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OF THE SELF-ADJOINT TRANSPORT OPERATOR

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Spatial and Angular Variation and Discretization of the Self-Adjoint Transport Operator

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1 Variational Derivation

1.1 Self-Adjoint Equation

The first-order equation for the angular flux, $\psi(\hat{\Omega}, \vec{x})$ is

$$\hat{\Omega} \cdot \vec{\nabla} \psi(\hat{\Omega}, \vec{x}) + \sigma_t \psi(\hat{\Omega}, \vec{x}) = \int d\hat{\Omega}' \sigma_s(\hat{\Omega} \cdot \hat{\Omega}', \vec{x}) \psi(\hat{\Omega}', \vec{x}) + q(\vec{x}) \quad (1)$$

$$= \mathbf{S} \psi(\hat{\Omega}, \vec{x}) + q(\vec{x}). \quad (2)$$

This equation may be rearranged as

$$\psi = (\sigma_t - \mathbf{S})^{-1} [q - \hat{\Omega} \cdot \vec{\nabla} \psi]. \quad (3)$$

Combining these equations we obtain the second-order, self-adjoint, form of the transport equation,

$$\hat{\Omega} \cdot \vec{\nabla} [(\sigma_t - \mathbf{S})^{-1} (q - \hat{\Omega} \cdot \vec{\nabla} \psi)] + \sigma_t \psi - \mathbf{S} \psi - q = 0. \quad (4)$$

1.2 Space Variational Functional

Now that we have the self-adjoint form of the transport equation we can find a functional, $\Gamma[\psi]$, whose minimization solves the transport equation, i.e.

$$\delta \Gamma[\psi] = 0 \quad (5)$$

implies ψ is a solution of Equation 4. Additionally the functional's minimization should also lead to ψ having the correct boundary conditions. The correct boundary conditions for the transport equation will be explained later.

A Ritz procedure will be used to obtain the desired functional. We define the functional, $W[\psi, \delta\psi]$, as

$$W[\psi, \delta\psi] = \iint \delta\psi \mathcal{L}(\psi) d^3x d\hat{\Omega} \quad (6)$$

$$= 0 \quad \forall \delta\psi, \quad (7)$$

where $\mathcal{L}(\psi) = 0$ corresponds to Equation 4.

For the self-adjoint equation $W[\psi, \delta\psi]$ becomes,

$$\begin{aligned} W[\psi, \delta\psi] &= \iint \delta\psi \hat{\Omega} \cdot \vec{\nabla} [(\sigma_t - \mathbf{S})^{-1} (q - \hat{\Omega} \cdot \vec{\nabla} \psi)] d^3x d\hat{\Omega} \\ &\quad + \iint \delta\psi (\sigma_t \psi - \mathbf{S} \psi - q) d^3x d\hat{\Omega} \end{aligned} \quad (8)$$

$$\begin{aligned} &= \iint \left[(\hat{\Omega} \cdot \vec{\nabla} \delta\psi) (\sigma_t - \mathbf{S})^{-1} (\hat{\Omega} \cdot \vec{\nabla} \psi - q) \right] d^3x d\hat{\Omega} \\ &\quad + \iint_S \delta\psi (\sigma_t - \mathbf{S})^{-1} (q - \hat{\Omega} \cdot \vec{\nabla} \psi) \hat{\Omega} \cdot \hat{n} d^2x d\hat{\Omega} \\ &\quad + \iint \delta\psi (\sigma_t \psi - \mathbf{S} \psi - q) d^3x d\hat{\Omega}. \end{aligned} \quad (9)$$

The boundary conditions for the integral are derived from the term inside the surface integral,

$$(\sigma_t - \mathbf{S})^{-1} (q - \hat{\Omega} \cdot \vec{\nabla} \psi),$$

which from Equation 3 is a ψ -like term. If we choose the value of $\psi(\hat{\Omega})$ on the boundary to be ψ_b for $\hat{\Omega} \cdot \hat{n} < 0$ and ψ otherwise, the equation for $W[\psi, \delta\psi]$ becomes,

$$\begin{aligned} W[\psi, \delta\psi] = & \iint \left[(\hat{\Omega} \cdot \vec{\nabla} \delta\psi) (\sigma_t - \mathbf{S})^{-1} (\hat{\Omega} \cdot \vec{\nabla} \psi - q) \right] d^3x d\hat{\Omega} \\ & + \int d^2x \int_{\hat{\Omega}^-} d\hat{\Omega} \delta\psi \psi_b \hat{\Omega} \cdot \hat{n} + \int d^2x \int_{\hat{\Omega}^+} d\hat{\Omega} \delta\psi \psi \hat{\Omega} \cdot \hat{n} \\ & + \iint \delta\psi (\sigma_t \psi - \mathbf{S}\psi - q) d^3x d\hat{\Omega}, \end{aligned} \quad (10)$$

where $\hat{\Omega}^-$ is defined as the set of angles at the surfaces where $\hat{\Omega} \cdot \hat{n} < 0$, and $\hat{\Omega}^+$ are angles at the surfaces where $\hat{\Omega} \cdot \hat{n} > 0$.

