Title: | Hexahedron, Wedge, Tetrahedron, and Pyramid Diffusion Operator Discretization

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Submitted to: | For electronic distribution upon request.

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Hexahedron, Wedge, Tetrahedron, and Pyramid Diffusion Operator Discretization

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December 11, 1995

1 General Variational Function

We are looking for the solution of the diffusion equation, $\phi(\vec{x})$, by finding the extrema of the following functional

$$\Gamma[\phi] = \int \left(\frac{1}{2} D \vec{\nabla}\phi \cdot \vec{\nabla}\phi + \frac{1}{2}\sigma_a \phi^2 - Q\phi \right) d^3x. \tag{1}$$

At this point I will concentrate only on the first term in the integral, and so take

$$\Gamma[\phi] = \int \frac{1}{2} D \vec{\nabla}\phi \cdot \vec{\nabla}\phi \ d^3x. \tag{2}$$

Also surface integrals arising from the boundaries of the problem will be ignored. These will be treated in a later section.

We will now discretize the above equation in terms of the values for $\phi(\vec{x})$ at each of the corners of the cell, ϕ_i. The functional, Γ, is replaced by a function of these corner values

$$\Gamma(\phi_1, \phi_2, \ldots) = \frac{1}{2} D \sum_k w_k \left\| \vec{\nabla}_k \phi \right\|^2, \tag{3}$$

where the sum is over the corners of the cell, and $\vec{\nabla}_k \phi$ is itself a function of the ϕ_is, and w_k are weights that sum to the volume of the cell. The form of the expression for $\vec{\nabla}_i \phi$ is

$$\vec{\nabla}_i \phi = \sum_{k'} (\phi_{k'} - \phi_i) \vec{\alpha}_{ik'}. \tag{4}$$

The sum extends only over the 3 nearest neighbors of the point, i. The $\vec{\alpha}_{ik'}$ is defined by

$$\vec{\alpha}_{ij} = \frac{\vec{r}_{ik} \times \vec{r}_{il}}{\vec{r}_{ij} \cdot (\vec{r}_{ik} \times \vec{r}_{il})}, \tag{5}$$

where k and l are the two neighbor corners of i that are not j.

The extrema of Γ is found by solving the following set of simultaneous equations for the ϕ_is

$$\frac{\partial \Gamma}{\partial \phi_i} = 0. \tag{6}$$

Since Γ has the form of Equation 3 with $\vec{\nabla}_i \phi$ in the form of Equation 4, the above equation becomes

$$\sum_j \frac{\partial^2 \Gamma}{\partial \phi_i \partial \phi_j} \phi_j = 0. \tag{7}$$

Substituting the above expressions for Γ and $\vec{\nabla}_i \phi$ we arrive at an expression for the matrix element, A_{ij}

$$A_{ij} = \frac{\partial^2 \Gamma}{\partial \phi_i \partial \phi_j} = D \sum_k w_k \frac{\partial \vec{\nabla}_k \phi}{\partial \phi_i} \cdot \frac{\partial \vec{\nabla}_k \phi}{\partial \phi_j}. \tag{8}$$

In the following sections we will investigate this matrix for the hexahedron, wedge, tetrahedron, and pyramid cells.
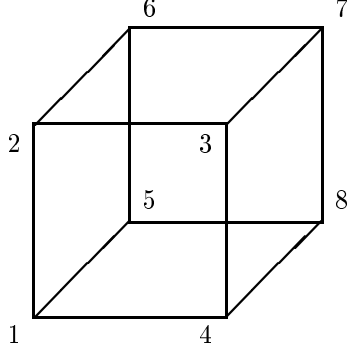
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Figure 1: The corner numbering scheme for the hexahedron.

2 Hexahedron Matrix Elements

For the hexahedron we will be looking at the following matrix elements, A_{11}, A_{12}, A_{16}, and A_{17}. By looking at these matrix elements we have covered those matrix elements that are fundamentally different. All other matrix elements may be found by a suitable topology-preserving permutation of the corner indices.

