Explorations of Options for Radiation Transport in Draco

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December 2000

UWFDM-1146

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Introduction

As with most radiation hydrodynamic simulation codes, the time taken in Draco to compute the physics of radiation transport dominates the computational time for a complete simulation. As a result, a thorough analysis and re-engineering of the radiation transport physics package is to be undertaken. This report summarizes a survey of available methods for radiation transport and computational techniques to accelerate this phase of the simulation.

Radiation transport is an important physical process in many laser fusion problems. In particular, the experiments being conducted and simulated at LLE are strongly influenced by the transport of radiation through the target. Radiation transport describes a pathway for energy to be transferred between different regions of a target plasma, drastically altering the way that the target as a whole behaves. Furthermore, various diagnostic techniques are based on the emission or absorption of radiation within the target as a function of time.

Review of Radiative Transfer

The radiative transfer equation has the following form

$$\frac{1}{c}\frac{\partial I_\nu(\vec{r},\hat{\Omega},t)}{\partial t} + \hat{\Omega}\cdot\nabla I_\nu(\vec{r},\hat{\Omega},t) = -\kappa I_\nu(\vec{r},\hat{\Omega},t) + J_\nu(\vec{r},\hat{\Omega},t)\,, \tag{1}$$

where $I_\nu(\vec{r},\hat{\Omega},t)$ is the specific intensity and is a function of seven independent variables $(x, y, z, \theta, \phi, h\nu, t)$, as shown in Figure 1.

Since analytic solutions to this equation are only possible in a small number of special circumstances, a number of approximations are available to solve for $I_\nu(\vec{r},\hat{\Omega},t)$, including:

- P_n spherical harmonics
- multigroup flux limited diffusion
- S_n discrete ordinates
- Monte Carlo
- variable Eddington
- multigroup-gray.

P_n Approximation

The basis for the P_n approximation is an expansion of the solution $I_\nu(\vec{r},\hat{\Omega},t)$ as a sum of orthogonal functions, in this case spherical harmonics. For simplicity, if we consider only one dimension, the spherical harmonics reduce to the Legendre polynomials, $P_n(\mu)$, which is complete for $\cos(\theta) = \mu = [-1,1]$. In 2 and 3-dimensions, the full spherical harmonics, $Y_m^l(\theta,\phi)$, would be necessary.

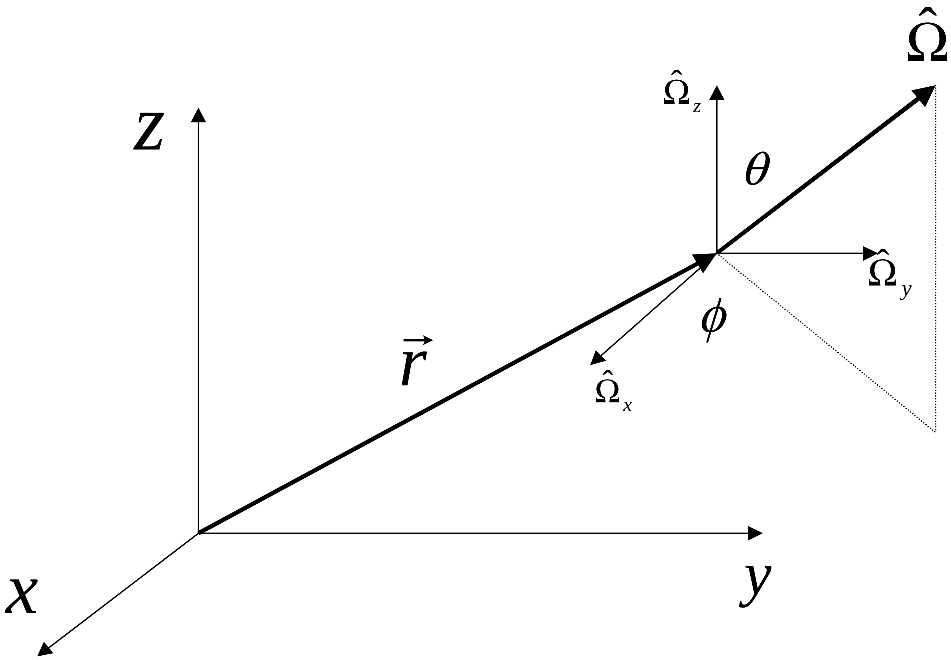

Figure 1. Description of spatial and angular variables.

The infinite expansion on this set of basis functions has the form

$$I_\nu(\vec{r},\hat{\Omega},t) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} I_n(\vec{r},\nu,t) P_n(\mu). \tag{2}$$

Substituting this into (1) and invoking the orthogonality of the Legendre polynomials

$$I_n(\vec{r},\nu,t) = 2\pi \int_{-1}^{1} d\mu P_n(\mu) I_\nu(\vec{r},\mu,t), \tag{3}$$

gives an infinite set of equations

$$\begin{aligned} &\frac{1}{c}\frac{\partial I_0}{\partial t} + \frac{\partial I_1}{\partial z} = -\kappa I_o + J_o \\ &\frac{2n+1}{c}\frac{\partial I_n}{\partial t} + n\frac{\partial I_{n-1}}{\partial z} + (n+1)\frac{\partial I_{n+1}}{\partial z} = -(2n+1)\kappa I_n, \quad \forall n \geq 1 \end{aligned} . \tag{4}$$

The set of equations is made manageable by truncating to some maximum value of n. For example, the P_1 approximation derives from setting all values of $I_n = 0, \quad \forall n \geq 2$, giving

$$\begin{aligned} &\frac{1}{c}\frac{\partial I_0}{\partial t} + \frac{\partial I_1}{\partial z} = -\kappa I_o + J_o \\ &\frac{3}{c}\frac{\partial I_1}{\partial t} + \frac{\partial I_0}{\partial z} = -3\kappa I_1 \end{aligned} . \tag{5}$$

The P_n approximation can, in principle, handle any degree of anisotropy, both in the specific radiation intensity and in the radiation transfer coefficient (opacities, cross-sections). However, in practice, highly anisotropic problems require many equations, that is many Legendre terms, in order to accurately predict the solution. The P_1 approximation, for example, estimates the specific intensity as linearly anisotropic.

Multigroup Flux Limited Diffusion

The P_1 approximation can be further simplified by assuming that the time derivative of the I_1 component is zero. Thus, the second equation of (5) becomes

$$\frac{\partial I_0}{\partial z} = -3\kappa I_1 \text{ or } I_1 = \frac{-1}{3\kappa}\frac{\partial I_0}{\partial z},$$

allowing the substitution into the first equation of (5), giving

$$\frac{1}{c}\frac{\partial I_0}{\partial t} - \frac{\partial}{\partial z}\frac{1}{3\kappa}\frac{\partial I_0}{\partial z} = -\kappa I_o + J_o, \tag{6}$$

or, for an arbitrary coordinate system,

$$\frac{1}{c}\frac{\partial I_0}{\partial t} - \nabla\frac{1}{3\kappa}\nabla I_0 = -\kappa I_o + J_o. \tag{7}$$

This is the radiation diffusion equation, with diffusion coefficient $D = -1/3\kappa$, and is the basis for the current radiation transport model in Draco. More specifically, the continuous energy spectrum is divided into a finite number of discrete energy groups, and the diffusion equation is applied to each energy group.

The simplifications made to derive the diffusion equation disrupt causality, permitting solutions with infinite propagation speeds. In order to mitigate this a correction is introduced to limit the flux to be no higher than the free streaming limit. This so-called *flux limiter* is typically implemented by replacing the diffusion coefficient D with an expression that varies between the physical diffusion coefficient in optically thick media and the asymptotic free streaming limit in optically thin media.

This method is well characterized, with a large base of experience using it for this kind of problem. While the issue of causality is addressed by implementing flux limiters, the mathematical assumptions made to derive this method translate to physical assumptions of optically thick media and isotropic intensities.

Variable Eddington

This method, also based on the P_n approximation, has seen some success in astrophysical applications. By including the P_1 term, it is slightly more flexible than the diffusion approximation, but there is little experience implementing this method for time-dependent radiation hydrodynamics problems and little numerical improvement over multigroup diffusion.

Multigroup-Gray Diffusion Approximation

As the methods used to solve the implicitly differenced diffusion equations for each energy group can be costly, there are benefits to solving as few different energy groups as possible. Since the derivation of group constants requires an energy dependent spectrum, many energy groups are typically used in order to minimize the effects of differences between the real spectrum and the characteristic spectrum used for calculating group constants.

One solution to this dichotomy is to employ a computationally efficient method to determine the normalized energy dependent spectrum. This detailed spectral information can be used to derive a small number of group constants for use in the solution to the implicitly differenced diffusion equation. The method used in the first phase of this approach need not be subject to the same restrictions as required of a general radiation transport method. For example, it need not conserve the total energy of the system, as long as it accurately generates the spectral information. The method of the second phase will ensure conservation using the normalized information of the first phase.

Depending on the method used in the first phase, this has the potential to be extremely parallelizable. For example, a fully explicit differencing of the diffusion equations would allow for an efficient domain decomposition in problems with large spatial domains. Of course, it is subject to all the same limitations as the diffusion approximation, namely, questionable validity in optically thin regions.

Discrete Ordinates (S_n) Approximation

The basis of the discrete ordinates, or S_n, approximation is the discretization of the angular variables in the transport equation (1). A number of different directions are chosen in the interval $\cos\theta = \mu = [-1,1]$, and the spatial mesh is swept from the left boundary condition tracking the forward streaming directions and then swept back tracking the backward streaming directions. This is repeated until the solution converges.

This method is particularly well suited for strongly anisotropic intensities and anisotropic cross-sections. The cross-sections are expanded on the Legendre polynomial basis set, which means the roots of those polynomials are prudent values for the discrete directions chosen in this approximation.

While these methods have seen a great deal of success for time independent neutron-gamma transport problems in 1- and 2-dimensions [1], they are less suited to radiative transfer problems of radiation hydrodynamics. In optically thin media, the well known ray effects lead to artificially preferential transport along the chosen discrete directions, and thus artificially low intensities between those directions. Conversely, in optically thick regions, this method can be very slow to converge unless some acceleration is used, such as diffusion synthetic acceleration (DSA). Finally, this approximation can be very complex when applied to distorted meshes. All of these mean that the S_n approximation is much more costly than diffusion with questionable benefit for the type of problems found in radiation hydrodynamics.