This equation $W[\psi, \delta\psi] = 0 \forall \delta\psi$ can be obtained from minimizing the functional, $\Gamma[\psi]$,

$$\begin{aligned} \Gamma[\psi] = & \iint (\hat{\Omega} \cdot \vec{\nabla} \psi) (\sigma_t - \mathbf{S})^{-1} \left[\frac{1}{2} (\hat{\Omega} \cdot \vec{\nabla} \psi) - q \right] d^3x d\hat{\Omega} \\ & + \int d^2x \int_{\hat{\Omega}^-} d\hat{\Omega} \psi_b \psi \hat{\Omega} \cdot \hat{n} + \int d^2x \int_{\hat{\Omega}^+} d\hat{\Omega} \frac{1}{2} \psi^2 \hat{\Omega} \cdot \hat{n} \\ & + \iint \frac{\sigma_t}{2} \psi^2 - \frac{1}{2} \psi \mathbf{S} \psi - q \psi d^3x d\hat{\Omega} \end{aligned} \quad (11)$$

where we have made use of the self-adjoint property of the operators, $\mathbf{S}$, and $(\sigma_t - \mathbf{S})^{-1}$.

2 1-D Example

Let's choose a 1-D example with $\mathbf{S} = 0$ and $q = 0$ to demonstrate the choice of boundary conditions. We will look at the boundary conditions from the left and right sides of the problem, with $\mu \equiv \hat{\Omega} \cdot \hat{x} > 0$. At $x = x_l$, $\hat{n} = -\hat{x}$, and at $x = x_r$, $\hat{n} = \hat{x}$. The next vertex to the right of $x = x_l$ is $x = x_r = x_l + h$. The values of the angular flux at $x = x_l$ and $x = x_r$ are ψ_l and ψ_r , respectively.

We can ignore the area perpendicular to the x-axis. Our expression for $\Gamma[\psi]$ becomes,

$$\Gamma[\psi] = -\mu \psi_b \psi_l + \frac{\mu}{2} \psi_r^2 + \int_{x_l}^{x_r} \left[\frac{\mu^2}{2\sigma_t} \left(\frac{d\psi}{dx} \right)^2 + \frac{\sigma_t}{2} \psi^2 \right] dx \quad (12)$$

$$\approx -\mu \psi_b \psi_l + \frac{\mu}{2} \psi_r^2 + \frac{\mu^2}{2\sigma_t h} (\psi_r - \psi_l)^2 + \frac{\sigma_t h}{4} (\psi_l^2 + \psi_r^2). \quad (13)$$

Defining $\tau \equiv \sigma_t h / \mu$ the above expression becomes,

$$\frac{1}{\mu} \Gamma[\psi] \approx \left(\frac{1}{2} \psi_r^2 - \psi_b \psi_l \right) + \frac{1}{2\tau} (\psi_r - \psi_l)^2 + \frac{\tau}{4} (\psi_l^2 + \psi_r^2). \quad (14)$$

The solution for ψ_l and ψ_r that minimizes $\Gamma[\psi]$ is

$$\psi_l = \frac{\psi_b \left(1 + \tau + \frac{\tau^2}{2} \right)}{1 + \tau + \frac{\tau^2}{2} + \frac{\tau^3}{4}} \quad (15)$$

$$\psi_r = \frac{\psi_b}{1 + \tau + \frac{\tau^2}{2} + \frac{\tau^3}{4}}. \quad (16)$$

The value of ψ_r can be compared with the exponential of τ by,

$$\psi_r = \psi_b e^{-\tau} + O(\tau^3). \quad (17)$$

3 S_N Discretized Functional

For this section we will concentrate on the volume contribution to the functional, $\Gamma_v[\psi]$,

$$\begin{aligned} \Gamma_v[\psi] = & \iint (\hat{\Omega} \cdot \vec{\nabla} \psi) (\sigma_t - \mathbf{S})^{-1} \left[\frac{1}{2} (\hat{\Omega} \cdot \vec{\nabla} \psi) - q \right] d^3x d\hat{\Omega} \\ & + \iint \frac{\sigma_t}{2} \psi^2 - \frac{1}{2} \psi \mathbf{S} \psi - q \psi d^3x d\hat{\Omega} \end{aligned} \quad (18)$$

We will be expressing the discretized functional in terms of $\psi(\hat{\Omega}, \vec{x})$ evaluated at the corners of the cells,

$$\psi(\hat{\Omega}, \vec{x}) \rightarrow \psi_i(\hat{\Omega}). \quad (19)$$

For the i 'th corner of a cell we will define an approximation to the gradient of ψ as

$$\vec{\nabla}_i \psi = \sum_j (\psi_j(\hat{\Omega}) - \psi_i(\hat{\Omega})) \vec{\alpha}_{ij}, \quad (20)$$

with the sum extending over the three neighbors sharing an edge with the i 'th corner. The expression $\vec{\alpha}_{ik}$ is defined by

$$\vec{\alpha}_{ij} = \frac{\vec{r}_{ik} \times \vec{r}_{il}}{\vec{r}_{ij} \cdot (\vec{r}_{ik} \times \vec{r}_{il})}, \quad (21)$$

where k and l are the two neighbor corners of i that are not j . For later convenience, the expression for $\hat{\Omega} \cdot \vec{\nabla}_i \psi$ may be expressed as

$$\hat{\Omega} \cdot \vec{\nabla}_i \psi = \sum_j \hat{\Omega} \cdot \vec{D}_{ij} \psi_j(\hat{\Omega}), \quad (22)$$

where the sum over j has been extended to all corners in a cell. The expression,

$$\hat{\Omega} \cdot \vec{D}_{ki},$$

implies a 3-vector dot product of a 3-vector with a 3-vector of matrices, i.e.