For the hexahedron the expressions for the $\vec{\nabla}_i \phi$s are

$$\vec{\nabla}_1 \phi = (\phi_2 - \phi_1)\vec{\alpha}_{12} + (\phi_4 - \phi_1)\vec{\alpha}_{14} + (\phi_5 - \phi_1)\vec{\alpha}_{15} \tag{9}$$

$$\vec{\nabla}_2 \phi = (\phi_1 - \phi_2)\vec{\alpha}_{21} + (\phi_3 - \phi_2)\vec{\alpha}_{23} + (\phi_6 - \phi_2)\vec{\alpha}_{26} \tag{10}$$

$$\vec{\nabla}_3 \phi = (\phi_2 - \phi_3)\vec{\alpha}_{32} + (\phi_4 - \phi_3)\vec{\alpha}_{34} + (\phi_7 - \phi_3)\vec{\alpha}_{37} \tag{11}$$

$$\vec{\nabla}_4 \phi = (\phi_1 - \phi_4)\vec{\alpha}_{41} + (\phi_3 - \phi_4)\vec{\alpha}_{43} + (\phi_8 - \phi_4)\vec{\alpha}_{48} \tag{12}$$

$$\vec{\nabla}_5 \phi = (\phi_1 - \phi_5)\vec{\alpha}_{51} + (\phi_6 - \phi_5)\vec{\alpha}_{56} + (\phi_8 - \phi_5)\vec{\alpha}_{58} \tag{13}$$

$$\vec{\nabla}_6 \phi = (\phi_2 - \phi_6)\vec{\alpha}_{62} + (\phi_5 - \phi_6)\vec{\alpha}_{65} + (\phi_7 - \phi_6)\vec{\alpha}_{67} \tag{14}$$

$$\vec{\nabla}_7 \phi = (\phi_3 - \phi_7)\vec{\alpha}_{73} + (\phi_6 - \phi_7)\vec{\alpha}_{76} + (\phi_8 - \phi_7)\vec{\alpha}_{78} \tag{15}$$

$$\vec{\nabla}_8 \phi = (\phi_4 - \phi_8)\vec{\alpha}_{84} + (\phi_5 - \phi_8)\vec{\alpha}_{85} + (\phi_7 - \phi_8)\vec{\alpha}_{87}. \tag{16}$$

Only $\vec{\nabla}_k \phi$ for $k \in \{1, 2, 4, 5\}$ will contribute to the calculation of A_{1j}, therefore,

$$
\begin{aligned}
A_{11} &= D\left[w_1 \left\| \frac{\partial \vec{\nabla}_1 \phi}{\partial \phi_1} \right\|^2 + w_2 \left\| \frac{\partial \vec{\nabla}_2 \phi}{\partial \phi_1} \right\|^2 + w_4 \left\| \frac{\partial \vec{\nabla}_4 \phi}{\partial \phi_1} \right\|^2 \right. \\
&\quad \left. + w_5 \left\| \frac{\partial \vec{\nabla}_5 \phi}{\partial \phi_1} \right\|^2 \right] \\
&= D\left[w_1 \|\vec{\alpha}_{12} + \vec{\alpha}_{14} + \vec{\alpha}_{15}\|^2 + w_2 \|\vec{\alpha}_{21}\|^2 + w_4 \|\vec{\alpha}_{41}\|^2 \right.
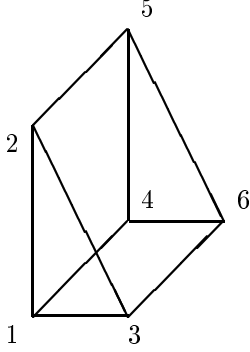\end{aligned}
\tag{17}
$$

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Figure 2: The corner numbering scheme for the wedge.

$$+ w_5 \|\vec{\alpha}_{51}\|^2 \Big] \tag{18}$$

$$A_{12} = D \left[w_1 \frac{\partial \vec{\nabla}_1 \phi}{\partial \phi_1} \cdot \frac{\partial \vec{\nabla}_1 \phi}{\partial \phi_2} + w_2 \frac{\partial \vec{\nabla}_2 \phi}{\partial \phi_1} \cdot \frac{\partial \vec{\nabla}_2 \phi}{\partial \phi_2} \right] \tag{19}$$

$$= -D \left[w_1 (\vec{\alpha}_{12} + \vec{\alpha}_{14} + \vec{\alpha}_{15}) \cdot \vec{\alpha}_{12} + w_2 \vec{\alpha}_{21} \cdot (\vec{\alpha}_{21} + \vec{\alpha}_{23} + \vec{\alpha}_{26}) \right] \tag{20}$$

