Discussion of the Telluride Diffusion Discretization

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Telluride Solver WG Presentation
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(later expanded version)

Telluride LSLR Method Derivation

(Gleaned from looking at the code itself! May be incorrect.)

Assume a diffusion equation of the form:

$$\frac{\partial \Phi}{\partial t} - \overrightarrow{\nabla} \cdot D \overrightarrow{\nabla} \Phi = 0$$

Integrate over the cell and use Green's Theorem to yield:

$$\frac{\partial \Phi_c}{\partial t} V_c - \oint D \overrightarrow{\nabla} \Phi \cdot \overrightarrow{dA} = 0$$

Discretize spatially by looping over faces:

$$\frac{\partial \Phi_c}{\partial t} V_c - \sum_f D_f \left. \overrightarrow{\nabla} \Phi \right|_f \cdot \overrightarrow{A_f} = 0$$

Everything here is known except $\left. \overrightarrow{\nabla} \Phi \right|_f$, so that must be expressed in terms of our unknowns, chosen to be the set of cell-center variables, $\{\Phi_c\}$.

Telluride LSLR Method Derivation

Assume a Taylor series expansion for Φ around the value at a face:

$$\Phi = \Phi_f + \frac{\partial \Phi}{\partial x}\Delta x + \frac{\partial \Phi}{\partial y}\Delta y + \frac{\partial \Phi}{\partial z}\Delta z + \mathcal{O}\left(\Delta x^2\right)$$

Define a set of "neighbor" cells for this face, denoted by "c of f", with a total number of C cells.

Use the linearized Taylor series expansion at each of the neighbor cells.†

Do a least squares fit of the linearized Taylor series expansion, using all of the neighbor cells, to determine Φ_f and $\overrightarrow{\nabla}\Phi$. The χ^2 function for each individual face is:

$$\chi_f^2 = \sum_{c \text{ of } f} w_{cf}\left[\Phi_c - \Phi_f - \left.\frac{\partial \Phi}{\partial x}\right|_f \Delta x_{cf} - \left.\frac{\partial \Phi}{\partial y}\right|_f \Delta y_{cf} - \left.\frac{\partial \Phi}{\partial z}\right|_f \Delta z_{cf}\right]^2$$

where w_{cf} is a weight applied to each neighbor cell for a given face.

† Note that this assumes that the gradient is the same over this set of cells, which is strictly true only if D is constant over all of these cells. If D varies slowly, then this may be a good assumption. This is the "material discontinuity" issue. Since D represents density in Telluride, this is probably a good assumption for liquid/solid flow of similar materials, but is *not* a good assumption for gas/liquid flow, where densities may differ by a factor of 10^3.

Telluride LSLR Method Derivation

Take derivatives wrt the constants to be determined (Φ_f, $\left.\frac{\partial\Phi}{\partial x}\right|_f$, $\left.\frac{\partial\Phi}{\partial y}\right|_f$, and $\left.\frac{\partial\Phi}{\partial z}\right|_f$) and set equal to zero:

$$
\begin{aligned}
0 &= -2 \sum_{c \text{ of } f} w_{cf} \left[\Phi_c - \Phi_f - \left.\frac{\partial\Phi}{\partial x}\right|_f \Delta x_{cf} - \left.\frac{\partial\Phi}{\partial y}\right|_f \Delta y_{cf} - \left.\frac{\partial\Phi}{\partial z}\right|_f \Delta z_{cf} \right] \\
0 &= -2 \sum_{c \text{ of } f} w_{cf} \left[\Phi_c \Delta x_{cf} - \Phi_f \Delta x_{cf} - \left.\frac{\partial\Phi}{\partial x}\right|_f \Delta x_{cf} \Delta x_{cf} \right. \\
&\quad \left. - \left.\frac{\partial\Phi}{\partial y}\right|_f \Delta y_{cf} \Delta x_{cf} - \left.\frac{\partial\Phi}{\partial z}\right|_f \Delta z_{cf} \Delta x_{cf} \right] \\
0 &= -2 \sum_{c \text{ of } f} w_{cf} \left[\Phi_c \Delta y_{cf} - \Phi_f \Delta y_{cf} - \left.\frac{\partial\Phi}{\partial x}\right|_f \Delta x_{cf} \Delta y_{cf} \right. \\
&\quad \left. - \left.\frac{\partial\Phi}{\partial y}\right|_f \Delta y_{cf} \Delta y_{cf} - \left.\frac{\partial\Phi}{\partial z}\right|_f \Delta z_{cf} \Delta y_{cf} \right] \\
0 &= -2 \sum_{c \text{ of } f} w_{cf} \left[\Phi_c \Delta z_{cf} - \Phi_f \Delta z_{cf} - \left.\frac{\partial\Phi}{\partial x}\right|_f \Delta x_{cf} \Delta z_{cf} \right. \\
&\quad \left. - \left.\frac{\partial\Phi}{\partial y}\right|_f \Delta y_{cf} \Delta z_{cf} - \left.\frac{\partial\Phi}{\partial z}\right|_f \Delta z_{cf} \Delta z_{cf} \right]
\end{aligned}
$$