$$\hat{\Omega} \cdot \vec{D}_{ki} = \mu D_{xki} + \eta D_{yki} + \xi D_{zki}. \quad (23)$$

With these definitions the volume functional (over one cell)¹ can be approximated by

$$\begin{aligned} \Gamma_v[\psi] \approx & \int d\hat{\Omega} \sum_k v_{ck} \left(\left(\hat{\Omega} \cdot \vec{\nabla}_k \psi \right) (\sigma_t - \mathbf{S})^{-1} \left[\frac{1}{2} \left(\hat{\Omega} \cdot \vec{\nabla}_k \psi \right) - q_{ck} \right] \right) \\ & + \int d\hat{\Omega} \sum_k v_{ck} \left(\frac{\sigma_t}{2} \psi_k^2 - \frac{1}{2} \psi_k \mathbf{S} \psi_k - q_k \psi_k \right). \end{aligned} \quad (24)$$

In the above expression the corner weights, v_{ck} , evaluated in the cell, sum to the total volume of the cell, and the q_{ck} expression is evaluated within the cells². The extrema of Γ_v is found by letting ψ contain a variation around the extrema value,

$$\psi_i(\hat{\Omega}) \rightarrow \psi_i(\hat{\Omega}) + \epsilon u_i(\hat{\Omega}), \quad (25)$$

and setting the coefficient of first order term in ϵ to 0,

$$\lim_{\epsilon \rightarrow 0} \frac{\partial}{\partial \epsilon} \Gamma_v[\psi + \epsilon u] = 0. \quad (26)$$

Since the ψ_i 's extremize Γ , Equation 26 should hold for any choice of u_i 's. A set of simultaneous equations can be found by setting $u_i(\hat{\Omega}) = 1$ for a particular choice of i with $u_j(\hat{\Omega}) = 0$ for $j \neq i$.

Putting Equation 24 into Equation 26 we have,

$$\begin{aligned} & \int d\hat{\Omega} \sum_k v_{ck} \left(\left(\hat{\Omega} \cdot \vec{\nabla}_k u \right) (\sigma_t - \mathbf{S})^{-1} \left[\left(\hat{\Omega} \cdot \vec{\nabla}_k \psi \right) - q_{ck} \right] \right) \\ & + \int d\hat{\Omega} \sum_k v_{ck} (\sigma_t u_k \psi_k - u_k \mathbf{S} \psi_k - q_k u_k) = 0, \end{aligned} \quad (27)$$

where we have again made use of the self-adjoint properties of $\mathbf{S}$ and $(\sigma_t - \mathbf{S})^{-1}$. The $(\sigma_t - \mathbf{S})^{-1} \left[\left(\hat{\Omega} \cdot \vec{\nabla}_k \psi \right) - q_{ck} \right]$ term in the above equation may be evaluated inside the cell using Equation 3. The above equation becomes,

$$\int d\hat{\Omega} \sum_k v_{ck} \left(- \left(\hat{\Omega} \cdot \vec{\nabla}_k u \right) \psi_{ck} + \sigma_t u_k \psi_k - u_k \mathbf{S} \psi_k - q_k u_k \right) = 0, \quad (28)$$

¹The sum over k can be viewed as a double sum, first over the cells, and then over the corners of the cell. The other sums over corners can then be restricted to the current cell.

²For the steady-state problem q_{ck} is evaluated on the vertices. For time-dependent problems q_{ck} will include $\psi_{ck}/c\Delta t$, evaluated at the previous iteration.

where $\psi_{ck}(\hat{\Omega})$ is evaluated within the cell.

We will use Equation 2 to evaluate ψ_{ck} in Equation 28,

$$\psi_{ck}^{(n+1)} = -\frac{1}{\sigma_t} \left(\hat{\Omega} \cdot \vec{\nabla}_k \psi^{(n+1)} \right)_c + \frac{1}{\sigma_t} \mathbf{S} \psi_{ck}^{(n)} + \frac{1}{\sigma_t} q_{ck}^{(n)}. \quad (29)$$

The superscripts represent iterations, since $\mathbf{S}$ is not easily invertable in the S_N representation. If we introduce a new source term to represent the previous iteration the above equation may be expressed as

$$\psi_{ck} = -\frac{1}{\sigma_t} \left(\hat{\Omega} \cdot \vec{\nabla}_k \psi \right) + \frac{1}{\sigma_t} Q_{ck}, \quad (30)$$

it is implied that $\vec{\nabla}_k \psi$ is evaluated within the cell. Additionally, in order to decouple the angles, the $\mathbf{S} \psi_k$ term in Equation 28 will be evaluated at the previous iteration, resulting in a $Q_{vk} = \mathbf{S} \psi_k^{(n)} + q_k^{(n)}$ term. These equations are inserted into Equation 28 to yield

$$\begin{aligned} \int d\hat{\Omega} \sum_k v_{ck} \left(\frac{1}{\sigma_t} \left(\hat{\Omega} \cdot \vec{\nabla}_k u \right) \left[\left(\hat{\Omega} \cdot \vec{\nabla}_k \psi \right) - Q_{ck} \right] \right) \\ + \int d\hat{\Omega} \sum_k v_{ck} (\sigma_t u_k \psi_k - Q_{vk} u_k) = 0. \end{aligned} \quad (31)$$

We introduce the matrix expression for $\hat{\Omega} \cdot \vec{\nabla}_k$ from Equation 22,

$$\begin{aligned} \int d\hat{\Omega} \sum_k v_{ck} \left(\frac{1}{\sigma_t} \sum_{i'} D_{ki'} u_{i'} \left[\sum_j D_{kj} \psi_j - Q_{ck} \right] \right) \\ + \int d\hat{\Omega} \sum_k v_{ck} (\sigma_t u_k \psi_k - Q_{vk} u_k) = 0, \end{aligned} \quad (32)$$

where $D_{ki}(\hat{\Omega}) \equiv \hat{\Omega} \cdot \vec{D}_{ki}$ (c.f. Equation 23).