$$A_{16} = D \left[w_2 \frac{\partial \vec{\nabla}_2 \phi}{\partial \phi_1} \cdot \frac{\partial \vec{\nabla}_2 \phi}{\partial \phi_6} + w_5 \frac{\partial \vec{\nabla}_5 \phi}{\partial \phi_1} \cdot \frac{\partial \vec{\nabla}_5 \phi}{\partial \phi_6} \right] \tag{21}$$

$$= D \left[w_2 \vec{\alpha}_{21} \cdot \vec{\alpha}_{26} + w_5 \vec{\alpha}_{51} \cdot \vec{\alpha}_{56} \right] \tag{22}$$

$$A_{17} = 0. \tag{23}$$

In general this leads to a 19 point diffusion operator. For a rectangular hexahedral mesh it is easy to see that A_{16} vanishes, leaving one with the standard 7 point operator.

3   Wedge Matrix Elements

For the wedge we will be looking at the following matrix elements, A_{11}, A_{12}, A_{14}, and A_{15}. By looking at these matrix elements we have covered those matrix elements that are fundamentally different. All other matrix elements may be found by a suitable topology-preserving permutation of the corner indices.

For the wedge the expressions for the $\vec{\nabla}_i \phi$s are

$$\vec{\nabla}_1 \phi = (\phi_2 - \phi_1)\vec{\alpha}_{12} + (\phi_3 - \phi_1)\vec{\alpha}_{13} + (\phi_4 - \phi_1)\vec{\alpha}_{14} \tag{24}$$

$$\vec{\nabla}_2 \phi = (\phi_1 - \phi_2)\vec{\alpha}_{21} + (\phi_3 - \phi_2)\vec{\alpha}_{23} + (\phi_5 - \phi_2)\vec{\alpha}_{25} \tag{25}$$

$$\vec{\nabla}_3 \phi = (\phi_1 - \phi_3)\vec{\alpha}_{31} + (\phi_2 - \phi_3)\vec{\alpha}_{32} + (\phi_6 - \phi_3)\vec{\alpha}_{36} \tag{26}$$

$$\vec{\nabla}_4 \phi = (\phi_1 - \phi_4)\vec{\alpha}_{41} + (\phi_5 - \phi_4)\vec{\alpha}_{45} + (\phi_6 - \phi_4)\vec{\alpha}_{46} \tag{27}$$

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$$\vec{\nabla}_5\phi \quad = \quad (\phi_2 - \phi_5)\vec{\alpha}_{52} + (\phi_4 - \phi_5)\vec{\alpha}_{54} + (\phi_6 - \phi_5)\vec{\alpha}_{56} \qquad (28)$$

$$\vec{\nabla}_6\phi \quad = \quad (\phi_3 - \phi_6)\vec{\alpha}_{63} + (\phi_4 - \phi_6)\vec{\alpha}_{64} + (\phi_5 - \phi_6)\vec{\alpha}_{65}. \qquad (29)$$

Following the same procedures as for the hexahedron, we find the matrix elements to be

$$A_{11} \quad = \quad D\left[w_1\|\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}\|^2 + w_2\|\vec{\alpha}_{21}\|^2 + w_3\|\vec{\alpha}_{31}\|^2\right.$$
$$\left. + w_4\|\vec{\alpha}_{41}\|^2\right] \qquad (30)$$

$$A_{12} \quad = \quad -D\left[w_1(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) \cdot \vec{\alpha}_{12} + w_2\vec{\alpha}_{21} \cdot (\vec{\alpha}_{21} + \vec{\alpha}_{23} + \vec{\alpha}_{25})\right] \quad (31)$$

$$A_{14} \quad = \quad -D\left[w_1(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}) \cdot \vec{\alpha}_{14} + w_4\vec{\alpha}_{41} \cdot (\vec{\alpha}_{41} + \vec{\alpha}_{45} + \vec{\alpha}_{46})\right] \quad (32)$$

$$A_{15} \quad = \quad D\left[w_2\vec{\alpha}_{21} \cdot \vec{\alpha}_{25} + w_4\vec{\alpha}_{41} \cdot \vec{\alpha}_{45}\right]. \qquad (33)$$

One can see that all the corner points couple to all of the others. In a general logically orthogonal grid connected as wedges this would yield a 15 point diffusion operator. If the wedge was created from an orthogonal grid then it is easy to see that A_{15} vanishes, and that each point is coupled only with its neighbors. This again yields the standard 7 point operator.

