf{I}}_1 - \widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \vec{S}_I\right]\ldots \\ + c\Delta t a_{11}\mathbf{M}^{-1}\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a*}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right]\right]\end{aligned}$$

Multiply by $\frac{1}{c\Delta t a_{11}}\mathbf{M}$

$$\begin{aligned}\frac{1}{c\Delta t a_{11}}\mathbf{M}\vec{\mathbf{I}}_1 = \frac{1}{c\Delta t a_{11}}\mathbf{M}\vec{\mathbf{I}}_n + \left[\frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^* - \widehat{\mathbf{M}}_{\sigma_t,*}\vec{\mathbf{I}}_1 - \widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \vec{S}_I\right]\ldots \\ + \widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a*}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right]\right]\end{aligned}$$

and move some terms over to the LHS:

$$\begin{aligned}\widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \left(\frac{1}{c\Delta t a_{11}}\mathbf{M} + \widehat{\mathbf{M}}_{\sigma_t,*}\right)\vec{\mathbf{I}}_1 = \frac{1}{c\Delta t a_{11}}\mathbf{M}\vec{\mathbf{I}}_n + \frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^* + \vec{S}_I\ldots \\ + \widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a*}\left(\vec{\phi}_1 - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right]\right]\end{aligned}$$

Further manipulating to pull all of the $\vec{\phi}_1$ terms together:

$$\begin{aligned}\widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \left(\frac{1}{c\Delta t a_{11}}\mathbf{M} + \widehat{\mathbf{M}}_{\sigma_t,*}\right)\vec{\mathbf{I}}_1 = \dots \\ \frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_1 + \Delta t a_{11}\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\mathbf{D}^*\right]^{-1}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\vec{\phi}_1 \dots \\ + \frac{1}{c\Delta t a_{11}}\mathbf{M}\vec{\mathbf{I}}_n + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^* + \vec{S}_I \dots \\ + \widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\vec{S}_T - 4\pi\widehat{\mathbf{M}}_{\sigma_a*}\vec{\mathbf{B}}^*\right]\right]\end{aligned} \quad (16)$$

Though it does not look that familiar, Eq. (16) can be made to resemble the canonical mono-energetic neutron fission equation. Let us define the following terms:

$$\bar{\bar{\nu}} = 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\mathbf{D}^*\right]^{-1}\widehat{\mathbf{M}}_{C_v}^{-1} \quad (17a)$$

$$\begin{aligned}\bar{\bar{\xi}}_d = \frac{1}{c\Delta t a_{11}}\mathbf{M}\vec{\mathbf{I}}_n + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^* + \vec{S}_I \dots \\ + \widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a*}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t a_{11}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\vec{S}_T - 4\pi\widehat{\mathbf{M}}_{\sigma_a}\vec{\mathbf{B}}^*\right]\right]\end{aligned} \quad (17b)$$

$$\bar{\bar{\mathbf{M}}}_{\sigma_t} = \frac{1}{c\Delta t a_{11}}\mathbf{M} + \widehat{\mathbf{M}}_{\sigma_t,*} \quad (17c)$$

Inserting Eqs. (17) into Eq. (16) gives our final form:

$$\widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \bar{\bar{\mathbf{M}}}_{\sigma_t}\vec{\mathbf{I}}_1 = \frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_1 + \frac{1}{4\pi}\bar{\bar{\nu}}\widehat{\mathbf{M}}_{\sigma_a*}\vec{\phi}_1 + \bar{\bar{\xi}}_d \quad (18)$$

Having found $\vec{\mathbf{I}}_1$ by solving Eq. (18), we use Eq. (15) to find $\vec{\mathbf{T}}_1$. There are two options to proceed at this point

1. use the new value of $\vec{\mathbf{T}}_1$ as the next iterate for $\vec{\mathbf{T}}_*$ or
2. do not iterate on $\vec{\mathbf{T}}_*$, and proceed with the calculation