Telluride LSLR Method Derivation

Grouping terms:

$$\begin{bmatrix} \sum w_{cf} & \sum w_{cf}\Delta x_{cf} & \sum w_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf} \\ \sum w_{cf}\Delta x_{cf} & \sum w_{cf}\Delta x_{cf}\Delta x_{cf} & \sum w_{cf}\Delta y_{cf}\Delta x_{cf} & \sum w_{cf}\Delta z_{cf}\Delta x_{cf} \\ \sum w_{cf}\Delta y_{cf} & \sum w_{cf}\Delta x_{cf}\Delta y_{cf} & \sum w_{cf}\Delta y_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf}\Delta y_{cf} \\ \sum w_{cf}\Delta z_{cf} & \sum w_{cf}\Delta x_{cf}\Delta z_{cf} & \sum w_{cf}\Delta y_{cf}\Delta z_{cf} & \sum w_{cf}\Delta z_{cf}\Delta z_{cf} \end{bmatrix} \times$$

$$\begin{bmatrix} \Phi_f \\ \left.\frac{\partial \Phi}{\partial x}\right|_f \\ \left.\frac{\partial \Phi}{\partial y}\right|_f \\ \left.\frac{\partial \Phi}{\partial z}\right|_f \end{bmatrix} = \begin{bmatrix} \sum w_{cf}\Phi_c \\ \sum w_{cf}\Phi_c\Delta x_{cf} \\ \sum w_{cf}\Phi_c\Delta y_{cf} \\ \sum w_{cf}\Phi_c\Delta y_{cf} \end{bmatrix}$$

Scale first column and first row by an average Δx, $\langle \Delta x \rangle$, presumably to improve the condition number of the matrix and/or to make all terms have the same units:

$$\begin{bmatrix} \langle \Delta x \rangle^2 \sum w_{cf} & \langle \Delta x \rangle \sum w_{cf}\Delta x_{cf} & \langle \Delta x \rangle \sum w_{cf}\Delta y_{cf} & \langle \Delta x \rangle \sum w_{cf}\Delta z_{cf} \\ \langle \Delta x \rangle \sum w_{cf}\Delta x_{cf} & \sum w_{cf}\Delta x_{cf}\Delta x_{cf} & \sum w_{cf}\Delta y_{cf}\Delta x_{cf} & \sum w_{cf}\Delta z_{cf}\Delta x_{cf} \\ \langle \Delta x \rangle \sum w_{cf}\Delta y_{cf} & \sum w_{cf}\Delta x_{cf}\Delta y_{cf} & \sum w_{cf}\Delta y_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf}\Delta y_{cf} \\ \langle \Delta x \rangle \sum w_{cf}\Delta z_{cf} & \sum w_{cf}\Delta x_{cf}\Delta z_{cf} & \sum w_{cf}\Delta y_{cf}\Delta z_{cf} & \sum w_{cf}\Delta z_{cf}\Delta z_{cf} \end{bmatrix} \times$$

$$\begin{bmatrix} \Phi_f / \langle \Delta x \rangle \\ \left.\frac{\partial \Phi}{\partial x}\right|_f \\ \left.\frac{\partial \Phi}{\partial y}\right|_f \\ \left.\frac{\partial \Phi}{\partial z}\right|_f \end{bmatrix} = \begin{bmatrix} \langle \Delta x \rangle \sum w_{cf}\Phi_c \\ \sum w_{cf}\Phi_c\Delta x_{cf} \\ \sum w_{cf}\Phi_c\Delta y_{cf} \\ \sum w_{cf}\Phi_c\Delta y_{cf} \end{bmatrix}$$

This is where the present Telluride coding stops. When fluxes are needed, the current values for Φ_c are inserted into the RHS, the summations are done, and the matrix on the LHS is inverted via LU to get the gradient vector.