To obtain a set of simultaneous equations we set the $u_{i'}$'s,

$$u_{i'}(\hat{\Omega}) = \begin{cases} 1 & i' = i \\ 0 & i' \neq i \end{cases}, \quad (33)$$

and Equation 32 becomes,

$$\begin{aligned} \int d\hat{\Omega} \sum_k v_{ck} \left(\frac{1}{\sigma_t} D_{ki} \left[\sum_j D_{kj} \psi_j - Q_{ck} \right] \right) \\ + \int d\hat{\Omega} v_{ci} (\sigma_t \psi_i - Q_{vi}) = 0, \end{aligned} \quad (34)$$

$$\begin{aligned} \int d\hat{\Omega} \sum_j \left[\sum_k \frac{v_{ck}}{\sigma_t} D_{ki} D_{kj} + \delta_{ij} v_{ci} \sigma_t \right] \psi_j \\ - \int d\hat{\Omega} \left[\sum_k \frac{v_{ck}}{\sigma_t} D_{ki} Q_{ck} + v_{ci} Q_{vi} \right] = 0, \end{aligned} \quad (35)$$

$$\begin{aligned} \int d\hat{\Omega} \sum_j \left[\sum_k \frac{v_{ck}}{\sigma_t} D_{ik}^T D_{kj} + \delta_{ij} v_{ci} \sigma_t \right] \psi_j \\ - \int d\hat{\Omega} \left[\sum_k \frac{v_{ck}}{\sigma_t} D_{ik}^T Q_{ck} + v_{ci} Q_{vi} \right] = 0. \end{aligned} \quad (36)$$

We continue by introducing the Hessian matrix, $\vec{\vec{H}}$,

$$\begin{aligned} \int d\hat{\Omega} \sum_j \left[\frac{\hat{\Omega} \cdot \vec{\vec{H}}_{ij} \cdot \hat{\Omega}}{\sigma_t} + \delta_{ij} v_{ci} \sigma_t \right] \psi_j \\ - \int d\hat{\Omega} \left[\sum_k \frac{v_{ck}}{\sigma_t} D_{ik}^T Q_{ck} + v_{ci} Q_{vi} \right] = 0, \end{aligned} \quad (37)$$

where $\vec{\vec{H}}_{ij}$ is the dyadic,

$$\vec{\vec{H}}_{ij} = \sum_k v_{ck} \vec{D}_{ik}^T \vec{D}_{kj}. \quad (38)$$

In matrix form S_N equation becomes,

$$\int d\hat{\Omega} \left[\sum_j A_{ij}(\hat{\Omega}) \psi_j(\hat{\Omega}) - b_i(\hat{\Omega}) \right] = 0, \quad (39)$$

where the functions $A_{ij}(\hat{\Omega})$ and $b_i(\hat{\Omega})$ do not explicitly depend on the ψ 's from this iteration.

If we assume some angular discretization, the matrix equation becomes

$$\sum_{lj} w_l A_{ij}^l \psi_{jl} - \sum_l w_l b_{il} = 0, \quad (40)$$

where

$$\psi_{jl} = \psi_j(\hat{\Omega}_l), \quad (41)$$

and w_l are the weightings for the integral over $\hat{\Omega}$. Since there is no explicit coupling between different values of l , Equation 40 must hold separately for each l , i.e.

$$\sum_j A_{ij}^l \psi_{jl} - b_{il} = 0. \quad (42)$$

4 P_N Discretized Functional

The P_N discretization begins as does the S_N up to Equation 27,

$$\begin{aligned} \int d\hat{\Omega} \sum_k v_{ck} \left((\hat{\Omega} \cdot \vec{\nabla}_k u) (\sigma_t - \mathbf{S})^{-1} \left[(\hat{\Omega} \cdot \vec{\nabla}_k \psi) - q_{ck} \right] \right) \\ + \int d\hat{\Omega} \sum_k v_{ck} (\sigma_t u_k \psi_k - u_k \mathbf{S} \psi_k - q_k u_k) = 0, \end{aligned} \quad (43)$$

where q_{ck} is evaluated within the cell. There is no need to substitute ψ_{ck} into this equation³. In the P_N formalism $(\sigma_t - \mathbf{S})^{-1}$ is easily invertible.