Having found $\vec{\mathbf{T}}_1$, either by iterating or solving once, the values of $k_{I,1}$ and $k_{T,1}$ are found by applying the definitions of Eq. (11) and Eq. (12) respectively (noting that since we now know $\vec{\mathbf{T}}_1$, we also know $\widehat{\mathbf{B}}_1$, and do not need to linearize)

$$k_{I,1} = c\mathbf{M}^{-1}\left[\frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,1}\vec{\phi}_1 + \widehat{\mathbf{M}}_{\sigma_a,1}\widehat{\mathbf{B}}_1 - \widehat{\mathbf{M}}_{\sigma_t,1}\vec{\mathbf{I}}_1 - \widehat{\mathbf{L}}\vec{\mathbf{I}}_1 + \vec{S}_I\right]$$

$$k_{T,1} = \widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a}\left(\vec{\phi}_1 - 4\pi\widehat{\mathbf{B}}_1\right) + \vec{S}_T\right]$$

2.2 i-th RK step

Moving on to the i-th RK step, we first write the equation for $\vec{\mathbf{I}}_i$ and $\vec{\mathbf{T}}_i$:

$$\vec{\mathbf{I}}_i = \vec{\mathbf{I}}_n + \Delta t\sum_{j=1}^{i-1}a_{ij}k_{I,j} + \Delta t a_{ii}c\mathbf{M}^{-1}\left[\frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_i + \widehat{\mathbf{M}}_{\sigma_a,*}\left(\vec{\mathbf{B}}^* + \widehat{\mathbf{D}}^*\left(\vec{\mathbf{T}}_i - \vec{\mathbf{T}}^*\right)\right) - \widehat{\mathbf{M}}_{\sigma_t,*}\vec{\mathbf{I}}_i - \widehat{\mathbf{L}}\vec{\mathbf{I}}_i + \vec{S}_I\right] \quad (19)$$

$$\vec{\mathbf{T}}_i = \vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} + \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* - 4\pi \mathbf{D}^* \left(\vec{\mathbf{T}}_i - \vec{\mathbf{T}}^* \right) \right) + \vec{S}_T \right] \tag{20}$$

Proceeding in a similar fashion as before, we solve Eq. (20) for $\vec{\mathbf{T}}_i$.

$$\vec{\mathbf{T}}_i + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \vec{\mathbf{T}}_i = \vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} + \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* + 4\pi \mathbf{D}^* \vec{\mathbf{T}}^* \right) + \vec{S}_T \right]$$

$$\left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a} \mathbf{D}^* \right] \vec{\mathbf{T}}_i = \vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} + \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* + 4\pi \mathbf{D}^* \vec{\mathbf{T}}^* \right) + \vec{S}_T \right]$$

$$\begin{aligned} \vec{\mathbf{T}}_i = & \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \left[\vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} \right] \dots \\ & + \Delta t a_{ii} \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* + 4\pi \mathbf{D}^* \vec{\mathbf{T}}^* \right) + \vec{S}_T \right] \end{aligned}$$

$$\begin{aligned} \vec{\mathbf{T}}_i = & \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \left[\vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} \right] \dots \\ & + \Delta t a_{ii} \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* \right) + \vec{S}_T \right] \dots \\ & + 4\pi \Delta t a_{ii} \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \vec{\mathbf{T}}^* \end{aligned}$$

Adding nothing:

$$\begin{aligned} \vec{\mathbf{T}}_i = & \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \left[\vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} \right] \dots \\ & + \Delta t a_{ii} \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* \right) + \vec{S}_T \right] \dots \\ & + \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \left[4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \vec{\mathbf{T}}^* \right] \dots \\ & + \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \mathbf{I} \left(\vec{\mathbf{T}}^* - \vec{\mathbf{T}}^* \right) \end{aligned}$$