It is possible, however, to solve for the gradient in terms of the set of Φ_c variables, so that a global matrix may be formed.

Telluride LSLR Method - Matrix Formation

Re-write the RHS:

$$\begin{bmatrix} \langle\Delta x\rangle^2 \sum w_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta x_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta y_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta z_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta x_{cf} & \sum w_{cf}\Delta x_{cf}\Delta x_{cf} & \sum w_{cf}\Delta y_{cf}\Delta x_{cf} & \sum w_{cf}\Delta z_{cf}\Delta x_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta y_{cf} & \sum w_{cf}\Delta x_{cf}\Delta y_{cf} & \sum w_{cf}\Delta y_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf}\Delta y_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta z_{cf} & \sum w_{cf}\Delta x_{cf}\Delta z_{cf} & \sum w_{cf}\Delta y_{cf}\Delta z_{cf} & \sum w_{cf}\Delta z_{cf}\Delta z_{cf} \end{bmatrix} \times$$

$$\begin{bmatrix} \Phi_f / \langle\Delta x\rangle \\ \left.\frac{\partial\Phi}{\partial x}\right|_f \\ \left.\frac{\partial\Phi}{\partial y}\right|_f \\ \left.\frac{\partial\Phi}{\partial z}\right|_f \end{bmatrix} = \begin{bmatrix} \langle\Delta x\rangle w_{1f} & \langle\Delta x\rangle w_{2f} & \langle\Delta x\rangle w_{3f} & \dots & \langle\Delta x\rangle w_{Cf} \\ w_{1f}\Delta x_{1f} & w_{2f}\Delta x_{2f} & w_{3f}\Delta x_{3f} & \dots & w_{Cf}\Delta x_{Cf} \\ w_{1f}\Delta y_{1f} & w_{2f}\Delta y_{2f} & w_{3f}\Delta y_{3f} & \dots & w_{Cf}\Delta y_{Cf} \\ w_{1f}\Delta z_{1f} & w_{2f}\Delta z_{2f} & w_{3f}\Delta z_{3f} & \dots & w_{Cf}\Delta z_{Cf} \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \dots \\ \Phi_C \end{bmatrix}$$

Symbolicly, this can be written:

$$\mathbf{B}_f \mathbf{F}_f = \mathbf{G}_f \mathbf{\Phi}_{c \text{ of } f}$$

where $\mathbf{\Phi}_{c \text{ of } f}$ signifies that the Φ vector contains all the neighbor cells for a given face. The unknowns in this equation are $\mathbf{F}_f$ and $\mathbf{\Phi}_{c \text{ of } f}$. We want to write the unknowns $\mathbf{F}_f$ in terms of the unknowns $\mathbf{\Phi}_{c \text{ of } f}$. $\mathbf{B}_f$ is small (4x4), so we can invert it to get:

$$\mathbf{F}_f = \mathbf{B}_f^{-1} \mathbf{G}_f \mathbf{\Phi}_{c \text{ of } f}$$

Parts of $\mathbf{F}_f$ are the flux components that we are looking for. The rectangular matrix $\mathbf{B}_f^{-1}\mathbf{G}_f$ gives the coefficients for the cell-center Φ_c's needed to represent the flux components in a matrix. We don't need the first entry of $\mathbf{F}_f$ (which contains $\Phi_f / \langle\Delta x\rangle$), but only the 2^{nd} through 4^{th} entries, which comprise the gradient. So, we only need the 2^{nd} through 4^{th} rows of $\mathbf{B}_f^{-1}\mathbf{G}_f$, which we will denote by $\left(\mathbf{B}_f^{-1}\mathbf{G}_f\right)_{234}$, such that

$$\begin{bmatrix} \left.\frac{\partial\Phi}{\partial x}\right|_f \\ \left.\frac{\partial\Phi}{\partial y}\right|_f \\ \left.\frac{\partial\Phi}{\partial z}\right|_f \end{bmatrix} = \left(\mathbf{B}_f^{-1}\mathbf{G}_f\right)_{234} \mathbf{\Phi}_{c \text{ of } f}$$

Telluride LSLR Method - Matrix Formation

Now, look back at this equation from slide 2:

$$\frac{\partial \Phi_c}{\partial t} V_c - \sum_f D_f \left. \overrightarrow{\nabla} \Phi \right|_f \cdot \overrightarrow{A_f} = 0$$