The next step is instead to define ψ_k by its spherical harmonic series,

$$\psi_k(\hat{\Omega}) = \sum_l Y_l(\hat{\Omega}) \phi_{kl} \quad (44)$$

$$u_k(\hat{\Omega}) = \sum_l Y_l(\hat{\Omega}) u_{kl}. \quad (45)$$

In this equation the l index represents both the polar and azimuthal moments, i.e. l represents the (l, m) tuple. The spherical harmonics are orthonormal,

$$\int d\hat{\Omega} Y_l(\hat{\Omega}) Y_{l'}(\hat{\Omega}) = \delta_{ll'}. \quad (46)$$

Before we begin to include the spherical harmonic series in the discretization we need to find the expansion for $\hat{\Omega} \cdot \vec{f}$. We may express $\vec{f}$ in terms of its spherical harmonics, $\vec{f}_l$,

$$\hat{\Omega} \cdot \vec{f} = \sum_{l'} Y_{l'}(\hat{\Omega}) \hat{\Omega} \cdot \vec{f}_{l'} \quad (47)$$

$$= \sum_{l'} Y_{l'}(\hat{\Omega}) \int d\hat{\Omega}' Y_{l'}(\hat{\Omega}') Y_{l'}(\hat{\Omega}') \hat{\Omega}' \cdot \vec{f}_{l'} \quad (48)$$

$$= \sum_{l'} Y_{l'}(\hat{\Omega}) \hat{\Lambda}_{l'} \cdot \vec{f}_{l'}, \quad (49)$$

where $\hat{\Lambda}_{l'}$ is a matrix of vectors representing the l' th coefficient of $Y_{l'}(\hat{\Omega}) \hat{\Omega}$.

With these definitions Equation 43 becomes,

$$0 = \int d\hat{\Omega} \left\{ \sum_{k m' l} v_{ck} Y_{m'} \hat{\Lambda}_{m'l} \cdot \vec{\nabla}_k u_l \right. \quad (50)$$

$$\times \sum_{l'} \frac{Y_{l'}}{(\sigma_t - \sigma_{l'})} \left[\sum_m \hat{\Lambda}_{l'm} \cdot \vec{\nabla}_k \phi_m - q_{ckl'} \right] \Bigg\} \\ + \int d\hat{\Omega} \sum_{k m'} v_{ck} Y_{m'} u_{km'} \sum_{l'} Y_{l'} [(\sigma_t - \sigma_{l'}) \phi_{kl'} - q_{kl'}]. \quad (51)$$

The l' , m , and m' indices are also single index representations of both the polar and azimuthal spherical moments. In the above equation we used the property that $\mathbf{S}$ is diagonal in the space of Y_l 's, i.e.

$$\mathbf{S} Y_l = \sigma_l Y_l \quad (52)$$

$$(\sigma_t - \mathbf{S})^{-1} Y_l = \frac{1}{(\sigma_t - \sigma_l)} Y_l. \quad (53)$$

³For time-dependent problems you will still need to evaluate and store the spherical moments of ψ_{ck} (c.f. Equation 29). The moments of q_{ck} terms will include the corresponding moments of $\psi_{ck}/c\Delta t$, evaluated at the previous iteration.

The only remaining functions of $\hat{\Omega}$ are the $Y_l(\hat{\Omega})$'s. Due to the orthonormality conditions the variation equation becomes,

$$0 = \sum_{k'l'l} v_{ck} \hat{\Lambda}_{l'l} \cdot \vec{\nabla}_k u_l \frac{1}{(\sigma_t - \sigma_{l'})} \left[\sum_m \hat{\Lambda}_{l'm} \cdot \vec{\nabla}_k \phi_m - q_{ckl'} \right] + \sum_{k'l'} v_{ck} u_{kl'} [(\sigma_t - \sigma_{l'}) \phi_{kl'} - q_{kl'}] \quad (54)$$

$$= \sum_{k'l'il} v_{ck} \hat{\Lambda}_{l'l} \cdot \vec{D}_{ki} u_{il} \frac{1}{(\sigma_t - \sigma_{l'})} \left[\sum_{j,m} \hat{\Lambda}_{l'm} \cdot \vec{D}_{kj} \phi_{jm} - q_{ckl'} \right] + \sum_{k'l'} v_{ck} u_{kl'} [(\sigma_t - \sigma_{l'}) \phi_{kl'} - q_{kl'}]. \quad (55)$$

It is important to realize that the expression,

$$\hat{\Lambda}_{l'l} \cdot \vec{D}_{ki},$$

implies a 3-vector dot product of two 3-vectors of matrices, i.e.

$$\hat{\Lambda}_{l'l} \cdot \vec{D}_{ki} = \Lambda_{\mu l'l} D_{xki} + \Lambda_{\eta l'l} D_{yki} + \Lambda_{\xi l'l} D_{zki}. \quad (56)$$

Since the variation in Γ is 0 for u taking on any values, we now set

$$u_{i'l'} = \begin{cases} 1 & i' = i, l' = l \\ 0 & \text{otherwise} \end{cases}, \quad (57)$$

and the (i, l) 'th variation equation becomes,

$$0 = \sum_{k'l'} v_{ck} \frac{\hat{\Lambda}_{l'l} \cdot \vec{D}_{ki}}{(\sigma_t - \sigma_{l'})} \left[\sum_{j,m} \hat{\Lambda}_{l'm} \cdot \vec{D}_{kj} \phi_{jm} - q_{ckl'} \right] + v_{ci} [(\sigma_t - \sigma_l) \phi_{il} - q_{il}]. \quad (58)$$