Monte Carlo

The Monte Carlo method consists of tracking the path and interactions undergone by a statistical sample of individual photons. This method can be extremely accurate, as it is essentially a pure physical simulation of the individual microscopic processes. To achieve this accuracy, however, a statistically large sample must be used, resulting in significant computational time.

Furthermore, Monte Carlo methods are best suited to solutions with a few individual solutions in space. To calculate an entire field of solutions on a fine spatial resolution, the statistical sample would have to be even larger, resulting in even more computational time. Finally, there are significant complexities involved with implementing Monte Carlo methods in multi-dimensional problems with distorted and mobile zone boundaries separating fine grained heterogeneities.

While Monte Carlo methods are intrinsically favorable to parallelization, the accuracy and spatial resolution required for radiation hydrodynamics problems would still require enough computational time to preclude their use.

Summary and Selection

The first choice for near-term implementation within Draco is multigroup flux limited diffusion. A long history of this method in radiation hydrodynamics has not only shown its value and applicability, but provides an extensive body of literature in which to find recommendations and suggestions for its implementation. There are some other methods which are slightly better that diffusion for anisotropic problems, but the benefit of these methods does not match the short-term development risk in implementing them. There is some concern for the efficiency of this method, particularly since a substantial and costly matrix inversion must be performed for each group in the multigroup expansion. This can be somewhat mitigated by exploring various parallelization paradigms for this part of the total radiation hydrodynamics problem.

For medium term consideration, particularly in 3-dimensions, the multigroup-gray diffusion approach deserves some attention. Since it builds upon the underlying infrastructure of the diffusion approximation for its second phase, research can be performed into various alternatives for the first phase without impacting the development of radiation transport in general.

With extensive experience outside the radiation hydrodynamics field, both S_n and Monte Carlo methods may also have some role to play in the long term. Neither of these methods builds directly upon the infrastructure of the multigroup diffusion approximation, and thus represent a larger development risk and longer development time.

Implementation of Multigroup Diffusion

This section will discuss the implementation of a multigroup flux-limited diffusion method in Cartesian coordinate systems.

The 1-D 3-point Stencil

Starting with the diffusion equation in one-dimension (equation 6),

$$\frac{1}{c}\frac{\partial I}{\partial t} - \frac{\partial}{\partial z} D \frac{\partial I}{\partial z} = -\kappa I + J \,, \tag{6}$$

and integrating over the dimension of cell *i*, gives

$$\int_{Z_i} dz \left(\frac{1}{c}\frac{\partial I}{\partial t} - \frac{\partial}{\partial z} D \frac{\partial I}{\partial z} \right) = \int_{Z_i} dz \left(-\kappa I + J \right)$$

$$(\hat{z}_{i+1} - \hat{z}_i)\frac{1}{c}\frac{\partial \langle I \rangle}{\partial t} - \int_{Z_i} dz \left(\frac{\partial}{\partial z} D \frac{\partial I}{\partial z} \right) = (\hat{z}_{i+1} - \hat{z}_i)\left(-\kappa \langle I \rangle + \langle J \rangle \right) \quad \text{(mean value theorem)}$$

$$\frac{1}{c}\frac{\partial \langle I \rangle}{\partial t} - \frac{1}{\Delta z_{i+1/2}} \left[\hat{D}\frac{\partial \hat{I}}{\partial z}\bigg|_{i+1} - \hat{D}\frac{\partial \hat{I}}{\partial z}\bigg|_{i} \right] = -\kappa \langle I \rangle + \langle J \rangle$$

where accented variables (e.g. $\hat{D}$) denote vertex-centered values and unaccented variables are cell-centered. Until now, no assumptions or approximations have been made about the function form of the radiation intensity, *I*. In order to change the derivative operator into a difference operator, it is necessary to know the value of the radiation intensity at the center of the cell. Therefore, we will define (assume) that the cell-centered radiation intensity, I_i, is identical to the mean value in that cell, $\langle I \rangle_i$.

Central differencing of the spatial derivative and forward differencing the time derivative give:

$$\frac{1}{c}\frac{I_i^{n+1}-I_i^n}{\Delta t^{n+1/2}}-\frac{1}{\Delta z_{i+1/2}}\left[\hat{D}_{i+1}\frac{I_{i+1}^{n+1}-I_i^{n+1}}{z_{i+1}-z_i}-\hat{D}_i\frac{I_i^{n+1}-I_{i-1}^{n+1}}{z_i-z_{i-1}}\right]=-\kappa I_i^{n+1}+J_i^{n+1}\ ,$$

where the superscript, *n*, denotes the time step index.

Written as a 3-point stencil:

$$\begin{aligned}&\frac{1}{c}\frac{I_i^{n+1}-I_i^n}{\Delta t^{n+1/2}}-\frac{1}{\Delta z_{i+1/2}}\left[\frac{\hat{D}_{i+1}}{\delta z_{i+1/2}}I_{i+1}^{n+1}-\left(\frac{\hat{D}_{i+1}}{\delta z_{i+1/2}}+\frac{\hat{D}_i}{\delta z_{i-1/2}}\right)I_i^{n+1}+\frac{\hat{D}_i}{\delta z_{i-1/2}}I_{i-1}^{n+1}\right]=-\kappa I_i^{n+1}+J_i^{n+1}\\&-\frac{\lambda_{i+1/2}}{\Delta z_{i+1/2}}I_{i+1}^{n+1}+\left[\frac{1}{c\Delta t^{n+1/2}}+\frac{\left(\lambda_{i+1/2}+\lambda_{i-1/2}\right)}{\Delta z_{i+1/2}}+\kappa\right]I_i^{n+1}-\frac{\lambda_{i-1/2}}{\Delta z_{i+1/2}}I_{i-1}^{n+1}=J_i^{n+1}+\frac{I_i^n}{c\Delta t^{n+1/2}}\end{aligned}\quad ,(8)$$

where $\lambda_{i+1/2}=\hat{D}_{i+1}/\delta z_{i+1/2}$, $\Delta z_{i+1/2}=\hat{z}_{i+1}-\hat{z}_i$, and $\delta z_{i+1/2}=z_{i+1}-z_i$.

As a summarizing note, the only assumption made in this derivation is that the mean value of the radiation intensity in the cell is identical to the value at the cell center.

The 2-D 9-point Stencil

Note: the derivation presented in this section is based entirely on the work of Richard Bruce Hickman, presented in his Ph.D. thesis of May, 1978[2].

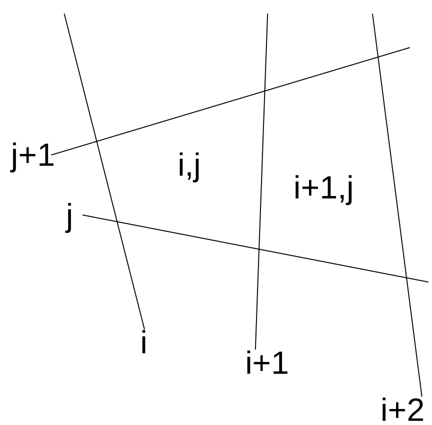

Figure 2. Sample Lagrangian mesh providing reference for mathematical derivation.

Starting with the diffusion equation in 2 (or more) dimensions (equation 7),

$$\frac{1}{c}\frac{\partial I}{\partial t}-\vec{\nabla}\cdot D\vec{\nabla}I=-\kappa I+J\ , \tag{7}$$

and integrating over the area of cell *ij*, gives

$$\int_{A_{ij}} dA\left(\frac{1}{c}\frac{\partial I}{\partial t} - \vec{\nabla}\cdot D\vec{\nabla}I\right) = \int_{A_{ij}} dA\left(-\kappa I + J\right)$$

$$\left|A_{ij}\right|\frac{1}{c}\frac{\partial\langle I\rangle}{\partial t} - \int_{A} dA\left(\vec{\nabla}\cdot D\vec{\nabla}I\right) = \left|A_{ij}\right|\left(-\kappa\langle I\rangle + \langle J\rangle\right) \qquad \text{(mean value theorem)}.$$

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{\left|A_{ij}\right|}\oint_{S_{ij}} dS\left(\vec{n}\cdot D\vec{\nabla}I\right) = -\kappa I_{ij} + J_{ij} \qquad \text{(Gauss' Theorem)}$$

As in the 1-dimensional case, the most basic assumption is that the cell-centered radiation intensity, I_{ij}, is identical to the mean value in that cell, $\langle I\rangle_{ij}$.

Since this line integral is around the perimeter of an arbitrary quadrilateral, it can be replaced by a summation:

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{\left|A_{ij}\right|}\left(F_{i+1,j+1/2} + F_{i+1/2,j+1} + F_{i,j+1/2} + F_{i+1/2,j}\right) = -\kappa I_{ij} + J_{ij}, \tag{9}$$

where

$$\begin{aligned} F_{i+1,j+1/2} &= \int_{i+1,j}^{i+1,j+1} ds\left[\vec{n}_{i+1,j+1/2}\cdot\left(D\vec{\nabla}I\right)_{i+1,j+1/2}\right] \\ &= L_{i+1,j+1/2}\vec{n}_{i+1,j+1/2}\cdot\left\langle D\vec{\nabla}I\right\rangle_{i+1,j+1/2} \\ &= \Delta y_{i+1,j+1/2}\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,j+1/2} - \Delta x_{i+1,j+1/2}\left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+1,j+1/2}, \end{aligned} \tag{10}$$

and

$$\begin{aligned} L_{i+1,j+1/2} &= \sqrt{(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j})^2 + (\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j})^2} \\ \vec{n}_{i+1,j+1/2} &= \left(\frac{\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}}{L_{i+1,j+1/2}}, -\frac{\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}}{L_{i+1,j+1/2}}\right) \\ \left\langle D\vec{\nabla}I\right\rangle_{i+1,j+1/2} &= \left(\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,j+1/2}, \left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+1,j+1/2}\right). \end{aligned}$$

It is now necessary to consider the determination of the mean value, $\left\langle D\vec{\nabla}I\right\rangle$. The two dimensional version of Stoke's theorem states

$$\int_{B}\left(\frac{\partial f}{\partial x} - \frac{\partial g}{\partial y}\right)dxdy = \oint_{\partial B}(f dy + g dx),$$

which implies

$$\int_B \frac{\partial f}{\partial x} dxdy = \oint_{\partial B} f dy \quad \text{and} \quad \int_B \frac{\partial g}{\partial y} dxdy = -\oint_{\partial B} g dx \, ,$$

which for this problem can be invoked as:

$$\int_B \frac{\partial I}{\partial \tau_x} d\tau_x dy = \oint_{\partial B} I dy \quad \text{and} \quad \int_B \frac{\partial I}{\partial \tau_y} dx d\tau_y = -\oint_{\partial B} I dx \, ,$$

where $d\tau_x = dx / D$ and $d\tau_y = dy / D$. The mean value theorem gives

$$\int_B \frac{\partial I}{\partial \tau_x} d\tau_x dy = \left\langle D \frac{\partial I}{dx} \right\rangle \int_B \frac{dxdy}{D} = \oint_{\partial B} I dy$$
$$\left\langle D \frac{\partial I}{dx} \right\rangle = \frac{\oint_{\partial B} I dy}{\int_B \frac{dxdy}{D}} \, , \tag{11}$$

and similarly for the *y*-derivative term.