We can now represent $\left. \overrightarrow{\nabla} \Phi \right|_f$ in terms of the global set of cell-center variables, $\{\Phi_c\}$. Changing from vector representation to matrix representation:

$$\frac{\partial \Phi_c}{\partial t} V_c - \sum_f D_f \begin{bmatrix} \left.\frac{\partial \Phi}{\partial x}\right|_f \\ \left.\frac{\partial \Phi}{\partial y}\right|_f \\ \left.\frac{\partial \Phi}{\partial z}\right|_f \end{bmatrix}^T \mathbf{A}_f = 0$$

Or,

$$\frac{\partial \Phi_c}{\partial t} V_c - \sum_f D_f \mathbf{A}_f^T \begin{bmatrix} \left.\frac{\partial \Phi}{\partial x}\right|_f \\ \left.\frac{\partial \Phi}{\partial y}\right|_f \\ \left.\frac{\partial \Phi}{\partial z}\right|_f \end{bmatrix} = 0$$

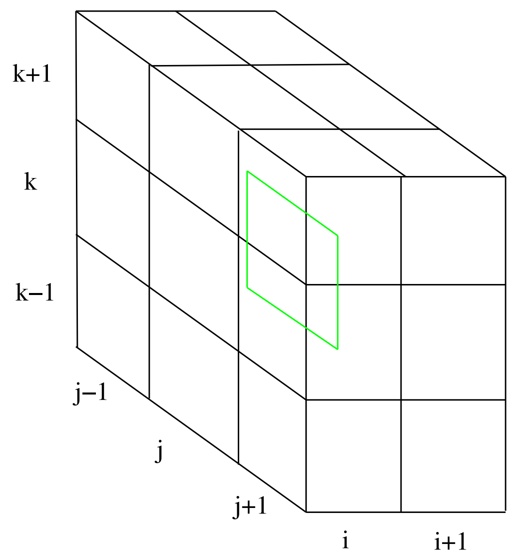
Substituting our derived LSLR form gives

$$\frac{\partial \Phi_c}{\partial t} V_c - \sum_f D_f \mathbf{A}_f^T \left(\mathbf{B}_f^{-1} \mathbf{G}_f \right)_{234} \mathbf{\Phi}_{c \text{ of } f} = 0$$

Building a matrix by going further than this step is easy in practise, but cumbersome using matrix representation. Basically, we first calculate the coefficient vector denoted by $D_f \mathbf{A}_f^T \left(\mathbf{B}_f^{-1} \mathbf{G}_f \right)_{234}$ for each face (note that it is a row vector with length equal to the number of neighbor cells for a given face). Then, we distribute this vector of coefficients into the global matrix, adding an entry for each neighbor cell of the currect face in the proper location. The entries are gotten by looping over cells, then looping over faces for each cell, then looping over neighbor cells for each face for each cell.

Telluride LSLR Method - Orthogonal Mesh Stencils

On an orthogonal, uniform mesh, with constant D, the method reduces to a simple stencil.† On this (i, j, k) mesh, the neighbor cells for a face at $\left(i + \frac{1}{2}, j, k\right)$, are taken to be the 18 cells (in a 2x3x3 block) within the range $(i : i + 1, j - 1 : j + 1, k - 1 : k + 1)$



Similarly, in 2-D there are 6 cells in a 2x3 block within the range $(i : i + 1, j - 1 : j + 1)$, and in 1-D there are 2 cells in the range $(i : i + 1)$.

We label the mesh spacing h in each direction and we refer to the cells in the following ranges by these names:

Major axis cells	$(i : i + 1, j, k)$
Edge cells	$(i : i + 1, j - 1, k)\,, (i : i + 1, j + 1, k)\,,$
	$(i : i + 1, j, k - 1)\,, (i : i + 1, j, k + 1)$
Corner cells	$(i : i + 1, j - 1, k - 1)\,, (i : i + 1, j - 1, k + 1)\,,$
	$(i : i + 1, j + 1, k - 1)\,, (i : i + 1, j + 1, k + 1)$

Note that 2-D has no corner cells, and 1-D consists only of major axis cells.

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†Doug Kothe's notes from 12/01/01 show this reduction explicitly for the 2-D, $w_{cf} = \frac{1}{d_{cf}^2}$ situation (where d_{cf} is the distance between cell-center c and face-center f).