Consolidating terms in ϕ we arrive at

$$0 = \sum_{j,m} \left[\sum_{k,l'} v_{ck} \frac{\hat{\Lambda}_{l'l} \cdot \vec{D}_{ki} \hat{\Lambda}_{l'm} \cdot \vec{D}_{kj}}{(\sigma_t - \sigma_{l'})} + \delta_{ij} \delta_{lm} v_{ci} (\sigma_t - \sigma_l) \right] \phi_{jm} - \left[\sum_{k,l'} v_{ck} \frac{\hat{\Lambda}_{l'l} \cdot \vec{D}_{ki}}{(\sigma_t - \sigma_{l'})} q_{ckl'} + v_{ci} q_{il} \right], \quad (59)$$

$$0 = \sum_{j,m} \left[\sum_{k,l'} v_{ck} \frac{\hat{\Lambda}_{l'l}^T \cdot \vec{D}_{ik}^T \vec{D}_{kj} \cdot \hat{\Lambda}_{l'm}}{(\sigma_t - \sigma_{l'})} + \delta_{ij} \delta_{lm} v_{ci} (\sigma_t - \sigma_l) \right] \phi_{jm} - \left[\sum_{k,l'} v_{ck} \frac{\hat{\Lambda}_{l'l}^T \cdot \vec{D}_{ik}^T}{(\sigma_t - \sigma_{l'})} q_{ckl'} + v_{ci} q_{il} \right]. \quad (60)$$

The above equation is written in terms of $\hat{\Lambda}^T$, even though $\hat{\Lambda}$ is symmetric, in order to expose the symmetry of the final matrix. We continue by introducing the Hessian matrix, $\overset{\leftrightarrow}{H}$,

$$0 = \sum_{jm} \left[\sum_{l'} \frac{\hat{\Lambda}_{ll'}^T \cdot \overset{\leftrightarrow}{H}_{ij} \cdot \hat{\Lambda}_{l'm}}{(\sigma_t - \sigma_{l'})} + \delta_{ij} \delta_{lm} v_{ci} (\sigma_t - \sigma_l) \right] \phi_{jm} - \left[\sum_{kl'} v_{ck} \frac{\hat{\Lambda}_{ll'}^T \cdot \vec{D}_{ik}^T}{(\sigma_t - \sigma_{l'})} q_{ckl'} + v_{ci} q_{il} \right]. \quad (61)$$

where $\overset{\leftrightarrow}{H}_{ij}$ is the dyadic,

$$\overset{\leftrightarrow}{H}_{ij} = \sum_k v_{ck} \vec{D}_{ik}^T \vec{D}_{kj}. \quad (62)$$

This definition is identical to that used in the S_N formalism.

Like Equation 37, Equation 61 may be written as a matrix equation,

$$\sum_{jm} A_{ij}^{lm} \phi_{jm} - b_{il} = 0, \quad (63)$$

where A_{ij}^{lm} and b_{il} do not explicitly depend on the ϕ 's from this iteration.

5 Surface Discretization

From Equation 11 the surface contribution the Γ functional, Γ_s , is

$$\Gamma_s[\psi] = \int d^2x \int_{\hat{\Omega}^-} d\hat{\Omega} \psi_b \psi \hat{\Omega} \cdot \hat{n} + \int d^2x \int_{\hat{\Omega}^+} d\hat{\Omega} \frac{1}{2} \psi^2 \hat{\Omega} \cdot \hat{n}. \quad (64)$$

We shall discretize Γ_s over boundary faces as follows,

$$\Gamma_s[\psi] \approx \sum_j \int_{\hat{\Omega}^-} d\hat{\Omega} \hat{\Omega} \cdot \vec{a}_{cj} \psi_{bj} \psi_j + \sum_j \int_{\hat{\Omega}^+} d\hat{\Omega} \hat{\Omega} \cdot \vec{a}_{cj} \frac{1}{2} \psi_j^2, \quad (65)$$

where the sum over j extends first to all boundary faces, and then to the corners of faces, $\vec{a}_{cj}$ is the area vector associated with that face and corner.

5.1 S_N Surface Angular Discretization

For the S_N treatment the integrals over angle are replaced by weighted sums,

$$\Gamma_s[\psi] \approx \sum_j \sum_{\hat{\Omega}_l \cdot \hat{n}_{cj} < 0} w_l \hat{\Omega}_l \cdot \vec{a}_{cj} \psi_{bjl} \psi_{jl} + \sum_j \sum_{\hat{\Omega}_l \cdot \hat{n}_{cj} > 0} w_l \hat{\Omega}_l \cdot \vec{a}_{cj} \frac{1}{2} \psi_{jl}^2. \quad (66)$$

Minimization of this equation with respect to ψ_{il} , on the boundary, for a particular value of $\hat{\Omega}_l$ leads to

$$0 = \text{volume terms} + \sum_c \begin{cases} \hat{\Omega}_l \cdot \vec{a}_{ci} \psi_{bil} & \hat{\Omega}_l \cdot \hat{n}_{ci} < 0 \\ \hat{\Omega}_l \cdot \vec{a}_{ci} \psi_{jl} & \hat{\Omega}_l \cdot \hat{n}_{ci} > 0 \end{cases}, \quad (67)$$

where the sum is over all boundary surfaces containing vertex i . The first of these surface terms will be added to the b_{il} term of Equation 42, the second term is added to the $\sum_j A_{ij}^l \psi_{jl}$ of that equation.