simplifying

$$\begin{aligned} \vec{\mathbf{T}}_i = & \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \left[\vec{\mathbf{T}}_n + \Delta t \sum_{j=1}^{i-1} a_{ij} k_{T,j} \right] \dots \\ & + \Delta t a_{ii} \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \widehat{\mathbf{M}}_{C_v}^{-1} \left[\widehat{\mathbf{M}}_{\sigma_a *} \left(\vec{\phi}_i - 4\pi \vec{\mathbf{B}}^* \right) + \vec{S}_T \right] \dots \\ & + \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right] \vec{\mathbf{T}}^* \dots \\ & - \left[\mathbf{I} + 4\pi \Delta t a_{ii} \widehat{\mathbf{M}}_{C_v}^{-1} \widehat{\mathbf{M}}_{\sigma_a *} \mathbf{D}^* \right]^{-1} \mathbf{I} \vec{\mathbf{T}}^* \end{aligned}$$

$$\vec{\mathbf{T}}_i = \vec{\mathbf{T}}^* + \left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{T,j}\right]\dots$$

$$+ \Delta t a_{ii}\left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{D}^*\right]^{-1}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a *}\left(\vec{\phi}_i - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right] \quad (21)$$

Multiplying Eq. (19) by $\frac{1}{c\Delta t a_{ii}}\mathbf{M}$:

$$\frac{1}{c\Delta t a_{ii}}\mathbf{M}\vec{\mathbf{I}}_i = \frac{1}{c\Delta t a_{ii}}\mathbf{M}\vec{\mathbf{I}}_n + \frac{1}{c a_{ii}}\mathbf{M}\sum_{j=1}^{i-1} a_{ij}k_{I,j}\dots$$

$$+ \frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_i + \widehat{\mathbf{M}}_{\sigma_a,*}\left(\vec{\mathbf{B}}^* + \widehat{\mathbf{D}}^*\left(\vec{\mathbf{T}}_i - \vec{\mathbf{T}}^*\right)\right) - \widehat{\mathbf{M}}_{\sigma_t,*}\vec{\mathbf{I}}_i - \widehat{\mathbf{L}}\vec{\mathbf{I}}_i + \vec{S}_I \quad (22)$$

Inserting Eq. (21) into Eq. (22):

$$\widehat{\mathbf{L}}\vec{\mathbf{I}}_i + \left(\frac{1}{c\Delta t a_{ii}}\mathbf{M} + \widehat{\mathbf{M}}_{\sigma_t,*}\right)\vec{\mathbf{I}}_i = \frac{1}{c\Delta t a_{ii}}\mathbf{M}\vec{\mathbf{I}}_n + \frac{1}{c a_{ii}}\mathbf{M}\sum_{j=1}^{i-1} a_{ij}k_{I,j} + \frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_i + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^*\dots$$

$$+ \widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left\{\left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{D}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{T,j}\right]\dots\right.$$

$$\left. + \Delta t a_{ii}\left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{D}^*\right]^{-1}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a *}\left(\vec{\phi}_i - 4\pi\vec{\mathbf{B}}^*\right) + \vec{S}_T\right]\right\}$$

Re-arranging to isolate $\vec{\phi}_i$:

$$\widehat{\mathbf{L}}\vec{\mathbf{I}}_i + \left(\frac{1}{c\Delta t a_{ii}}\mathbf{M} + \widehat{\mathbf{M}}_{\sigma_t,*}\right)\vec{\mathbf{I}}_i = \frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,*}\vec{\phi}_i\dots$$

$$+ \Delta t a_{ii}\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a,*}\mathbf{D}^*\right]^{-1}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\vec{\phi}_i\dots$$

$$+ \frac{1}{c\Delta t a_{ii}}\mathbf{M}\vec{\mathbf{I}}_n + \frac{1}{c a_{ii}}\mathbf{M}\sum_{j=1}^{i-1} a_{ij}k_{I,j} + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^*\dots$$

$$+\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\widehat{\mathbf{D}}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{T,j} + \Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\vec{S}_T - 4\pi\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{B}^*\right]\right] \quad (23)$$