Given this, we can then define a region, *B*, upon which to apply Stoke's theorem on the side, *i+1,j+1/2*, using the centers of the two cells separated by this side and the vertices of the side itself.

In the case where the radiation intensity varies linearly between adjacent vertices of the region *B*,

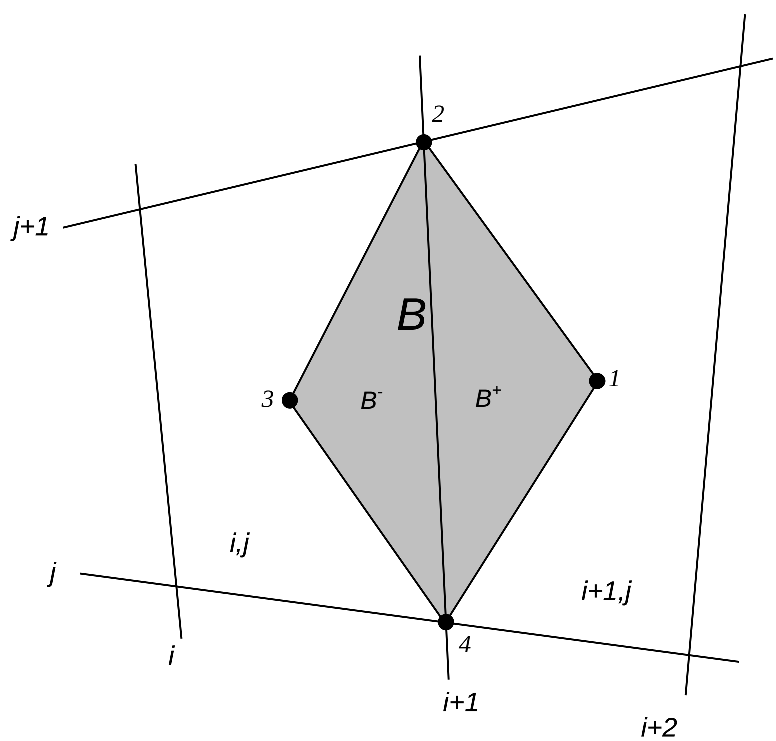

Figure 3. Sub-region defined for determination of mean value gradient on side i+1,j+1/2 using Stoke's theorem.

$$\oint_{\partial B} I dy = \frac{1}{2}\left[\left(I_{i+1,j} - I_{ij}\right)\left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right) - \left(\hat{I}_{i+1,j+1} - \hat{I}_{i+1,j}\right)\left(y_{i+1,j} - y_{ij}\right)\right]$$
$$\oint_{\partial B} I dx = \frac{1}{2}\left[\left(I_{i+1,j} - I_{ij}\right)\left(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}\right) - \left(\hat{I}_{i+1,j+1} - \hat{I}_{i+1,j}\right)\left(x_{i+1,j} - x_{ij}\right)\right] \quad (12)$$

Furthermore, if region B is divided into two sub-regions, one on each side of the side $i+1,j+1/2$,

$$\int_B \frac{dxdy}{D} = \int_{B^-_{i+1,j+1/2}} \frac{dxdy}{D} + \int_{B^+_{i+1,j+1/2}} \frac{dxdy}{D} = \frac{\left|B^-_{i+1,j+1/2}\right|}{D^{B-}_{i+1,j+1/2}} + \frac{\left|B^+_{i+1,j+1/2}\right|}{D^{B+}_{i+1,j+1/2}},$$

using the mean value theorem.

For the purpose of implementation, we can define an effective diffusion coefficient:

$$\frac{1}{D^*_{i+1,j+1/2}} \equiv \frac{\left|B^-_{i+1,j+1/2}\right|}{D^-_{i+1,j+1/2}} + \frac{\left|B^+_{i+1,j+1/2}\right|}{D^+_{i+1,j+1/2}}$$

and assume that the vertex-centered values of the radiation intensity are a linear combination of the cell-centered values from the four adjacent cells:

$$\hat{I}_{i+1,j+1} = \gamma^{i+1,j+1}_{ij} I_{ij} + \gamma^{i+1,j+1}_{i+1,j} I_{i+1,j} + \gamma^{i+1,j+1}_{i,j+1} I_{i,j+1} + \gamma^{i+1,j+1}_{i+1,j+1} I_{i+1.j+1}.$$

Substituting these into equation 10, we get:

$$F_{i+1,j+1/2} = \frac{D^*_{i+1,j+1/2}\Delta y_{i+1,j+1/2}}{2}\left[\begin{array}{l}\left(I_{i+1,j} - I_{ij}\right)\Delta y_{i+1,j+1/2} \\ -\left(\begin{array}{l}\gamma^{i+1,j+1}_{ij} I_{ij} + \gamma^{i+1,j+1}_{i+1,j} I_{i+1,j} + \gamma^{i+1,j+1}_{i,j+1} I_{i,j+1} + \gamma^{i+1,j+1}_{i+1,j+1} I_{i+1.j+1} \\ -\gamma^{i+1,j}_{i,j-1} I_{i,j-1} - \gamma^{i+1,j}_{i+1,j-1} I_{i+1,j-1} - \gamma^{i+1,j}_{ij} I_{ij} - \gamma^{i+1,j}_{i+1,j} I_{i+1.j}\end{array}\right)\delta y_{i+1,j+1/2}\end{array}\right]$$
$$+ \frac{D^*_{i+1,j+1/2}\Delta x_{i+1,j+1/2}}{2}\left[\begin{array}{l}\left(I_{i+1,j} - I_{ij}\right)\Delta x_{i+1,j+1/2} \\ -\left(\begin{array}{l}\gamma^{i+1,j+1}_{ij} I_{ij} + \gamma^{i+1,j+1}_{i+1,j} I_{i+1,j} + \gamma^{i+1,j+1}_{i,j+1} I_{i,j+1} + \gamma^{i+1,j+1}_{i+1,j+1} I_{i+1.j+1} \\ -\gamma^{i+1,j}_{i,j-1} I_{i,j-1} - \gamma^{i+1,j}_{i+1,j-1} I_{i+1,j-1} - \gamma^{i+1,j}_{ij} I_{ij} - \gamma^{i+1,j}_{i+1,j} I_{i+1.j}\end{array}\right)\delta x_{i+1,j+1/2}\end{array}\right].$$

If this is continued for all 4 sides (see Appendix) the result is the 9-pt stencil:

$$\begin{aligned}&\beta_{i-1,j-1}I_{i-1,j-1}+\beta_{i,j-1}I_{i,j-1}+\beta_{i+1,j-1}I_{i+1,j-1}\\&+\beta_{i-1,j}I_{i-1,j}+\alpha_{ij}I_{ij}+\beta_{i+1,j}I_{i+1,j}\\&+\beta_{i-1,j+1}I_{i-1,j+1}+\beta_{i,j+1}I_{i,j+1}+\beta_{i+1,j+1}I_{i+1,j+1}\end{aligned} \quad = \quad \frac{I_{ij}^{n-1}}{c\Delta t^{n-1/2}}+J_{ij}\ ,$$

where:

$$\alpha_{ij}=\left(\beta_{ij}+\frac{1}{c\Delta t^{n-1/2}}+\kappa\right)$$

$$\beta_{i-1.j-1}=\frac{1}{2|A_{ij}|}\gamma_{i-1,j-1}^{ij}\left(D_{i-}^{*}\Lambda_{i-}^{*}+D_{j-}^{*}\Lambda_{j-}^{*}\right)$$

$$\beta_{i.j-1}=\frac{-1}{2|A_{ij}|}\left(D_{j-}^{*}L_{j-}^{2}+\gamma_{i,j-1}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2}+D_{j-}^{*}\Lambda_{j-}^{2}\right]-\gamma_{i,j-1}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2}+D_{j-}^{*}\Lambda_{j-}^{2}\right]\right)$$

$$\beta_{i+1.j-1}=\frac{-1}{2|A_{ij}|}\gamma_{i+1,j-1}^{i,j+1}\left(D_{i+}^{*}\Lambda_{i+}^{*}+D_{j-}^{*}\Lambda_{j-}^{*}\right)$$

$$\beta_{i-1.j}=\frac{-1}{2|A_{ij}|}\left(D_{i-}^{*}L_{i-}^{2}+\gamma_{i-1,j}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2}+D_{i-}^{*}\Lambda_{i-}^{2}\right]-\gamma_{i-1,j}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2}+D_{j-}^{*}\Lambda_{j-}^{2}\right]\right)$$

$$\beta_{ij}=\frac{1}{2|A_{ij}|}\begin{pmatrix}D_{j+}^{*}L_{j+}^{2}+D_{i-}^{*}L_{i-}^{2}+D_{i+}^{*}L_{i+}^{2}+D_{j-}^{*}L_{j-}^{2}\\-\gamma_{ij}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2}+D_{j-}^{*}\Lambda_{j-}^{2}\right]-\gamma_{ij}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2}+D_{i-}^{*}\Lambda_{i-}^{2}\right]\\+\gamma_{ij}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2}+D_{j+}^{*}\Lambda_{j+}^{2}\right]+\gamma_{ij}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2}+D_{j-}^{*}\Lambda_{j-}^{2}\right]\end{pmatrix}$$

$$\beta_{i+1.j}=\frac{-1}{2|A_{ij}|}\left(D_{i+}^{*}L_{i+}^{2}+\gamma_{i+1,j}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2}+D_{j-}^{*}\Lambda_{j-}^{2}\right]-\gamma_{i+1,j}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2}+D_{j+}^{*}\Lambda_{j+}^{2}\right]\right)$$