At one point we were considering treating the wedge as a degenerate hexahedron, e.g. a hexahedron with points 2 and 6 approaching points 1 and 5, respectively. This approach will not yield the same matrix elements that were derived in this section. This can be seen by looking at the expression for A_{15} for the hexahedron, corresponding to A_{14} for the wedge, with Equations 9–16 modified as follows,

$$\phi_2 \quad \rightarrow \quad \phi_1 \qquad (34)$$

$$\phi_6 \quad \rightarrow \quad \phi_5 \qquad (35)$$

$$\vec{r}_2 \quad \rightarrow \quad \vec{r}_1 \qquad (36)$$

$$\vec{r}_6 \quad \rightarrow \quad \vec{r}_5 \qquad (37)$$

$$w_1 \quad = \quad 0 \qquad (38)$$

$$w_2 \quad = \quad 0 \qquad (39)$$

$$w_5 \quad = \quad 0 \qquad (40)$$

$$w_6 \quad = \quad 0. \qquad (41)$$

The reason for setting the w_k to zero for points 1, 2, 5, and 6 is that the w_k represent the volume weight of those points *on the hexahedron*. When w_k goes to zero as the parallelpiped volume of the corner then the $w_k\left\|\vec{\nabla}_k\phi\right\|^2$ terms go to zero. By inspection of $\vec{\nabla}_3\phi$, $\vec{\nabla}_4\phi$, $\vec{\nabla}_7\phi$, and $\vec{\nabla}_8\phi$, modified as above, one sees that there is no coupling between ϕ_1 and ϕ_5; therefore, the A_{15} matrix element is zero. For the wedge A_{14} is not, in general, zero. This shows that the wedge cannot be treated as a degenerate hex to obtain the wedge results of this section.
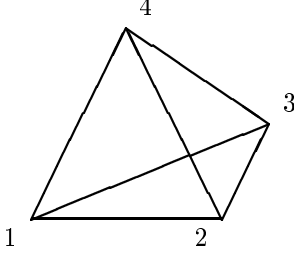
Figure 3: The corner numbering scheme for the tetrahedron.

4   Tetrahedron Matrix Elements

For the tetrahedron we will only have to look at the A_{11} and A_{12} matrix elements. They are

$$
\begin{aligned}
A_{11} &= D\left[w_1\|\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14}\|^2 + w_2\|\vec{\alpha}_{21}\|^2 + w_3\|\vec{\alpha}_{31}\|^2 \right. \\
&\quad \left. + w_4\|\vec{\alpha}_{41}\|^2\right] \quad (42) \\
A_{12} &= D\left[-w_1(\vec{\alpha}_{12} + \vec{\alpha}_{13} + \vec{\alpha}_{14})\cdot\vec{\alpha}_{12} - w_2\vec{\alpha}_{21}\cdot(\vec{\alpha}_{21} + \vec{\alpha}_{23} + \vec{\alpha}_{24})\right. \\
&\quad \left. + w_3\vec{\alpha}_{31}\cdot\vec{\alpha}_{32} + w_4\vec{\alpha}_{41}\cdot\vec{\alpha}_{42}\right]. \quad (43)
\end{aligned}
$$

Up until this point the only specification for w_i was that its sum over corners equals the volume of the cell. It has been shown that a very good choice of w_i for a cell type is

$$
w_i = \frac{V_i}{\sum_j V_j}V, \quad (44)
$$

where V is the volume of the cell, and V_i is the volume of the parallelepiped formed by the three cell edges emanating from the corner i. For a tetrahedron w_i is independent of the corner,

$$
w_i = \frac{1}{4}V. \quad (45)
$$

With this choice of w_i the matrix element expressions simplify to

$$
\begin{aligned}
A_{11} &= \frac{1}{9}\frac{D}{V}\left\|\vec{A}_1\right\|^2 \quad (46) \\
A_{12} &= \frac{1}{9}\frac{D}{V}\vec{A}_1\cdot\vec{A}_2, \quad (47)
\end{aligned}
$$

where $\vec{A}_i$ is the area vector for the triangle face opposite corner i.
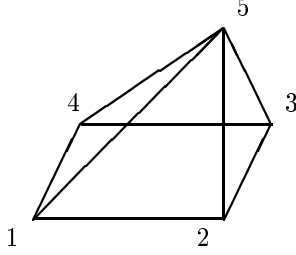
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Figure 4: The corner numbering scheme for the pyramid.