Make the following definitions:

$$\bar{\bar{\xi}}_{i,d} = \frac{1}{c\Delta t a_{ii}}\mathbf{M}\vec{\mathbf{I}}_n + \frac{1}{c a_{ii}}\mathbf{M}\sum_{j=1}^{i-1} a_{ij}k_{I,j} + \widehat{\mathbf{M}}_{\sigma_a,*}\vec{\mathbf{B}}^*\dots$$

$$+\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^*\left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\widehat{\mathbf{D}}^*\right]^{-1}\left[\vec{\mathbf{T}}_n - \vec{\mathbf{T}}^* + \Delta t\sum_{j=1}^{i-1} a_{ij}k_{T,j} + \Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\left[\vec{S}_T - 4\pi\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{B}^*\right]\right] \quad (24a)$$

$$\bar{\bar{\nu}}_i = 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{\sigma_a,*}\widehat{\mathbf{D}}^* \left[\mathbf{I} + 4\pi\Delta t a_{ii}\widehat{\mathbf{M}}_{C_v}^{-1}\widehat{\mathbf{M}}_{\sigma_a *}\mathbf{D}^*\right]^{-1}\widehat{\mathbf{M}}_{C_v}^{-1} \tag{24b}$$

$$\bar{\bar{\mathbf{M}}}_{\sigma_t,i} = \mathbf{M}_{\sigma_t,*} + \frac{1}{c\Delta t a_{ii}}\mathbf{M} \tag{24c}$$

This then gives us our final equation for the radiation intensity:

$$\widehat{\mathbf{L}}\vec{\mathbf{I}}_i + \bar{\bar{\mathbf{M}}}_{\sigma_t,i}\vec{\mathbf{I}}_i = \frac{1}{4\pi}\mathbf{M}_{\sigma_s,*}\vec{\phi}_i + \frac{1}{4\pi}\bar{\bar{\nu}}_i\widehat{\mathbf{M}}_{\sigma_a *}\vec{\phi}_i + \bar{\bar{\xi}}_{i,d} \tag{25}$$

Having found $\vec{\mathbf{I}}$ for the i-th RK time step, we solve for $\vec{\mathbf{T}}_i$ using Eq. (21). At this point, we again have the option to either iterate on $\vec{\mathbf{T}}_i$, or we only solve for $\vec{\mathbf{T}}_i$ once. Regardless of whether we iterate for $\vec{\mathbf{T}}_i$ or not, we evaluate all material properties at the final value of $\vec{\mathbf{T}}_i$, and apply the definitions of $k_{T,i}$ and $k_{I,i}$:

$$k_{I,i} = c\mathbf{M}^{-1}\left[\frac{1}{4\pi}\widehat{\mathbf{M}}_{\sigma_s,i}\vec{\phi}_i + \widehat{\mathbf{M}}_{\sigma_a,i}\widehat{\mathbf{B}}_i - \widehat{\mathbf{M}}_{\sigma_t}\vec{\mathbf{I}}_i - \widehat{\mathbf{L}}\vec{\mathbf{I}}_i + \vec{S}_I\right] \tag{26}$$

$$k_{T,i} = \widehat{\mathbf{M}}_{C_v}^{-1}\left[\widehat{\mathbf{M}}_{\sigma_a,i}\left(\vec{\phi}_i - 4\pi\widehat{\mathbf{B}}_i\right) + \vec{S}_T\right] \tag{27}$$

After completing all steps of the particular RK scheme, we advance $\vec{\mathbf{I}}_n \to \vec{\mathbf{I}}_{n+1}$ and $\vec{\mathbf{T}}_n \to \vec{\mathbf{T}}_{n+1}$:

$$\vec{\mathbf{I}}_{n+1} = \vec{\mathbf{I}}_n + \Delta t\sum_{i=1}^{s} b_i k_{I,i}$$

$$\vec{\mathbf{T}}_{n+1} = \vec{\mathbf{T}}_n + \Delta t\sum_{i=1}^{s} b_i k_{T,i}$$