$$\beta_{i-1.j+1}=\frac{-1}{2|A_{ij}|}\gamma_{i-1,j+1}^{i+1,j}\left(D_{i-}^{*}\Lambda_{i-}^{*}+D_{j+}^{*}\Lambda_{j+}^{*}\right)$$

$$\beta_{i.j+1}=\frac{-1}{2|A_{ij}|}\left(D_{j+}^{*}L_{j+}^{2}+\gamma_{i,j+1}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2}+D_{i-}^{*}\Lambda_{i-}^{2}\right]-\gamma_{i,j+1}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2}+D_{j+}^{*}\Lambda_{j+}^{2}\right]\right)$$

$$\beta_{i+1.j+1}=\frac{1}{2|A_{ij}|}\gamma_{i+1,j+1}^{i+1,j+1}\left(D_{i+}^{*}\Lambda_{i+}^{*}+D_{j+}^{*}\Lambda_{j+}^{*}\right),$$

and

$$\Delta y_{i-}^{2}=\Delta y_{i,j+1/2}\Delta y_{i,j+1/2} \qquad \Delta\delta y_{i-}=\Delta y_{i,j+1/2}\delta y_{i,j+1/2}$$

$$\Delta y_{i+}^{2}=\Delta y_{i+1,j+1/2}\Delta y_{i+1,j+1/2} \qquad \Delta\delta y_{i+}=\Delta y_{i+1,j+1/2}\delta y_{i+1,j+1/2}$$

$$\Delta y_{j-}^{2}=\Delta y_{i+1/2,j}\Delta y_{i+1/2,j} \qquad \Delta\delta y_{j-}=\Delta y_{i+1/2,j}\delta y_{i+1/2,j}$$

$$\Delta y_{j+}^{2}=\Delta y_{i+1/2,j+1}\Delta y_{i+1/2,j+1} \qquad \Delta\delta y_{j+}=\Delta y_{i+1/2,j+1}\delta y_{i+1/2,j+1}$$

and similarly for x, so that:

$$
\begin{array}{lll}
L_{i-}^2 = \Delta y_{i-}^2 + \Delta x_{i-}^2 & \Lambda_{i-}^2 = \Delta\delta y_{i-} + \Delta\delta x_{i-} & D_{i-} = D_{i,j+\frac{1}{2}}^* \\
L_{i+}^2 = \Delta y_{i+}^2 + \Delta x_{i+}^2 & \Lambda_{i+}^2 = \Delta\delta y_{i+} + \Delta\delta x_{i+} & D_{i+} = D_{i+1,j+\frac{1}{2}}^* \\
L_{j-}^2 = \Delta y_{j-}^2 + \Delta x_{j-}^2 & \Lambda_{j-}^2 = \Delta\delta y_{j-} + \Delta\delta x_{j-} & D_{j-} = D_{i+\frac{1}{2},j}^* \\
L_{j+}^2 = \Delta y_{j+}^2 + \Delta x_{j+}^2 & \Lambda_{j+}^2 = \Delta\delta y_{j+} + \Delta\delta x_{j+} & D_{j+} = D_{i+\frac{1}{2},j+1}^*
\end{array} .
$$

There are two issues yet to be resolved:

- the determination of sub-region mean values of the diffusion coefficients, and
- the determination of the weights for the vertex-centered values of the radiation intensity based on the adjacent cell-centered values.

The simplest solutions to these issues are to assume that the diffusion coefficient for each sub-region is equal to the diffusion coefficient for the whole grid region in question, and that the vertex-centered radiation intensities are found by simply averaging the 4 adjacent cell-centered values.

Future Development

Future development will focus on the following areas:

1. The investigation of alternative formulations for the diffusion coefficients, including the introduction of various flux limiters;
2. the investigation of alternative formulations for the linear weights used to calculate the vertex-centered radiation intensity;
3. the development of the difference equations for cylindrical (r-z) coordinate systems; and
4. the development of difference equations for various boundary conditions.

Options for Parallel Implementation

Introduction

In most traditional implementations of multigroup diffusion, each of the energy groups is solved in sequence: a matrix for that group is constructed based on the difference equations and then inverted. There are typically between 2 and 100 energy groups and the solution of each group is independent of the other groups.

For large problems with many groups, this can often dominate the computing time required for a solution. As a result, there is motivation for exploring different options for the parallelization of this process. There are two obvious approaches for parallelization:

- solving each group in sequence, inverting the matrix by use of parallel sparse matrix algebra libraries, or
- solving the groups in parallel, with each group's matrix being solved on a different processor.

This section will describe the issues related to each of these approaches, including some early testing of parallel sparse matrix libraries.

With all parallelization approaches, an important issue is that of communication of data among the processors, and specifically, the ratio between the time spent in communication and the time spent performing useful computation.

Parallel Sparse Matrix Algebra Libraries

With this approach, the matrix inversions occur sequentially, but the processing for each matrix inversion is spread across the available processors by invoking parallel libraries for sparse matrix algebra. While the libraries themselves typically handle all the communication internally, the process of setting up each matrix across the processors would represent the biggest communication penalty. Early testing has been performed with two candidate libraries, Aztec 2.1 and PETSc 2.0.24, using a matrix typical of a radiation diffusion problem created on a 100x100 spatial mesh. The Aztec parallel library is being developed at Sandia National Laboratory. PETSc is being developed at Argonne National Laboratory. Both offer a variety of methods and preconditioners for the solution of sparse linear systems. For all testing, the platform was an SGI Origen2000 machine located at LLE.

Testing with Aztec was performed on a range of processors, from 1 to 16d, using the default conjugate gradient method with no preconditioner. The results were generated by Aztec's built-in timing routines and averaged over 10 independent runs for each number of processors. The time taken to solve the system for a single processor was 2.1 ± 0.1 s in 570 iterations. The minimum reliable (small standard deviation) run time was 0.32 ± 0.06 s in 333 iterations with 6 processors. While it is unexpected for the number of iterations to be a function of the number of processors, this represents significant speed-up. For more than 6 processors, the speed-up is not substantial and the standard deviation in the results was significant. The library's authors are currently being contacted for their comments on the correlation between the number of processors and the number of iterations.

Testing with PETSc was somewhat less successful as it experienced convergence problems when running on more than one processor. However, single processor results were available with a run time of 1.3 s in 70 iterations using the default methods: GMRES with block Jacobi preconditioning.

It is important to restate that the run times reported in this testing did not include the time spent distributing the matrix elements to the various processors. A true analysis of this is being partially facilitated by integrating Aztec into the ORCHID radiation hydrodynamics code as an alternative to the existing solver.

Master/Slave Groupwise Processing

With this approach each group is solved using traditional sequential methods, but simultaneous to other groups on different processors. The maximum theoretical benefit of this method comes from having as many processors as there are energy groups, therefore solving all the groups simultaneously. Since the individual group calculations are independent of each other, the only communication is the sharing of the current state and geometry to all processors once before any group calculation and the collecting of the energy emission and deposition terms from all processors once after all the group calculations.

Single Processor Matrix Methods

When implementing the master/slave approach for parallelization, the single processor matrix inversion performance will be of utmost importance. One result of the testing with parallel matrix libraries was that the single processor performance of these libraries was better than the experience base with the existing methods. This indicated a need to better understand what single processor methods were being used and whether they were ideally tuned to the problems and computing platforms in question.

Most importantly, new classes of solution methodologies exist that may be well suited to these problems. Multi-grid methods, for example, have a physical analogue which suggests that they will result in rapid convergence to the final solution.

Future Development

More work will be done to characterize the different parallelization approaches and improve the implementation of matrix inversion, whether in parallel or on a single processor. This will include:

- testing of parallel libraries under application relevant conditions to achieve a measure of their total time, including communication of the initial matrices;
- investigation of the master/slave approach to better determine the balance between communication and computation; and
- investigation into and testing of alternative single processor matrix inversion methods and libraries.

While further characterization of these methods may indicate a preference of one method over the other, it is also possible to implement a combination of the two methods for increased flexibility.

Summary

A variety of approaches for the modeling of radiative transfer have been outlined. The numerical stencil for multigroup diffusion, as the preferred of these models, has been derived in detail for 1- and 2-dimensions in Cartesian coordinates. Three remaining issues have been identified for the implementation of the Cartesian diffusion model. A similar derivation will be necessary for cylindrical coordinate systems.

These numerical stencils result in large sparse matrices that are typically expensive to invert. Two approaches for parallelization have been described. Further characterization of these approaches will provide input on how to proceed. In particular, it is not yet clear whether one approach is preferred over the other or if they are complementary. The impact of highly efficient single processor matrix inversion will also be important.

References

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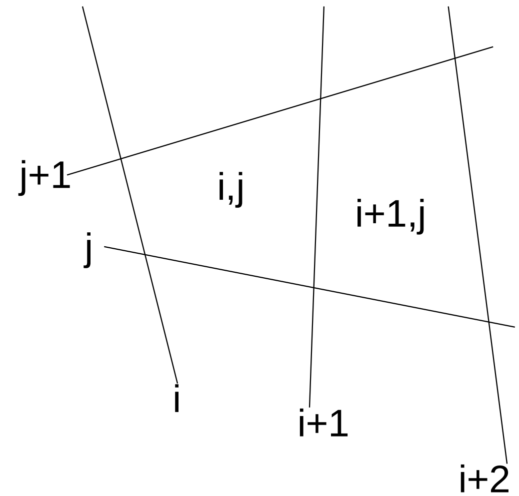
Acknowledgement

Funding for this work was provided by the U.S. Department of Energy through the University of Rochester Laboratory for Laser Energetics.