Telluride LSLR Method - Orthogonal Mesh Stencils

Examine the $\mathbf{B}_f$ matrix from the top of slide 6:

$$\begin{bmatrix} \langle\Delta x\rangle^2 \sum w_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta x_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta y_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta z_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta x_{cf} & \sum w_{cf}\Delta x_{cf}\Delta x_{cf} & \sum w_{cf}\Delta y_{cf}\Delta x_{cf} & \sum w_{cf}\Delta z_{cf}\Delta x_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta y_{cf} & \sum w_{cf}\Delta x_{cf}\Delta y_{cf} & \sum w_{cf}\Delta y_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf}\Delta y_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta z_{cf} & \sum w_{cf}\Delta x_{cf}\Delta z_{cf} & \sum w_{cf}\Delta y_{cf}\Delta z_{cf} & \sum w_{cf}\Delta z_{cf}\Delta z_{cf} \end{bmatrix}$$

Note that the neighbor cells can be grouped into $(\boldsymbol{i}, \boldsymbol{i}+1)$ pairs. These pairs have opposite signs for the $\Delta \boldsymbol{x}_{cf}$ factors, but exactly the same $\Delta \boldsymbol{y}_{cf}$ and $\Delta \boldsymbol{z}_{cf}$ factors. If we further assume that any weights are constants or functions of distance (which is the same for both members of a pair), then any sums which contain a single $\Delta \boldsymbol{x}_{cf}$ are identically zero:

$$\begin{bmatrix} \langle\Delta x\rangle^2 \sum w_{cf} & 0 & \langle\Delta x\rangle \sum w_{cf}\Delta y_{cf} & \langle\Delta x\rangle \sum w_{cf}\Delta z_{cf} \\ 0 & \sum w_{cf}\Delta x_{cf}\Delta x_{cf} & 0 & 0 \\ \langle\Delta x\rangle \sum w_{cf}\Delta y_{cf} & 0 & \sum w_{cf}\Delta y_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf}\Delta y_{cf} \\ \langle\Delta x\rangle \sum w_{cf}\Delta z_{cf} & 0 & \sum w_{cf}\Delta y_{cf}\Delta z_{cf} & \sum w_{cf}\Delta z_{cf}\Delta z_{cf} \end{bmatrix}$$

Similarly, $\sum \boldsymbol{w}_{cf}\Delta \boldsymbol{y}_{cf}$ consists of terms for $\boldsymbol{j}$, which have a zero $\Delta \boldsymbol{y}_{cf}$, and matched pairs for the $(\boldsymbol{j}-1, \boldsymbol{j}+1)$ terms, which are opposite in sign but otherwise equal. Ditto for $\sum \boldsymbol{w}_{cf}\Delta \boldsymbol{z}_{cf}$:

$$\begin{bmatrix} \langle\Delta x\rangle^2 \sum w_{cf} & 0 & 0 & 0 \\ 0 & \sum w_{cf}\Delta x_{cf}\Delta x_{cf} & 0 & 0 \\ 0 & 0 & \sum w_{cf}\Delta y_{cf}\Delta y_{cf} & \sum w_{cf}\Delta z_{cf}\Delta y_{cf} \\ 0 & 0 & \sum w_{cf}\Delta y_{cf}\Delta z_{cf} & \sum w_{cf}\Delta z_{cf}\Delta z_{cf} \end{bmatrix}$$

Telluride LSLR Method - Orthogonal Mesh Stencils

Finally, $\sum w_{cf} \Delta y_{cf} \Delta z_{cf}$ has zero entries for the j and k terms, since they have zero Δy_{cf} or Δz_{cf}. This leaves only the eight corner cells, which consist of two sets of four cells that have the same absolute values for $\Delta y_{cf} \Delta z_{cf}$, but these sign combinations: $++, --, -+, +-$. With this sum set to zero, we see that the matrix reduces to a diagonal matrix:

$$\mathbf{B}_f = \begin{bmatrix} \langle \Delta x \rangle^2 \sum w_{cf} & 0 & 0 & 0 \\ 0 & \sum w_{cf} \Delta x_{cf} \Delta x_{cf} & 0 & 0 \\ 0 & 0 & \sum w_{cf} \Delta y_{cf} \Delta y_{cf} & 0 \\ 0 & 0 & 0 & \sum w_{cf} \Delta z_{cf} \Delta z_{cf} \end{bmatrix}$$