In anticipation of the pyramid results we will modify our notation for the tetrahedron matrix elements to be explicit about which points w_i and $\vec{A}_i$ refer. We will define V_{ijkl} to be the volume of the tetrahedron with corners i, j, k, l, and $\vec{A}_{ijk}$ to be the area vector of triangle i j, k. The matrix elements for the tetrahedron containing points 1, 2, 3, 4 become

$$A_{11}^{1234} = \frac{1}{9}\frac{D}{V_{1234}}\left\|\vec{A}_{234}\right\|^2 \tag{48}$$

$$A_{12}^{1234} = \frac{1}{9}\frac{D}{V_{1234}}\vec{A}_{234}\cdot\vec{A}_{143}. \tag{49}$$

5   Pyramid Matrix Elements

In this section we calculate the matrix elements of the pyramid as the average of the matrix elements from the 4 tetrahedra, {1, 2, 4, 5}, {2, 3, 4, 5}, {1, 3, 4, 5}, and {1, 2, 3, 5},

$$A_{ij} = \frac{1}{4}\left[A_{ij}^{1245} + A_{ij}^{2345} + A_{ij}^{1345} + A_{ij}^{1235}\right]. \tag{50}$$

Due to the linearity of derivatives the same matrix elements would be recovered by first averaging the four tetrahedron functionals, Γ^{ijkl}, and then performing the variational procedure.

The distinct matrix elements for the pyramid are A_{11}, A_{12}, A_{13}, A_{15}, and A_{55},

$$A_{11} = \frac{D}{36}\left[\frac{1}{V_{1245}}\left\|\vec{A}_{245}\right\|^2 + \frac{1}{V_{1345}}\left\|\vec{A}_{345}\right\|^2 + \frac{1}{V_{1235}}\left\|\vec{A}_{235}\right\|^2\right] \tag{51}$$

$$A_{12} = \frac{D}{36}\left[\frac{1}{V_{1245}}\vec{A}_{245}\cdot\vec{A}_{154} + \frac{1}{V_{1235}}\vec{A}_{235}\cdot\vec{A}_{153}\right] \tag{52}$$

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$$A_{13} \quad = \quad \frac{D}{36} \left[\frac{1}{V_{1345}} \vec{A}_{345} \cdot \vec{A}_{154} + \frac{1}{V_{1235}} \vec{A}_{235} \cdot \vec{A}_{125} \right] \tag{53}$$

$$A_{15} \quad = \quad \frac{D}{36} \left[\frac{1}{V_{1245}} \vec{A}_{245} \cdot \vec{A}_{142} + \frac{1}{V_{1345}} \vec{A}_{345} \cdot \vec{A}_{143} + \frac{1}{V_{1235}} \vec{A}_{235} \cdot \vec{A}_{132} \right] \tag{54}$$

$$A_{55} \quad = \quad \frac{D}{36} \left[\frac{1}{V_{1245}} \left\| \vec{A}_{142} \right\|^2 + \frac{1}{V_{2345}} \left\| \vec{A}_{243} \right\|^2 + \frac{1}{V_{1345}} \left\| \vec{A}_{143} \right\|^2 \right.$$
$$\left. + \frac{1}{V_{1235}} \left\| \vec{A}_{132} \right\|^2 \right] \tag{55}$$

In general all points couple to all other points for the pyramid. There are conditions under which either A_{12} or A_{13} vanish. These matrix elements would both be zero only under unusual conditions, and then only for a few isolated pyramids.

6 Ignored and Surface Terms in the Γ Functional

In this section we will consider the terms that were dropped in going from Equation 1 to Equation 2. In addition, we will consider the effects of boundaries on the system. Up until this point we have been treating the system as infinite in extent. Treating the system as finite will introduce a surface integral term into Equation 1.

In order to discover the surface terms we must re-derive Equation 1 from the original diffusion equation,

$$-\vec{\nabla} \cdot D\vec{\nabla}\phi + \sigma_a \phi - Q = 0, \tag{56}$$

using the weighted residual method.