APPENDIX: Detailed Derivation of Diffusion Operator on Lagrangian Mesh



$$\frac{1}{c}\frac{\partial I}{\partial t} - \vec{\nabla}\cdot D\vec{\nabla} I = -\kappa I + J$$

$$\int_{A_{ij}} dA\left(\frac{1}{c}\frac{\partial I}{\partial t} - \vec{\nabla}\cdot D\vec{\nabla} I\right) = \int_{A_{ij}} dA\left(-\kappa I + J\right)$$

$$\left|A_{ij}\right|\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \int_{A} dA\left(\vec{\nabla}\cdot D\vec{\nabla} I\right) = \left|A_{ij}\right|\left(-\kappa I_{ij} + J_{ij}\right) \qquad \text{(mean value theorem)}$$

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{\left|A_{ij}\right|}\oint_{\partial A_{ij}} ds\left(\vec{n}\cdot D\vec{\nabla} I\right) = -\kappa I_{ij} + J_{ij} \qquad \text{(Gauss' Theorem)}$$

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{\left|A_{ij}\right|}\left(F_{i+1,j+\frac{1}{2}} + F_{i+\frac{1}{2},j+1} + F_{i,j+\frac{1}{2}} + F_{i+\frac{1}{2},j}\right) = -\kappa I_{ij} + J_{ij} \qquad \text{(4 sides of quadrilateral)}$$

$$F_{i+1,j+\frac{1}{2}} = \int_{i+1,j}^{i+1,j+1} ds\left[\vec{n}_{i+1,j+\frac{1}{2}}\cdot\left(D\vec{\nabla} I\right)_{i+1,j+\frac{1}{2}}\right]$$

$$= L_{i+1,j+\frac{1}{2}}\vec{n}_{i+1,j+\frac{1}{2}}\cdot\left\langle D\vec{\nabla} I\right\rangle_{i+1,j+\frac{1}{2}}$$

$$L_{i+1,j+\frac{1}{2}} = \sqrt{(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j})^2 + (\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j})^2}$$

$$\vec{n}_{i+1,j+\frac{1}{2}} = \left(\frac{\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}}{L_{i+1,j+\frac{1}{2}}}, -\frac{\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}}{L_{i+1,j+\frac{1}{2}}}\right)$$

$$\left\langle D\vec{\nabla} I\right\rangle_{i+1,j+\frac{1}{2}} = \left(\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,j+\frac{1}{2}}, \left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+1,j+\frac{1}{2}}\right)$$

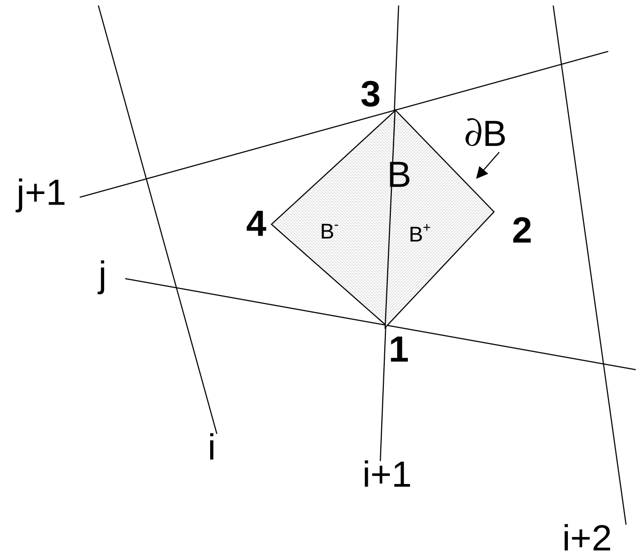
$$F_{i+1,j+\frac{1}{2}} = \left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right)\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,j+\frac{1}{2}} - \left(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}\right)\left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+1,j+\frac{1}{2}}$$

$$\int_B D\frac{\partial I}{\partial x}\frac{dx}{D}dy = \oint_{\partial B} Idy$$

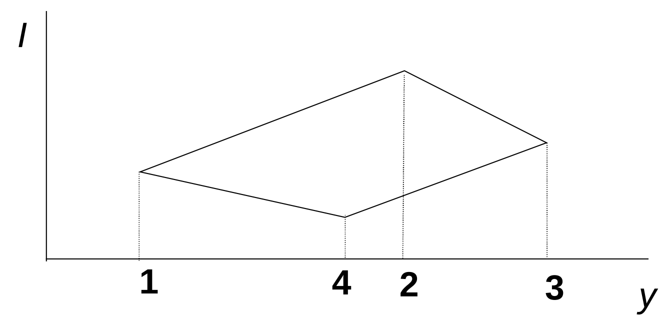
$$\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,\,j+1/2}\int_B \frac{dxdy}{D} = \oint_{\partial B} Idy$$

$$\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,\,j+1/2} = \frac{\oint_{\partial B} Idy}{\int_B \frac{dxdy}{D}}$$

$$\left(\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,\,j+1/2}, \left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+1,\,j+1/2}\right) = \frac{1}{\int_B \frac{dxdy}{D}}\left(\oint_{\partial B} Idy, -\oint_{\partial B} Idx\right)$$



If I varies linearly on the boundary, ∂B, as in the following figure:



$$\oint_{\partial B} Idy = \frac{1}{2}\left(I_{i+1,j} + \hat{I}_{i+1,j}\right)\left(y_{i+1,j} - \hat{y}_{i+1,j}\right) + \frac{1}{2}\left(\hat{I}_{i+1,j+1} + I_{i+1,j}\right)\left(\hat{y}_{i+1,j+1} - y_{i+1,j}\right) + \frac{1}{2}\left(I_{ij} + \hat{I}_{i+1,j+1}\right)\left(y_{ij} - \hat{y}_{i+1,j+1}\right) + \frac{1}{2}\left(\hat{I}_{i+1,j} + I_{ij}\right)\left(\hat{y}_{i+1,j} - y_{ij}\right)$$

$$= \frac{1}{2}\left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right)I_{i+1,j} + \frac{1}{2}\left(y_{i+1,j} - y_{ij}\right)\hat{I}_{i+1,j} + \frac{1}{2}\left(y_{ij} - y_{i+1,j}\right)\hat{I}_{i+1,j+1} + \frac{1}{2}\left(\hat{y}_{i+1,j} - \hat{y}_{i+1,j+1}\right)I_{ij}$$

$$= \frac{1}{2}\left[\left(I_{i+1,j} - I_{ij}\right)\left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right) - \left(\hat{I}_{i+1,j+1} - \hat{I}_{i+1,j}\right)\left(y_{i+1,j} - y_{ij}\right)\right]$$

and similarly

$$\oint_{\partial B} Idx = \frac{1}{2}\left[\left(I_{i+1,j} - I_{ij}\right)\left(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}\right) - \left(\hat{I}_{i+1,j+1} - \hat{I}_{i+1,j}\right)\left(x_{i+1,j} - x_{ij}\right)\right]$$

Definitions:

$$\Delta y_{i+1,j+\frac{1}{2}} \equiv \hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}$$

$$\delta y_{i+1,j+\frac{1}{2}} \equiv y_{i+1,j} - y_{ij}$$

$$\frac{1}{D^*_{i+1,j+\frac{1}{2}}} \equiv \frac{\left|B^-_{i+1,j+\frac{1}{2}}\right|}{D^-_{i+1,j+\frac{1}{2}}} + \frac{\left|B^+_{i+1,j+\frac{1}{2}}\right|}{D^+_{i+1,j+\frac{1}{2}}}$$

$$\int_B \frac{dxdy}{D} = \int_{B_{ij}} \frac{dxdy}{D} + \int_{B_{i+1,j}} \frac{dxdy}{D} = \frac{\left|B^-_{i+1,j+\frac{1}{2}}\right|}{D^-_{i+1,j+\frac{1}{2}}} + \frac{\left|B^+_{i+1,j+\frac{1}{2}}\right|}{D^+_{i+1,j+\frac{1}{2}}}$$

$$\left|B^-_{i+1,j+\frac{1}{2}}\right| = \frac{1}{2}\left|\left(\hat{x}_{i+1,j+1} - x_{ij}\right) * \left(\hat{y}_{i+1,j} - y_{ij}\right) - \left(\hat{x}_{i+1,j} - x_{ij}\right) * \left(\hat{y}_{i+1,j+1} - y_{ij}\right)\right|$$

$$\left|B^+_{i+1,j+\frac{1}{2}}\right| = \frac{1}{2}\left|\left(\hat{x}_{i+1,j+1} - x_{i+1,j}\right) * \left(\hat{y}_{i+1,j} - y_{i+1,j}\right) - \left(\hat{x}_{i+1,j} - x_{i+1,j}\right) * \left(\hat{y}_{i+1,j+1} - y_{i+1,j}\right)\right|$$

General Assumption:

$$\hat{I}_{i+1,j+1} = \gamma^{i+1,j+1}_{ij} I_{ij} + \gamma^{i+1,j+1}_{i+1,j} I_{i+1,j} + \gamma^{i+1,j+1}_{i,j+1} I_{i,j+1} + \gamma^{i+1,j+1}_{i+1,j+1} I_{i+1.j+1}$$

$$F_{i+1,j+\frac{1}{2}} = \left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right)\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+1,j+\frac{1}{2}} - \left(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}\right)\left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+1,j+\frac{1}{2}}$$

$$= \frac{\left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right)}{\frac{\left|B^-_{i+1,j+\frac{1}{2}}\right|}{D_{ij}} + \frac{\left|B^+_{i+1,j+\frac{1}{2}}\right|}{D_{i+1,j}}} \frac{1}{2}\left[\left(I_{i+1,j} - I_{ij}\right)\left(\hat{y}_{i+1,j+1} - \hat{y}_{i+1,j}\right) - \left(\hat{I}_{i+1,j+1} - \hat{I}_{i+1,j}\right)\left(y_{i+1,j} - y_{ij}\right)\right]$$

$$+ \frac{\left(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}\right)}{\frac{\left|B^-_{i+1,j+\frac{1}{2}}\right|}{D_{ij}} + \frac{\left|B^+_{i+1,j+\frac{1}{2}}\right|}{D_{i+1,j}}} \frac{1}{2}\left[\left(I_{i+1,j} - I_{ij}\right)\left(\hat{x}_{i+1,j+1} - \hat{x}_{i+1,j}\right) - \left(\hat{I}_{i+1,j+1} - \hat{I}_{i+1,j}\right)\left(x_{i+1,j} - x_{ij}\right)\right]$$

$$= \frac{D^*_{i+1,j+\frac{1}{2}} \Delta y_{i+1,j+\frac{1}{2}}}{2}\left[\begin{array}{l}\left(I_{i+1,j} - I_{ij}\right)\Delta y_{i+1,j+\frac{1}{2}} \\ -\left(\begin{array}{l}\gamma^{i+1,j+1}_{ij} I_{ij} + \gamma^{i+1,j+1}_{i+1,j} I_{i+1,j} + \gamma^{i+1,j+1}_{i,j+1} I_{i,j+1} + \gamma^{i+1,j+1}_{i+1,j+1} I_{i+1.j+1} \\ -\gamma^{i+1,j}_{i,j-1} I_{i,j-1} - \gamma^{i+1,j}_{i+1,j-1} I_{i+1,j-1} - \gamma^{i+1,j}_{ij} I_{ij} - \gamma^{i+1,j}_{i+1,j} I_{i+1.j}\end{array}\right)\delta y_{i+1,j+\frac{1}{2}}\end{array}\right]$$