which is easily inverted. The area vector for this face (where q is the dimensionality) is

$$\mathbf{A}_f = \begin{bmatrix} h^{q-1} \\ 0 \\ 0 \end{bmatrix}$$

which selects only the first row of $\left(\mathbf{B}_f^{-1} \mathbf{G}_f\right)_{234}$, such that

$$\mathbf{A}_f^T \left(\mathbf{B}_f^{-1} \mathbf{G}_f\right)_{234} =$$

$$\frac{h^{q-1}}{\sum w_{cf} \Delta x_{cf} \Delta x_{cf}} \begin{bmatrix} w_{1f} \Delta x_{1f} & w_{2f} \Delta x_{2f} & \ldots & w_{Cf} \Delta x_{Cf} \end{bmatrix}$$

When evaluating the summation, recognize that all neighbor cells have the same value for $\Delta x_{cf} \Delta x_{cf}$:

$$\sum w_{cf} \Delta x_{cf} \Delta x_{cf} = \frac{h^2}{4} \sum w_{cf}$$

Telluride LSLR Method - Orthogonal Mesh Stencils

All the neighbor cells also have the same Δx_{cf}, except for the sign. Denoting the sign as S_{cf}:

$$\mathbf{A}_f^T \left(\mathbf{B}_f^{-1} \mathbf{G}_f \right)_{234} = \frac{2h^{q-2}}{\sum w_{cf}} \begin{bmatrix} w_{1f}S_{1f} & w_{2f}S_{2f} & \dots & w_{Cf}S_{Cf} \end{bmatrix}$$

This leads to the following face stencils:

Dimension	$w_{cf} = 1$	$w_{cf} = 1/d_{cf}^2$
1-D	$\frac{1}{h} \begin{bmatrix} -1 & 1 \end{bmatrix}$	$\frac{1}{h} \begin{bmatrix} -1 & 1 \end{bmatrix}$
2-D	$\frac{1}{3} \begin{bmatrix} -1 & 1 \\ -1 & 1 \\ -1 & 1 \end{bmatrix}$	$\frac{1}{7} \begin{bmatrix} -1 & 1 \\ -5 & 5 \\ -1 & 1 \end{bmatrix}$
3-D	$\frac{h}{9} \begin{bmatrix} -1 & -1 & -1 \\ -1 & -1 & -1 \\ -1 & -1 & -1 \end{bmatrix}, \frac{h}{9} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	$\frac{h}{101} \begin{bmatrix} -5 & -9 & -5 \\ -9 & -45 & -9 \\ -5 & -9 & -5 \end{bmatrix}, \frac{h}{101} \begin{bmatrix} 5 & 9 & 5 \\ 9 & 45 & 9 \\ 5 & 9 & 5 \end{bmatrix}$

Telluride LSLR Method - Orthogonal Mesh Stencils

The face stencils are valid for all faces of the cell, due to the uniformity of the grid. For the negative faces of the cell, the area vector is negative, which flips the stencil so that the part with the negative numbers is always on the interior side of the face.

Evaulating this equation:

$$\frac{1}{V_c}\int_c \nabla^2\Phi\, dV = \frac{1}{h^q}\sum_f \mathbf{A}_f^T\left(\mathbf{B}_f^{-1}\mathbf{G}_f\right)_{234}\mathbf{\Phi}_{c\text{ of }f}$$

leads to the Laplacian stencils for the cell . . .

Telluride LSLR Method - Orthogonal Mesh Stencils

Dimension	$w_{cf} = 1$	$w_{cf} = 1/d_{cf}^2$
1-D	$\frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 \end{bmatrix}$	$\frac{1}{h^2}\begin{bmatrix} 1 & -2 & 1 \end{bmatrix}$
2-D	$\frac{1}{3h^2}\begin{bmatrix} 2 & -1 & 2 \\ -1 & -4 & -1 \\ 2 & -1 & 2 \end{bmatrix}$	$\frac{1}{7h^2}\begin{bmatrix} 2 & 3 & 2 \\ 3 & -20 & 3 \\ 2 & 3 & 2 \end{bmatrix}$
3-D	$\frac{1}{3h^2}\begin{bmatrix} 1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \frac{1}{3h^2}\begin{bmatrix} 0 & -1 & 0 \\ -1 & -2 & -1 \\ 0 & -1 & 0 \end{bmatrix}, \frac{1}{3h^2}\begin{bmatrix} 1 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 1 \end{bmatrix}$	$\frac{1}{101h^2}\begin{bmatrix} 15 & 8 & 15 \\ 8 & 9 & 8 \\ 15 & 8 & 15 \end{bmatrix}, \frac{1}{101h^2}\begin{bmatrix} 8 & 9 & 8 \\ 9 & -270 & 9 \\ 8 & 9 & 8 \end{bmatrix}, \frac{1}{101h^2}\begin{bmatrix} 15 & 8 & 15 \\ 8 & 9 & 8 \\ 15 & 8 & 15 \end{bmatrix}$