In this method we construct a functional, W, and find a solution to the differential equation, $\mathcal{L}(\phi) = 0$ by solving

$$W \quad = \quad \int \delta\phi \mathcal{L}(\phi) \ d^3x \tag{57}$$

$$= \quad 0 \ \forall \ \delta\phi. \tag{58}$$

For the diffusion equation this becomes

$$W \quad = \quad \int \delta\phi \left(-\vec{\nabla} \cdot D\vec{\nabla}\phi + \sigma_a \phi - Q \right) d^3x \tag{59}$$

$$= \quad \int \left(D\vec{\nabla}\delta\phi \cdot \vec{\nabla}\phi + \delta\phi(\sigma_a \phi - Q) \right) d^3x - \int_S \delta\phi D\vec{\nabla}\phi \cdot \hat{n} \ d^2x, \tag{60}$$

where we have integrated by parts to obtain the surface integral. Using Marshak boundary conditions,

$$D\vec{\nabla}\phi \cdot \hat{n} = 2J - \frac{\phi}{2}, \tag{61}$$

the expression for W becomes

$$W = \int \left(D \vec{\nabla} \delta\phi \cdot \vec{\nabla}\phi + \delta\phi(\sigma_a\phi - Q) \right) d^3x - \int_S \delta\phi \left(2J - \frac{\phi}{2} \right) d^2x. \qquad (62)$$

In order to produce a functional, $\Gamma[\phi]$, that when minimized produces Equation 62 we equate the variation of $\Gamma[\phi]$ to the terms in Equation 62. The variation of a functional $\Gamma[\phi]$ is

$$\delta\Gamma = \frac{\partial\Gamma}{\partial\phi}\delta\phi + \sum_{i=1}^{3} \frac{\partial\Gamma}{\partial\frac{\partial\phi}{\partial x_i}} \frac{\partial\delta\phi}{\partial x_i}. \qquad (63)$$

It is easily shown that the variation of the following functional,

$$\Gamma[\phi] = \int \left(\frac{1}{2}D\vec{\nabla}\phi \cdot \vec{\nabla}\phi + \frac{1}{2}\sigma_a\phi^2 - Q\phi \right) d^3x + \int_S \left(\frac{1}{4}\phi^2 - 2J\phi \right) d^2x, \qquad (64)$$

reproduces Equation 62.

With this functional Equation 3 becomes

$$\begin{aligned}
\Gamma(\phi_1, \phi_2, \ldots) &= \sum_k w_k \left(\frac{1}{2}D \left\| \vec{\nabla}_k\phi \right\|^2 + \frac{1}{2}\sigma_a\phi_k^2 - Q_k\phi_k \right) \\
&\quad + \sum_l a_l \left(\frac{1}{4}\phi_l^2 - 2J\phi_l \right),
\end{aligned} \qquad (65)$$

where the sum over l is over corners on the boundary of the system, and the sum of a_l over the corners on the face of a cell equals the area of that face.

The variation of $\Gamma[\phi]$ proceeds as before, by Equation 6. Using the above equation for Γ the volume contribution becomes

$$\frac{\partial\Gamma}{\partial\phi_i} = \sum_j (A_{ij} + w_i\sigma_a\delta_{ij})\phi_j - w_iQ_i, \qquad (66)$$

where the A_{ij} is the matrix element calculated for the appropriate cell type in the previous sections. The surface contribution is

$$\frac{\partial\Gamma}{\partial\phi_i} = \sum_j \left(\frac{a_i}{2}\delta_{ij} \right) \phi_j - a_i 2J. \qquad (67)$$

There are two cases for the surface term, one when the surface face is a quadralateral, the other when the surface face is a triangle. For the quadralateral case, the equation for $\frac{\partial\Gamma}{\partial\phi_i}$ becomes