$$+ \frac{D^*_{i+1,j+\frac{1}{2}} \Delta x_{i+1,j+\frac{1}{2}}}{2}\left[\begin{array}{l}\left(I_{i+1,j} - I_{ij}\right)\Delta x_{i+1,j+\frac{1}{2}} \\ -\left(\begin{array}{l}\gamma^{i+1,j+1}_{ij} I_{ij} + \gamma^{i+1,j+1}_{i+1,j} I_{i+1,j} + \gamma^{i+1,j+1}_{i,j+1} I_{i,j+1} + \gamma^{i+1,j+1}_{i+1,j+1} I_{i+1.j+1} \\ -\gamma^{i+1,j}_{i,j-1} I_{i,j-1} - \gamma^{i+1,j}_{i+1,j-1} I_{i+1,j-1} - \gamma^{i+1,j}_{ij} I_{ij} - \gamma^{i+1,j}_{i+1,j} I_{i+1.j}\end{array}\right)\delta x_{i+1,j+\frac{1}{2}}\end{array}\right]$$

$$
\begin{aligned}
F_{i+1,j+\frac{1}{2}} = &-\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \gamma^{i+1,j+1}_{i,j+1} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i,j+1} \\
&-\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \gamma^{i+1,j+1}_{i+1,j+1} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i+1,j+1} \\
&-\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \begin{pmatrix} \Delta y_{i+1,j+\frac{1}{2}} \Delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \Delta x_{i+1,j+\frac{1}{2}} \\ + \left(\gamma^{i+1,j+1}_{ij} - \gamma^{i+1,j}_{ij} \right) \Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} \\ + \left(\gamma^{i+1,j+1}_{ij} - \gamma^{i+1,j}_{ij} \right) \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \end{pmatrix} I_{ij} \\
&+\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \begin{pmatrix} \Delta y_{i+1,j+\frac{1}{2}} \Delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \Delta x_{i+1,j+\frac{1}{2}} \\ + \left(\gamma^{i+1,j+1}_{i+1,j} - \gamma^{i+1,j}_{i+1,j} \right) \Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} \\ + \left(\gamma^{i+1,j+1}_{i+1,j} - \gamma^{i+1,j}_{i+1,j} \right) \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \end{pmatrix} I_{i+1,j} \\
&+\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \gamma^{i+1,j}_{i,j-1} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i,j-1} \\
&+\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \gamma^{i+1,j}_{i+1,j-1} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i+1,j-1}
\end{aligned}
$$

Simplest assumptions

$$
\gamma^{kl}_{ij} = \frac{1}{4} \forall \left(i, j, k = [i-1, i, i+1], l = [j-1, j, j+1] \right)
$$

$$
\begin{aligned}
F_{i+1,j+\frac{1}{2}} = &-\frac{1}{8} D^*_{i+1,j+\frac{1}{2}} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i,j+1} \\
&-\frac{1}{8} D^*_{i+1,j+\frac{1}{2}} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i+1,j+1} \\
&-\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \left(\Delta y_{i+1,j+\frac{1}{2}} \Delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \Delta x_{i+1,j+\frac{1}{2}} \right) I_{ij} \\
&+\frac{1}{2} D^*_{i+1,j+\frac{1}{2}} \left(\Delta y_{i+1,j+\frac{1}{2}} \Delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \Delta x_{i+1,j+\frac{1}{2}} \right) I_{i+1,j} \\
&+\frac{1}{8} D^*_{i+1,j+\frac{1}{2}} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i,j-1} \\
&+\frac{1}{8} D^*_{i+1,j+\frac{1}{2}} \left(\Delta y_{i+1,j+\frac{1}{2}} \delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}} \delta x_{i+1,j+\frac{1}{2}} \right) I_{i+1,j-1}
\end{aligned}
$$

Looking at an alternative variation on $F_{i+1,j+\frac{1}{2}}$:

$$F_{i+1,j+\frac{1}{2}} = \frac{D^*_{i+1,j+\frac{1}{2}}}{2}\begin{bmatrix} \left(\Delta y_{i+1,j+\frac{1}{2}}\Delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}}\Delta x_{i+1,j+\frac{1}{2}}\right) I_{i+1,j} \\ -\left(\Delta y_{i+1,j+\frac{1}{2}}\Delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}}\Delta x_{i+1,j+\frac{1}{2}}\right) I_{ij} \\ +\left(\Delta y_{i+1,j+\frac{1}{2}}\delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}}\delta x_{i+1,j+\frac{1}{2}}\right) \hat{I}_{i+1,j} \\ -\left(\Delta y_{i+1,j+\frac{1}{2}}\delta y_{i+1,j+\frac{1}{2}} + \Delta x_{i+1,j+\frac{1}{2}}\delta x_{i+1,j+\frac{1}{2}}\right) \hat{I}_{i+1,j+1} \end{bmatrix}$$

Now looking at another side of the cell:

$$F_{i+\frac{1}{2},j} = \int_{ij}^{i+1,j} ds\left[\vec{n}_{i+\frac{1}{2},j}\cdot\left(D\vec{\nabla}I\right)_{i+\frac{1}{2},j}\right]$$

$$= L_{i+\frac{1}{2},j}\vec{n}_{i+\frac{1}{2},j}\cdot\left\langle D\vec{\nabla}I\right\rangle_{i+\frac{1}{2},j}$$

$$L_{i+\frac{1}{2},j} = \sqrt{(\hat{x}_{i+1,j}-\hat{x}_{ij})^2 + (\hat{y}_{i+1,j}-\hat{y}_{ij})^2}$$

$$\vec{n}_{i+\frac{1}{2},j} = \left(\frac{\hat{y}_{i+1,j}-\hat{y}_{ij}}{L_{i+\frac{1}{2},j}}, -\frac{\hat{x}_{i+1,j}-\hat{x}_{ij}}{L_{i+\frac{1}{2},j}}\right)$$

$$= \left(\frac{\Delta y_{i+\frac{1}{2},j}}{L_{i+\frac{1}{2},j}}, -\frac{\Delta x_{i+\frac{1}{2},j}}{L_{i+\frac{1}{2},j}}\right)$$

$$\left\langle D\vec{\nabla}I\right\rangle_{i+\frac{1}{2},j} = \left(\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+\frac{1}{2},j}, \left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+\frac{1}{2},j}\right)$$

$$F_{i+\frac{1}{2},j} = \Delta y_{i+\frac{1}{2},j}\left\langle D\frac{\partial I}{\partial x}\right\rangle_{i+\frac{1}{2},j} - \Delta x_{i+\frac{1}{2},j}\left\langle D\frac{\partial I}{\partial y}\right\rangle_{i+\frac{1}{2},j}$$

$$\left[\oint_{\partial B} I\,dy\right]$$

$$F_{i+\frac{1}{2},j} = \Delta y_{i+\frac{1}{2},j}D^*_{i+\frac{1}{2},j}\left[\oint_{\partial B} I\,dy\right]_{i+\frac{1}{2},j} - \Delta x_{i+\frac{1}{2},j}D^*_{i+\frac{1}{2},j}\left[-\oint_{\partial B} I\,dx\right]_{i+\frac{1}{2},j}$$

$$\left[\oint_{\partial B} I dy\right]_{i+\frac{1}{2},j} = \frac{1}{2}\left(I_{i,j-1} + \hat{I}_{ij}\right)\left(y_{i,j-1} - \hat{y}_{ij}\right) + \frac{1}{2}\left(\hat{I}_{i+1,j} + I_{i,j-1}\right)\left(\hat{y}_{i+1,j} - y_{i,j-1}\right) + \frac{1}{2}\left(I_{ij} + \hat{I}_{i+1,j}\right)\left(y_{ij} - \hat{y}_{i+1,j}\right) + \frac{1}{2}\left(\hat{I}_{ij} + I_{ij}\right)\left(\hat{y}_{ij} - y_{ij}\right)$$

$$= \frac{1}{2}\left(\hat{y}_{i+1,j} - \hat{y}_{ij}\right)I_{i,j-1} + \frac{1}{2}\left(y_{i,j-1} - y_{ij}\right)\hat{I}_{ij} + \frac{1}{2}\left(y_{ij} - y_{i,j-1}\right)\hat{I}_{i+1,j} + \frac{1}{2}\left(\hat{y}_{ij} - \hat{y}_{i+1,j}\right)I_{ij}$$

$$= \frac{1}{2}\left[\left(I_{i,j-1} - I_{ij}\right)\left(\hat{y}_{i+1,j} - \hat{y}_{ij}\right) - \left(\hat{I}_{i+1,j} - \hat{I}_{ij}\right)\left(y_{i,j-1} - y_{ij}\right)\right]$$

$$= \frac{1}{2}\left[\left(I_{i,j-1} - I_{ij}\right)\Delta y_{i+\frac{1}{2},j} + \left(\hat{I}_{i+1,j} - \hat{I}_{ij}\right)\delta y_{i+\frac{1}{2},j}\right]$$

$$\left[\oint_{\partial B} I dx\right]_{i+\frac{1}{2},j} = \frac{1}{2}\left[\left(I_{i,j-1} - I_{ij}\right)\Delta x_{i+\frac{1}{2},j} + \left(\hat{I}_{i+1,j} - \hat{I}_{ij}\right)\delta x_{i+\frac{1}{2},j}\right]$$

$$F_{i+\frac{1}{2},j} = \Delta y_{i+\frac{1}{2},j} D^{*}_{i+\frac{1}{2},j}\left[\oint_{\partial B} I dy\right]_{i+\frac{1}{2},j} - \Delta x_{i+\frac{1}{2},j} D^{*}_{i+\frac{1}{2},j}\left[-\oint_{\partial B} I dx\right]_{i+\frac{1}{2},j}$$

$$= \Delta y_{i+\frac{1}{2},j} D^{*}_{i+\frac{1}{2},j}\frac{1}{2}\left[\left(I_{i,j-1} - I_{ij}\right)\Delta y_{i+\frac{1}{2},j} + \left(\hat{I}_{i+1,j} - \hat{I}_{ij}\right)\delta y_{i+\frac{1}{2},j}\right]$$

$$+ \Delta x_{i+\frac{1}{2},j} D^{*}_{i+\frac{1}{2},j}\frac{1}{2}\left[\left(I_{i,j-1} - I_{ij}\right)\Delta x_{i+\frac{1}{2},j} + \left(\hat{I}_{i+1,j} - \hat{I}_{ij}\right)\delta x_{i+\frac{1}{2},j}\right]$$

$$= \frac{D^{*}_{i+\frac{1}{2},j}}{2}\begin{bmatrix} \left(\Delta y_{i+\frac{1}{2},j}\Delta y_{i+\frac{1}{2},j} + \Delta x_{i+\frac{1}{2},j}\Delta x_{i+\frac{1}{2},j}\right)I_{i,j-1} \\ -\left(\Delta y_{i+\frac{1}{2},j}\Delta y_{i+\frac{1}{2},j} + \Delta x_{i+\frac{1}{2},j}\Delta x_{i+\frac{1}{2},j}\right)I_{ij} \\ +\left(\Delta y_{i+\frac{1}{2},j}\delta y_{i+\frac{1}{2},j} + \Delta x_{i+\frac{1}{2},j}\delta x_{i+\frac{1}{2},j}\right)\hat{I}_{i+1,j} \\ -\left(\Delta y_{i+\frac{1}{2},j}\delta y_{i+\frac{1}{2},j} + \Delta x_{i+\frac{1}{2},j}\delta x_{i+\frac{1}{2},j}\right)\hat{I}_{ij} \end{bmatrix}$$