Telluride LSLR Method - Orthogonal Accuracy Order

To determine the accuracy order for the orthogonal stencils, start with the Taylor series expansion for Φ around the value at a cell center:

$$\Phi = \Phi_c + \sum_{n=1,\infty} \frac{1}{n!} \left\{ \Delta x \frac{\partial}{\partial x}\bigg|_c + \Delta y \frac{\partial}{\partial y}\bigg|_c + \Delta z \frac{\partial}{\partial z}\bigg|_c \right\}^n \Phi$$

Next, expand each of the six stencils using this series and cancel terms to see what remains.

The constant Φ_c term will be zero if the stencil sums to zero, which is true for all of the cases.

The $n = 1$ (linear) terms will be zero due to cancellations if the stencil is symmetric along the x, y, and z planes, which is also true for all of the cases.

The $n = 2$ terms can be grouped into 6 mixed terms (e.g. $\frac{1}{2}\ \Delta x \Delta y\ \frac{\partial^2 \Phi}{\partial x \partial y}\Big|_c$) and 3 squared terms (e.g. $\frac{1}{2}\ \Delta x^2\ \frac{\partial^2 \Phi}{\partial x^2}\Big|_c$).

Telluride LSLR Method - Orthogonal Accuracy Order

The 3 squared terms are all similar due to stencil symmetry. The "stencil multipliers" for the $\frac{1}{2}\,\Delta x^2\, \frac{\partial^2 \Phi}{\partial x^2}\Big|_c$ term are:

Dimension	Multiplier
1-D	$\frac{h^2}{2}\,\frac{\partial^2 \Phi}{\partial x^2}\Big|_c \begin{bmatrix} 1 & 0 & 1 \end{bmatrix}$
2-D	$\frac{h^2}{2}\,\frac{\partial^2 \Phi}{\partial x^2}\Big|_c \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$
3-D	$\frac{h^2}{2}\,\frac{\partial^2 \Phi}{\partial x^2}\Big|_c \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$, $\frac{h^2}{2}\,\frac{\partial^2 \Phi}{\partial x^2}\Big|_c \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$, $\frac{h^2}{2}\,\frac{\partial^2 \Phi}{\partial x^2}\Big|_c \begin{bmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$

Telluride LSLR Method - Orthogonal Accuracy Order

Multiplying term by term and summing yields:

Dimension	$w_{cf} = 1$	$w_{cf} = 1/d_{cf}^2$	Standard Discretization
1-D	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$
2-D	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$
3-D	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$	$\frac{\partial^2\Phi}{\partial x^2}\Big\vert_c$

The y and z dimensions are similar, so that the 3 squared terms yield the full Laplacian, regardless of discretization or dimensionality.

The mixed secord-order term $\frac{1}{2}\ \Delta x \Delta y \left.\frac{\partial^2\Phi}{\partial x \partial y}\right|_c$ is a representative case. This term can be grouped into z-planes (none for 1-D, one for 2-D, and three for 3-D). Each z-plane has this stencil multiplier:

$$\frac{h^2}{2} \left.\frac{\partial^2\Phi}{\partial x \partial y}\right|_c \begin{bmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix}$$

which sums to zero. Thus, all of the mixed second-order terms are zero.