$$\frac{\partial\Gamma}{\partial\phi_i} = \sum_j \left(\frac{1}{8} \left\| \vec{A}_i \right\|^2 \delta_{ij} \right) \phi_j - \frac{1}{2} \left\| \vec{A}_i \right\|^2 J, \qquad (68)$$
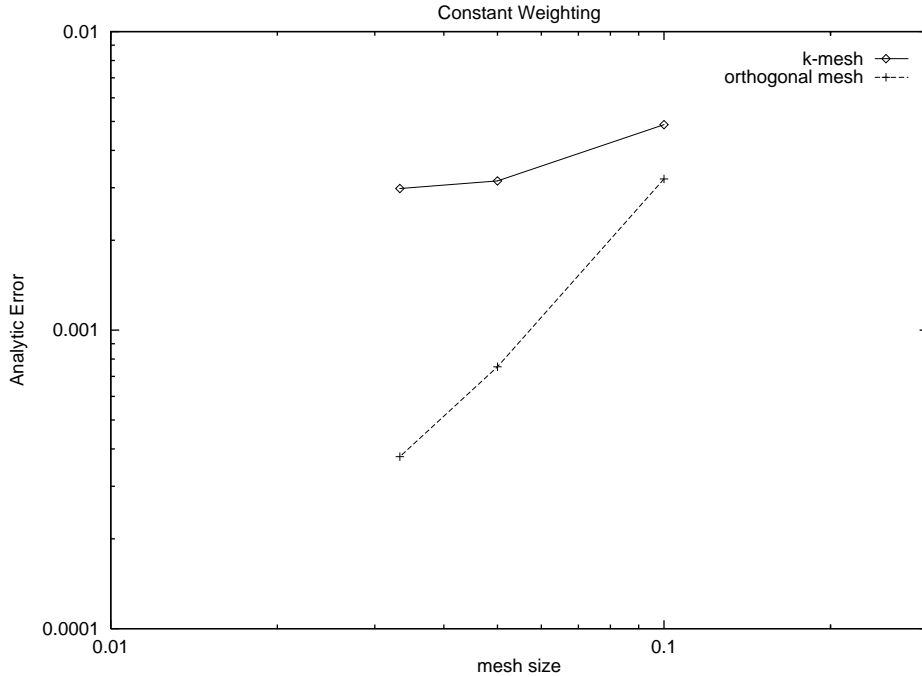
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Figure 5: Analytic Error for K-mesh $= .2$ and orthogonal mesh for $-D\frac{\partial^2 \phi}{\partial x^2} - Qx^2 = 0$ with $D = \frac{1}{30}$, $Q = 1$, and $J_0 = J_1 = 0$, w_k constant weighted.

where $\vec{A}_i$ is the area vector created from the two edge vectors at corner i on the face. For the triangal case, the equation for $\frac{\partial \Gamma}{\partial \phi_i}$ becomes

$$\frac{\partial \Gamma}{\partial \phi_i} = \sum_j \left(\frac{1}{6} \left\| \vec{A}_i \right\|^2 \delta_{ij} \right) \phi_j - \frac{2}{3} \left\| \vec{A}_i \right\|^2 J, \tag{69}$$

where $\vec{A}_i$ is the area vector for the triangle.

The volume contribution, Equation 66, is composed for each cell in the system. The surface contribution, either Equation 68 or Equation 69, is composed for each face on the boundary of the system. These equations can be seen to take the form of a matrix equation,

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \tag{70}$$

with $\mathbf{x}$ containing the vector of ϕ_is, and the right hand side, $\mathbf{b}$, containing the Q_i and J terms.
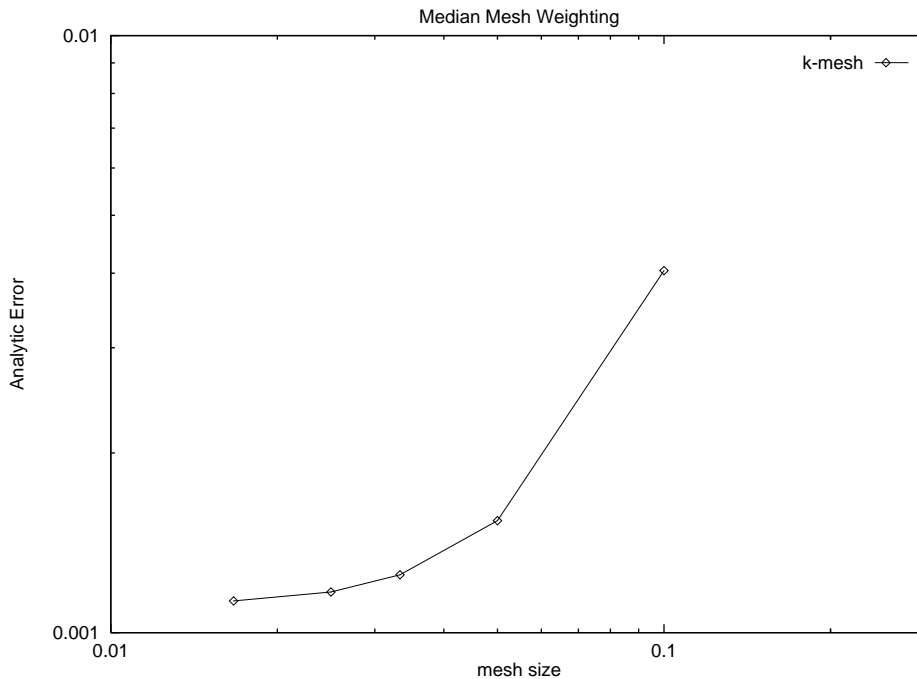
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Figure 6: Analytic Error for K-mesh = .2 for $-D\frac{\partial^2 \phi}{\partial x^2} - Qx^2 = 0$ with $D = \frac{1}{30}$, $Q = 1$, and $J_0 = J_1 = 0$, w_k median mesh weighted.