Until now, we have assumed that all these integrals are being evaluated for the solution of the diffusion equation at cell *i,j*. For integral $F_{i,j+\frac{1}{2}}$, consider the relationship between this integral for cell *i,j* and for cell *i-1,j*.

$$
\begin{aligned}
F^{ij}_{i,\,j+\frac{1}{2}} &= \int_{i,\,j+1}^{i,\,j} ds_{i,\,j+1\to i,\,j}\left[n^{ij}_{i,\,j+\frac{1}{2}}\cdot\left(D\vec{\nabla}I\right)_{i,\,j+\frac{1}{2}}\right] \\
&= -\int_{i,\,j}^{i,\,j+1}\left(-\,ds_{i,\,j\to i,\,j+1}\right)\left[n^{ij}_{i,\,j+\frac{1}{2}}\cdot\left(D\vec{\nabla}I\right)_{i,\,j+\frac{1}{2}}\right] \\
&= \int_{i,\,j}^{i,\,j+1} ds_{i,\,j\to i,\,j+1}\left[\left(-\,n^{i-1,\,j}_{i,\,j+\frac{1}{2}}\right)\cdot\left(D\vec{\nabla}I\right)_{i,\,j+\frac{1}{2}}\right] \\
&= -\int_{i,\,j}^{i,\,j+1} ds_{i,\,j\to i,\,j+1}\left[n^{i-1,\,j}_{i,\,j+\frac{1}{2}}\cdot\left(D\vec{\nabla}I\right)_{i,\,j+\frac{1}{2}}\right] \\
&= -F^{i-1,\,j}_{i,\,j+\frac{1}{2}}
\end{aligned}
$$

Since we know $F^{i-1,j}_{i,j+\frac{1}{2}}$ by induction from the first integral that was evaluated, we can re-use this for $F^{ij}_{i,j+\frac{1}{2}}$.

$$
F^{i-1,j}_{i,j+\frac{1}{2}} = \frac{D^{*}_{i,j+\frac{1}{2}}}{2}\begin{bmatrix}
\left(\Delta y_{i,j+\frac{1}{2}}\Delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\Delta x_{i,j+\frac{1}{2}}\right)I_{i,j} \\
-\left(\Delta y_{i,j+\frac{1}{2}}\Delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\Delta x_{i,j+\frac{1}{2}}\right)I_{i-1,j} \\
+\left(\Delta y_{i,j+\frac{1}{2}}\delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\delta x_{i,j+\frac{1}{2}}\right)\hat{I}_{i,j} \\
-\left(\Delta y_{i,j+\frac{1}{2}}\delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\delta x_{i,j+\frac{1}{2}}\right)\hat{I}_{i,j+1}
\end{bmatrix}
$$

$$
F^{ij}_{i,j+\frac{1}{2}} = \frac{D^{*}_{i,j+\frac{1}{2}}}{2}\begin{bmatrix}
\left(\Delta y_{i,j+\frac{1}{2}}\Delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\Delta x_{i,j+\frac{1}{2}}\right)I_{i,j} \\
-\left(\Delta y_{i,j+\frac{1}{2}}\Delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\Delta x_{i,j+\frac{1}{2}}\right)I_{i-1,j} \\
+\left(\Delta y_{i,j+\frac{1}{2}}\delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\delta x_{i,j+\frac{1}{2}}\right)\hat{I}_{i,j} \\
-\left(\Delta y_{i,j+\frac{1}{2}}\delta y_{i,j+\frac{1}{2}} + \Delta x_{i,j+\frac{1}{2}}\delta x_{i,j+\frac{1}{2}}\right)\hat{I}_{i,j+1}
\end{bmatrix}
$$

The same is true for $F^{ij}_{i+\frac{1}{2},j+1}$:

$$\begin{aligned}
F^{ij}_{i+\frac{1}{2},j+1} &= \int_{i+1,j+1}^{i,j+1} ds_{i+1,j+1\to i,j+1}\left[\vec{n}^{ij}_{i+\frac{1}{2},j+1}\cdot\left(D\vec{\nabla}I\right)_{i+\frac{1}{2},j+1}\right] \\
&= \int_{i,j+1}^{i+1,j+1} ds_{i,j+1\to i+1,j+1}\left[\left(-\vec{n}^{i,j+1}_{i+\frac{1}{2},j+1}\right)\cdot\left(D\vec{\nabla}I\right)_{i+\frac{1}{2},j+1}\right] \\
&= -F^{i,j+1}_{i+\frac{1}{2},j+1} \\
&= \frac{D^{*}_{i+\frac{1}{2},j+1}}{2}\begin{bmatrix}
\left(\Delta y_{i+\frac{1}{2},j+1}\Delta y_{i+\frac{1}{2},j+1}+\Delta x_{i+\frac{1}{2},j+1}\Delta x_{i+\frac{1}{2},j+1}\right)I_{ij} \\
-\left(\Delta y_{i+\frac{1}{2},j+1}\Delta y_{i+\frac{1}{2},j+1}+\Delta x_{i+\frac{1}{2},j+1}\Delta x_{i+\frac{1}{2},j+1}\right)I_{i,j+1} \\
+\left(\Delta y_{i+\frac{1}{2},j+1}\delta y_{i+\frac{1}{2},j+1}+\Delta x_{i+\frac{1}{2},j+1}\delta x_{i+\frac{1}{2},j+1}\right)\hat{I}_{i+1,j+1} \\
-\left(\Delta y_{i+\frac{1}{2},j+1}\delta y_{i+\frac{1}{2},j+1}+\Delta x_{i+\frac{1}{2},j+1}\delta x_{i+\frac{1}{2},j+1}\right)\hat{I}_{i,j+1}
\end{bmatrix}
\end{aligned}$$

Putting it all together with the following definitions:

$$\Delta y_{i-}^2 = \Delta y_{i,j+1/2}\Delta y_{i,j+1/2} \qquad \Delta y_{j-}^2 = \Delta y_{i+1/2,j}\Delta y_{i+1/2,j}$$

$$\Delta y_{i+}^2 = \Delta y_{i+1,j+1/2}\Delta y_{i+1,j+1/2} \qquad \Delta y_{j+}^2 = \Delta y_{i+1/2,j+1}\Delta y_{i+1/2,j+1}$$

$$\Delta\delta y_{i-} = \Delta y_{i,j+1/2}\delta y_{i,j+1/2} \qquad \Delta\delta y_{j-} = \Delta y_{i+1/2,j}\delta y_{i+1/2,j}$$

$$\Delta\delta y_{i+} = \Delta y_{i+1,j+1/2}\delta y_{i+1,j+1/2} \qquad \Delta\delta y_{j+} = \Delta y_{i+1/2,j+1}\delta y_{i+1/2,j+1}$$

and similarly for x, so that:

$$L_{i-}^2 = \Delta y_{i-}^2 + \Delta x_{i-}^2 \qquad L_{j-}^2 = \Delta y_{j-}^2 + \Delta x_{j-}^2$$

$$L_{i+}^2 = \Delta y_{i+}^2 + \Delta x_{i+}^2 \qquad L_{j+}^2 = \Delta y_{j+}^2 + \Delta x_{j+}^2$$

$$\Lambda_{i-}^2 = \Delta\delta y_{i-} + \Delta\delta x_{i-} \qquad \Lambda_{j-}^2 = \Delta\delta y_{j-} + \Delta\delta x_{j-} ,$$

$$\Lambda_{i+}^2 = \Delta\delta y_{i+} + \Delta\delta x_{i+} \qquad \Lambda_{j+}^2 = \Delta\delta y_{j+} + \Delta\delta x_{j+}$$

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{\left|A_{ij}\right|}\left(F_{i+1,j+1/2} - F_{i+1/2,j+1} - F_{i,j+1/2} + F_{i+1/2,j}\right) = -\kappa I_{ij} + J_{ij}$$

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{2\left|A_{ij}\right|}\begin{pmatrix} D^*_{i+1,j+1/2}\left[L_{i+}^2 I_{i+1,j} - L_{i+}^2 I_{ij} + \Lambda_{i+}^2 \hat{I}_{i+1,j} - \Lambda_{i+}^2 \hat{I}_{i+1,j+1}\right] \\ - D^*_{i+1/2,j+1}\left[- L_{j+}^2 I_{i,j+1} + L_{j+}^2 I_{ij} - \Lambda_{j+}^2 \hat{I}_{i,j+1} + \Lambda_{j+}^2 \hat{I}_{i+1,j+1}\right] \\ - D^*_{i,j+1/2}\left[- L_{i-}^2 I_{i-1,j} + L_{i-}^2 I_{ij} - \Lambda_{i-}^2 \hat{I}_{i,j+1} + \Lambda_{i-}^2 \hat{I}_{ij}\right] \\ + D^*_{i+1/2,j}\left[L_{j-}^2 I_{i,j-1} - L_{j-}^2 I_{ij} + \Lambda_{j-}^2 \hat{I}_{i+1,j} - \Lambda_{j-}^2 \hat{I}_{ij}\right] \end{pmatrix} = -\kappa I_{ij} + J_{ij}$$