5.2 P_N Surface Angular Discretization

For the P_N treatment we minimize Equation 65 using

$$\psi_j(\hat{\Omega}) \rightarrow \psi_j(\hat{\Omega}) + \epsilon u(\hat{\Omega}), \quad (68)$$

obtaining,

$$0 = \text{volume terms} + \sum_j \int_{\hat{\Omega}^-} d\hat{\Omega} \hat{\Omega} \cdot \vec{a}_{cj} \psi_{bj} u_j + \sum_j \int_{\hat{\Omega}^+} d\hat{\Omega} \hat{\Omega} \cdot \vec{a}_{cj} \psi_j u_j. \quad (69)$$

The equation is now expanded into its spherical harmonics,

$$\begin{aligned} 0 &= \text{volume terms} \\ &+ \sum_j \sum_{m'l'} \int_{\hat{\Omega}^-} d\hat{\Omega} \hat{\Omega} \cdot \vec{a}_{cj} Y_m \phi_{bjm} Y_{l'} u_{jl'} \\ &+ \sum_j \sum_{m'l'} \int_{\hat{\Omega}^+} d\hat{\Omega} \hat{\Omega} \cdot \vec{a}_{cj} Y_m \phi_{jlm} Y_{l'} u_{jl'} \end{aligned} \quad (70)$$

$$\begin{aligned} &= \text{volume terms} \\ &+ \sum_j \sum_{m'l'} \left[\left(\int_{\hat{\Omega}^-} d\hat{\Omega} Y_m(\hat{\Omega}) Y_{l'}(\hat{\Omega}) \hat{\Omega} \right) \cdot \vec{a}_{cj} u_{jl'} \right] \phi_{bjm} \\ &+ \sum_j \sum_{m'l'} \left[\left(\int_{\hat{\Omega}^+} d\hat{\Omega} Y_m(\hat{\Omega}) Y_{l'}(\hat{\Omega}) \hat{\Omega} \right) \cdot \vec{a}_{cj} u_{jl'} \right] \phi_{jlm} \end{aligned} \quad (71)$$

$$\begin{aligned} &= \text{volume terms} \\ &+ \sum_j \sum_{m'l'} \left[\hat{\Lambda}_{l'm}^{(-)}(\hat{n}_{cj}) \cdot \vec{a}_{cj} u_{jl'} \right] \phi_{bjm} \\ &+ \sum_j \sum_{m'l'} \left[\hat{\Lambda}_{l'm}^{(+)}(\hat{n}_{cj}) \cdot \vec{a}_{cj} u_{jl'} \right] \phi_{jlm}. \end{aligned} \quad (72)$$

Setting $u_{jl'} = \delta_{ij} \delta_{ll'}$ we arrive at

$$\begin{aligned} 0 &= \text{volume terms} \\ &+ \sum_c \sum_m \left[\hat{\Lambda}_{lm}^{(-)}(\hat{n}_{ci}) \cdot \vec{a}_{ci} \right] \phi_{bim} \\ &+ \sum_c \sum_m \left[\hat{\Lambda}_{lm}^{(+)}(\hat{n}_{ci}) \cdot \vec{a}_{ci} \right] \phi_{im}, \end{aligned} \quad (73)$$

Figure 1: The corner numbering scheme for the hexahedron.

where the sum over c indicates a sum over all boundary surfaces containing vertex i . The first of these surface terms will be added to the b_{il} term of Equation 63, the second term (multiplied by δ_{ij} and summed over j) is added to the $\sum_{jm} A_{ij}^{lm} \phi_{jm}$ of that equation.

6 Specific Element Geometries

In this section we will display the explicit forms of the $\vec{D}$ and $\vec{H}$ matrices that were defined above.

One important property of the $\vec{D}$ matrix is that its only non-zero elements are between indices that share an edge in the element in question. This also implies that the $\vec{D}$ matrix is “structurally” symmetric, meaning that if $\vec{D}_{ij} \neq 0$ then $\vec{D}_{ji} \neq 0$. The $\vec{H}$ matrix is truly symmetric.

6.1 Hexahedron

For the hexahedron we will look at the matrix elements associated with corner 1 of the hex (c.f. Figure 1). All other matrix elements may be derived by a suitable permutation of corner indices, corresponding to a rotation of the hex.

For corner 1 the only non-zero elements of $\vec{D}$ correspond to corners 1, 2, 4, and 5,

$$\vec{D}_{1k} = \begin{cases} -(\vec{\alpha}_{12} + \vec{\alpha}_{14} + \vec{\alpha}_{15}) & k = 1 \\ \vec{\alpha}_{1k} & k \in \{2, 4, 5\} \\ 0 & \text{otherwise} \end{cases} \quad (74)$$

For the $\vec{H}$ matrix there are 4 distinct types of elements associated with

corner 1. The diagonal element is

$$\vec{\vec{H}}_{11} = \sum_{k \in \{1,2,4,5\}} v_{ck} \vec{D}_{k1} \vec{D}_{k1} \quad (75)$$

$$= v_{c1} (\vec{\alpha}_{12} + \vec{\alpha}_{14} + \vec{\alpha}_{15})(\vec{\alpha}_{12} + \vec{\alpha}_{14} + \vec{\alpha}_{15}) \\ + v_{c2} \vec{\alpha}_{21} \vec{\alpha}_{21} + v_{c4} \vec{\alpha}_{41} \vec{\alpha}_{41} + v_{c5} \vec{\alpha}_{51} \vec{\alpha}_{51}. \quad (76)$$

The matrix elements from corner 1 to its nearest neighbors, corners 2, 4, and 5, are represented by $\vec{\vec{H}}_{12}$,

$$\vec{\vec{H}}_{12} = \sum_{k \in \{1,2\}} v_{ck} \vec{D}_{k1} \vec{D}_{k2} \quad (77)$$

$$= -v_{c1} (\vec{\alpha}_{12} + \vec{\alpha}_{14} + \vec{\alpha}_{15}) \vec{\alpha}_{12} - v_{c2} \vec{\alpha}_{21} (\vec{\alpha}_{21} + \vec{\alpha}_{23} + \vec{\alpha}_{26}). \quad (78)$$