7   Results

In this section we will present results for hexahedral meshes, and three weighting methods. The analytic error, defined as

$$\text{Analytic Error} = \left[\frac{\sum_i (\phi_i - \phi(\vec{x}_i))^2}{\sum_i \phi(\vec{x}_i)^2}\right]^{\frac{1}{2}}, \tag{71}$$

is plotted in Figures 5, 6, and 7.

In Figure 5 the weights, w_k, are constant. Results are shown for a random mesh, and an orthogonal mesh. The orthogonal mesh shows second order convergence. The convergence is less than second order for the random mesh.

In Figure 6 the weights, w_k, are the median mesh volumes surrounding the kth point. Results are shown for a random mesh. The convergence is again less than second order for the random mesh.

In Figure 7 the weights, w_k, are the parallelpiped volumes surrounding the kth point, c.f. Equation 44. Results are shown for a random mesh. The convergence, in this case, is second order for the random mesh. We have chosen parallelpiped volume weights for this reason.

The linear solution is not recovered using these weights. Using a random mesh, the 20x20x20 linear problem obtained an analytic error of 7.10×10^{-4}. In
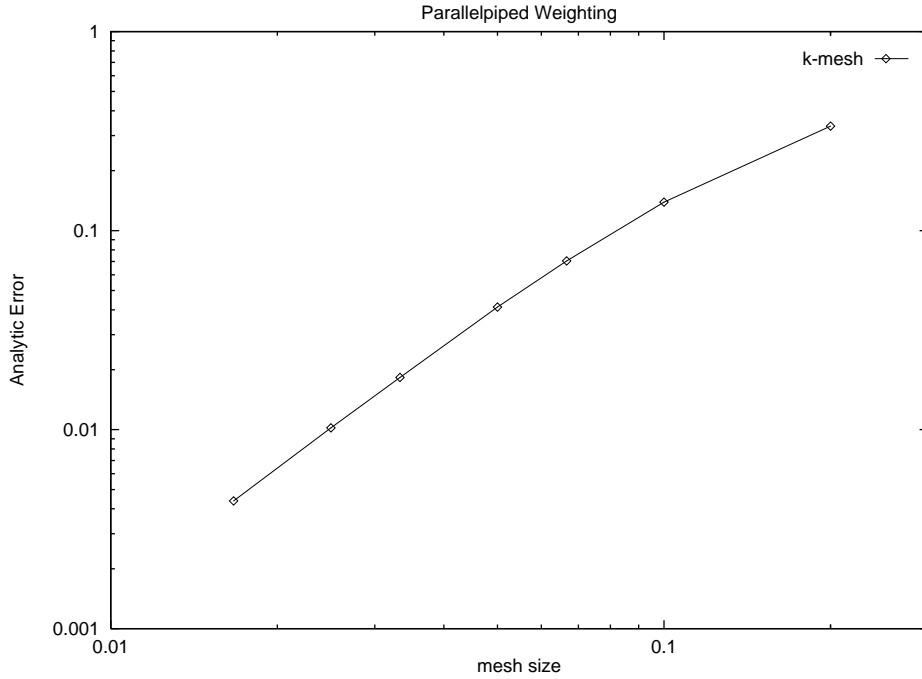
Figure 7: Analytic Error for K-mesh $= .2$ for $-D\frac{\partial^2 \phi}{\partial x^2} + \sigma_a \phi - Q x^2 = 0$ with $D = \frac{1}{30}$, $\sigma_a = 10$, $Q = 1$, $J_0 = 0.5$, and $J_1 = 1.0$, w_k parallelpiped weighted.

order to demonstrate that this error was not due to roundoff, we ran the same problem with

$$w_i = \frac{1}{8}V_i. \tag{72}$$

It can be shown that this choice of weighting will produce the exact linear solution, though it will yield incorrect results for the general diffusion equation. With this weighting we obtained an analytic error of 1.44×10^{-14}. This points out the inability to determine the exact linear equation with the preferred weights from Equation 44 even though we obtain second order convergence.