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{2\left|A_{ij}\right|}\begin{bmatrix} D^*_{i+}L_{i+}^2 I_{i+1,j} + D^*_{j+}L_{j+}^2 I_{i,j+1} + D^*_{i-}L_{i-}^2 I_{i-1,j} + D^*_{j-}L_{j-}^2 I_{i,j-1} \\ + \left(D^*_{i+}\Lambda_{i+}^2 + D^*_{j-}\Lambda_{j-}^2\right)\hat{I}_{i+1,j} + \left(D^*_{j+}\Lambda_{j+}^2 + D^*_{i-}\Lambda_{i-}^2\right)\hat{I}_{i,j+1} \\ - \left(D^*_{i+}\Lambda_{i+}^2 + D^*_{j+}\Lambda_{j+}^2\right)\hat{I}_{i+1,j+1} - \left(D^*_{i-}\Lambda_{i-}^2 + D^*_{j-}\Lambda_{j-}^2\right)\hat{I}_{ij} \\ - (D^*_{j+}L_{j+}^2 + D^*_{i-}L_{i-}^2 + D^*_{i+}L_{i+}^2 + D^*_{j-}L_{j-}^2) I_{ij} \end{bmatrix} = -\kappa I_{ij} + J_{ij}$$

If we now introduce the general assumption that the vertex-centered values are linear combinations of the 4 surrounding cell-centered values:

$\hat{I}_{i+1,j+1} = \gamma_{ij}^{i+1,j+1} I_{ij} + \gamma_{i+1,j}^{i+1,j+1} I_{i+1,j} + \gamma_{i,j+1}^{i+1,j+1} I_{i,j+1} + \gamma_{i+1,j+1}^{i+1,j+1} I_{i+1.j+1}$,

then,

$$\frac{1}{c}\frac{\partial I_{ij}}{\partial t} - \frac{1}{2|A_{ij}|}\left\{\begin{array}{l}
\left(D_{i+}^{*}L_{i+}^{2} + \gamma_{i+1,j}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right] - \gamma_{i+1,j}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j+}^{*}\Lambda_{j+}^{2}\right]\right) I_{i+1,j} \\
+\left(D_{j+}^{*}L_{j+}^{2} + \gamma_{i,j+1}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2} + D_{i-}^{*}\Lambda_{i-}^{2}\right] - \gamma_{i,j+1}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j+}^{*}\Lambda_{j+}^{2}\right]\right) I_{i,j+1} \\
+\left(D_{i-}^{*}L_{i-}^{2} + \gamma_{i-1,j}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2} + D_{i-}^{*}\Lambda_{i-}^{2}\right] - \gamma_{i-1,j}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right]\right) I_{i-1,j} \\
+\left(D_{j-}^{*}L_{j-}^{2} + \gamma_{i,j-1}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right] - \gamma_{i,j-1}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right]\right) I_{i,j-1} \\
-\left(\begin{array}{l}
D_{j+}^{*}L_{j+}^{2} + D_{i-}^{*}L_{i-}^{2} + D_{i+}^{*}L_{i+}^{2} + D_{j-}^{*}L_{j-}^{2} \\
-\gamma_{ij}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right] - \gamma_{ij}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2} + D_{i-}^{*}\Lambda_{i-}^{2}\right] \\
+\gamma_{ij}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j+}^{*}\Lambda_{j+}^{2}\right] + \gamma_{ij}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right]
\end{array}\right) I_{ij} \\
+\gamma_{i+1,j-1}^{i+1,j}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right] I_{i+1,j-1} \\
+\gamma_{i-1,j}^{i,j+1}\left[D_{j+}^{*}\Lambda_{j+}^{2} + D_{i-}^{*}\Lambda_{i-}^{2}\right] I_{i-1,j+1} \\
-\gamma_{i+1,j+1}^{i+1,j+1}\left[D_{i+}^{*}\Lambda_{i+}^{2} + D_{j+}^{*}\Lambda_{j+}^{2}\right] I_{i+1,j+1} \\
-\gamma_{i,j-1}^{ij}\left[D_{i-}^{*}\Lambda_{i-}^{2} + D_{j-}^{*}\Lambda_{j-}^{2}\right] I_{i-1,j-1}
\end{array}\right\} = -\kappa I_{ij} + J_{ij}$$

$$\frac{1}{c}\frac{I_{ij}^{n} - I_{ij}^{n-1}}{\Delta t^{n-1/2}} + \left(\beta_{i-1,j-1}I_{i-1,j-1} + \beta_{i,j-1}I_{i,j-1} + \beta_{i+1,j-1}I_{i+1,j-1} + \beta_{i-1,j}I_{i-1,j} + \beta_{ij}I_{ij} + \beta_{i+1,j}I_{i+1,j} + \beta_{i-1,j+1}I_{i-1,j+1} + \beta_{i,j+1}I_{i,j+1} + \beta_{i+1,j+1}I_{i+1,j+1}\right) = -\kappa I_{ij} + J_{ij}$$

$$\beta_{i-1,j-1}I_{i-1,j-1} + \beta_{i,j-1}I_{i,j-1} + \beta_{i+1,j-1}I_{i+1,j-1} + \beta_{i-1,j}I_{i-1,j} + \alpha_{ij}I_{ij} + \beta_{i+1,j}I_{i+1,j} + \beta_{i-1,j+1}I_{i-1,j+1} + \beta_{i,j+1}I_{i,j+1} + \beta_{i+1,j+1}I_{i+1,j+1} = \frac{I_{ij}^{n-1}}{c\Delta t^{n-1/2}} + J_{ij}$$

where

$$\alpha_{ij} = \left(\beta_{ij} + \frac{1}{c\Delta t^{n-½}} + \kappa \right)$$

$$\beta_{i-1.j-1} = \frac{1}{2|A_{ij}|} \gamma^{ij}_{i-1,j-1} \left(D^*_{i-}\Lambda^*_{i-} + D^*_{j-}\Lambda^*_{j-} \right)$$

$$\beta_{i.j-1} = \frac{-1}{2|A_{ij}|} \left(D^*_{j-}L^2_{j-} + \gamma^{i+1,j}_{i,j-1} \left[D^*_{i+}\Lambda^2_{i+} + D^*_{j-}\Lambda^2_{j-} \right] - \gamma^{ij}_{i,j-1} \left[D^*_{i-}\Lambda^2_{i-} + D^*_{j-}\Lambda^2_{j-} \right] \right)$$

$$\beta_{i+1.j-1} = \frac{-1}{2|A_{ij}|} \gamma^{i,j+1}_{i+1,j-1} \left(D^*_{i+}\Lambda^*_{i+} + D^*_{j-}\Lambda^*_{j-} \right)$$

$$\beta_{i-1.j} = \frac{-1}{2|A_{ij}|} \left(D^*_{i-}L^2_{i-} + \gamma^{i,j+1}_{i-1,j} \left[D^*_{j+}\Lambda^2_{j+} + D^*_{i-}\Lambda^2_{i-} \right] - \gamma^{ij}_{i-1,j} \left[D^*_{i-}\Lambda^2_{i-} + D^*_{j-}\Lambda^2_{j-} \right] \right)$$

$$\beta_{ij} = \frac{1}{2|A_{ij}|} \left(D^*_{j+}L^2_{j+} + D^*_{i-}L^2_{i-} + D^*_{i+}L^2_{i+} + D^*_{j-}L^2_{j-} - \gamma^{i+1,j}_{ij} \left[D^*_{i+}\Lambda^2_{i+} + D^*_{j-}\Lambda^2_{j-} \right] - \gamma^{i,j+1}_{ij} \left[D^*_{j+}\Lambda^2_{j+} + D^*_{i-}\Lambda^2_{i-} \right] + \gamma^{i+1,j+1}_{ij} \left[D^*_{i+}\Lambda^2_{i+} + D^*_{j+}\Lambda^2_{j+} \right] + \gamma^{ij}_{ij} \left[D^*_{i-}\Lambda^2_{i-} + D^*_{j-}\Lambda^2_{j-} \right] \right)$$

$$\beta_{i+1.j} = \frac{-1}{2|A_{ij}|} \left(D^*_{i+}L^2_{i+} + \gamma^{i+1,j}_{i+1,j} \left[D^*_{i+}\Lambda^2_{i+} + D^*_{j-}\Lambda^2_{j-} \right] - \gamma^{i+1,j+1}_{i+1,j} \left[D^*_{i+}\Lambda^2_{i+} + D^*_{j+}\Lambda^2_{j+} \right] \right)$$

$$\beta_{i-1.j+1} = \frac{-1}{2|A_{ij}|} \gamma^{i+1,j}_{i-1,j+1} \left(D^*_{i-}\Lambda^*_{i-} + D^*_{j+}\Lambda^*_{j+} \right)$$

$$\beta_{i.j+1} = \frac{-1}{2|A_{ij}|} \left(D^*_{j+}L^2_{j+} + \gamma^{i,j+1}_{i,j+1} \left[D^*_{j+}\Lambda^2_{j+} + D^*_{i-}\Lambda^2_{i-} \right] - \gamma^{i+1,j+1}_{i,j+1} \left[D^*_{i+}\Lambda^2_{i+} + D^*_{j+}\Lambda^2_{j+} \right] \right)$$

$$\beta_{i+1.j+1} = \frac{1}{2|A_{ij}|} \gamma^{i+1,j+1}_{i+1,j+1} \left(D^*_{i+}\Lambda^*_{i+} + D^*_{j+}\Lambda^*_{j+} \right)$$

Note that for an orthogonal mesh, either Δy or δy vanishes for all sides (and similarly for Δx or δx), and therefore Λ vanishes for all sides, leaving the 5-pt stencil:

$$-\frac{D^*_{j-}L^2_{j-}}{2|A_{ij}|} I_{i,j-1} - \frac{D^*_{i-}L^2_{i-}}{2|A_{ij}|} I_{i-1,j} + \left(\frac{D^*_{j-}L^2_{j-} + D^*_{i-}L^2_{i-} + D^*_{i+}L^2_{i+} + D^*_{j+}L^2_{j+}}{2|A_{ij}|} + \frac{1}{c\Delta t^{n-½}} + \kappa \right) I_{ij} - \frac{D^*_{i+}L^2_{i+}}{2|A_{ij}|} I_{i+1,j} - \frac{D^*_{j+}L^2_{j+}}{2|A_{ij}|} I_{i,j+1} = \frac{I^{n-1}_{ij}}{c\Delta t^{n-½}} + J_{ij}$$