The matrix elements from corner 1 to its next-nearest neighbors, corners 3, 6, and 8, are represented by $\vec{\vec{H}}_{13}$,

$$\vec{\vec{H}}_{13} = \sum_{k \in \{2,4\}} v_{ck} \vec{D}_{k1} \vec{D}_{k3} \quad (79)$$

$$= v_{c2} \vec{\alpha}_{21} \vec{\alpha}_{23} + v_{c4} \vec{\alpha}_{41} \vec{\alpha}_{43}. \quad (80)$$

The matrix element from corner 1 to its third-nearest neighbor, corner 7, is

$$\vec{\vec{H}}_{17} = 0. \quad (81)$$

This is because there are no nearest neighbor corners in common for corners 1 and 7.

6.2 Wedge

For the wedge we will look at the matrix elements associated with corner 1 (c.f. Figure 2). All other matrix elements may be derived by a suitable permutation of corner indices, corresponding to a rotation of the wedge.

For corner 1 the only non-zero elements of $\vec{D}$ correspond to corners 1, 2, 3, and 4,

$$\vec{D}_{1k} = \begin{cases} -(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) & k = 1 \\ \vec{\alpha}_{1k} & k \in \{2, 3, 4\} \\ 0 & \text{otherwise} \end{cases} \quad (82)$$

For the $\vec{\vec{H}}$ matrix there are 3 distinct types of elements associated with corner 1. The diagonal element is

$$\vec{\vec{H}}_{11} = \sum_{k \in \{1,2,3,4\}} v_{ck} \vec{D}_{k1} \vec{D}_{k1} \quad (83)$$

$$= v_{c1} (\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14})(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) \\ + v_{c2} \vec{\alpha}_{21} \vec{\alpha}_{21} + v_{c3} \vec{\alpha}_{31} \vec{\alpha}_{31} + v_{c4} \vec{\alpha}_{41} \vec{\alpha}_{41}. \quad (84)$$

Figure 2: The corner numbering scheme for the wedge.

The matrix elements from corner 1 to its nearest neighbors, corners 2, 3, and 4, are represented by $\vec{H}_{12}$,

$$\vec{H}_{12} = \sum_{k \in \{1,2,3\}} v_{ck} \vec{D}_{k1} \vec{D}_{k2} \quad (85)$$

$$= -v_{c1} (\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) \vec{\alpha}_{12} - v_{c2} \vec{\alpha}_{21} (\vec{\alpha}_{21} + \vec{\alpha}_{23} + \vec{\alpha}_{25}) + v_{c3} \vec{\alpha}_{31} \vec{\alpha}_{32}. \quad (86)$$

The matrix elements from corner 1 to its next-nearest neighbors, corners 5, and 6, are represented by $\vec{H}_{15}$,

$$\vec{H}_{15} = \sum_{k \in \{2,4\}} v_{ck} \vec{D}_{k1} \vec{D}_{k5} \quad (87)$$

$$= v_{c2} \vec{\alpha}_{21} \vec{\alpha}_{25} + v_{c4} \vec{\alpha}_{41} \vec{\alpha}_{45}. \quad (88)$$

6.3 Tetrahedron

For the tetrahedron we will look at the matrix elements associated with corner 1 (c.f. Figure 3). All other matrix elements may be derived by a suitable permutation of corner indices, corresponding to a rotation of the tet.

For corner 1 all matrix elements of $\vec{D}$ are non-zero,

$$\vec{D}_{1k} = \begin{cases} -(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) & k = 1 \\ \vec{\alpha}_{1k} & \text{otherwise} \end{cases} \quad (89)$$

For the $\vec{H}$ matrix there are 2 distinct types of elements associated with corner 1. The diagonal element is

$$\vec{H}_{11} = \sum_{k \in \{1,2,3,4\}} v_{ck} \vec{D}_{k1} \vec{D}_{k1} \quad (90)$$

Figure 3: The corner numbering scheme for the tetrahedron.

$$\begin{aligned}
 &= v_{c1} (\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14})(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) \\
 &\quad + v_{c2} \vec{\alpha}_{21} \vec{\alpha}_{21} + v_{c3} \vec{\alpha}_{31} \vec{\alpha}_{31} + v_{c4} \vec{\alpha}_{41} \vec{\alpha}_{41}.
 \end{aligned} \tag{91}$$

The matrix elements from corner 1 to its neighbors, corners 2, 3, and 4, are represented by $\vec{H}_{12}$,

$$\vec{H}_{12} = \sum_{k \in \{1,2,3,4\}} v_{ck} \vec{D}_{k1} \vec{D}_{k2} \tag{92}$$

$$\begin{aligned}
 &= -v_{c1} (\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) \vec{\alpha}_{12} - v_{c2} \vec{\alpha}_{21} (\vec{\alpha}_{21} + \vec{\alpha}_{23} + \vec{\alpha}_{24}) \\
 &\quad + v_{c3} \vec{\alpha}_{31} \vec{\alpha}_{32} + v_{c4} \vec{\alpha}_{41} \vec{\alpha}_{42}.
 \end{aligned} \tag{93}$$

6.4 Pyramid

Figure 4: The corner numbering scheme for the pyramid.