Telluride LSLR Method - Orthogonal Accuracy Order

The $n = 3$ terms can be grouped into these three categories:

- 3 cubed "3"† terms (e.g. $\frac{1}{6}\ \Delta x^3 \left.\frac{\partial^3 \Phi}{\partial x^3}\right|_c$), with 1-D stencil multipliers, $\begin{bmatrix} -1 & 0 & 1 \end{bmatrix}$, which sum to zero;
- 18 mixed "2-1"† terms (e.g. $\frac{1}{6}\ \Delta x^2 \Delta y \left.\frac{\partial^3 \Phi}{\partial x^2 \partial y}\right|_c$), grouped in z-planes with 2-D stencil multipliers,

$$\frac{h^3}{6} \left.\frac{\partial^3 \Phi}{\partial x^2 \partial y}\right|_c \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & -1 \end{bmatrix},$$

  which sum to zero; and
- 6 mixed "1-1-1"† terms (e.g. $\frac{1}{6}\ \Delta x \Delta y \Delta z \left.\frac{\partial^3 \Phi}{\partial x \partial y \partial z}\right|_c$), with 3-D stencil multipliers,

$$\frac{h^3}{6} \left.\frac{\partial^3 \Phi}{\partial x \partial y \partial z}\right|_c \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix},$$

  which also sum to zero.

Therefore, the third-order terms all cancel out.

†We can refer to term categories by listing the exponents of the terms.

Telluride LSLR Method - Orthogonal Accuracy Order

The $n = 4$ terms can be grouped into these four categories (two here):

- 4 quartic "4" terms (e.g. $\frac{1}{24}\ \Delta x^4 \frac{\partial^4 \Phi}{\partial x^4}\Big|_c$), with 1-D stencil multipliers, $\begin{bmatrix} 1 & 0 & 1 \end{bmatrix}$, which sum to:

Dimension	$w_{cf} = 1$	$w_{cf} = 1/d_{cf}^2$	Standard Discretization
1-D	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$
2-D	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$
3-D	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$	$\frac{h^2}{12} \frac{\partial^4 \Phi}{\partial x^4}\Big\|_c$

  The y and z dimensions are analogous;

- 24 mixed "3-1" terms (e.g. $\frac{1}{24}\ \Delta x^3 \Delta y\ \frac{\partial^4 \Phi}{\partial x^3 \partial y}\Big|_c$), grouped in z-planes with 2-D stencil multipliers,

$$\frac{h^4}{24} \frac{\partial^4 \Phi}{\partial x^3 \partial y}\Big|_c \begin{bmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix},$$

  which sum to zero;

Telluride LSLR Method - Orthogonal Accuracy Order

The $n = 4$ terms can be grouped into these four categories (two more here):

- 18 mixed "2-2" terms (e.g. $\frac{1}{24}\,\Delta x^2 \Delta y^2 \left.\frac{\partial^4 \Phi}{\partial x^2 \partial y^2}\right|_c$), grouped in z-planes with 2-D stencil multipliers,

$$\frac{h^4}{24}\left.\frac{\partial^4 \Phi}{\partial x^2 \partial y^2}\right|_c \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix},$$

which sum to:

Dimension	$w_{cf} = 1$	$w_{cf} = 1/d_{cf}^2$	Standard Discretization
1-D	0	0	0
2-D	$\frac{2h^2}{3}\left.\frac{\partial^4 \Phi}{\partial x^2 \partial y^2}\right\|_c$	$\frac{2h^2}{7}\left.\frac{\partial^4 \Phi}{\partial x^2 \partial y^2}\right\|_c$	0
3-D	$\frac{2h^2}{3}\left.\frac{\partial^4 \Phi}{\partial x^2 \partial y^2}\right\|_c$	$\frac{38h^2}{101}\left.\frac{\partial^4 \Phi}{\partial x^2 \partial y^2}\right\|_c$	0

The xz and yz combinations are analogous; and

- 36 mixed "2-1-1" terms (e.g. $\frac{1}{24}\,\Delta x^2 \Delta y \Delta z \left.\frac{\partial^4 \Phi}{\partial x^2 \partial y \partial z}\right|_c$), with 3-D stencil multipliers,

$$\frac{h^4}{24}\left.\frac{\partial^4 \Phi}{\partial x^2 \partial y \partial z}\right|_c \begin{bmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & -1 \end{bmatrix},$$

which sum to zero.

Telluride LSLR Method - Orthogonal Accuracy Order

Therefore, the leading error terms are:

Dimension and Discretization	Leading Error Terms
1-D, Standard	$\frac{h^2}{12}\left.\frac{\partial^4\Phi}{\partial x^4}\right\|_c$
1-D, $w_{cf} = 1$	$\frac{h^2}{12}\left.\frac{\partial^4\Phi}{\partial x^4}\right\|_c$
1-D, $w_{cf} = 1/d_{cf}^2$	$\frac{h^2}{12}\left.\frac{\partial^4\Phi}{\partial x^4}\right\|_c$
2-D, Standard	$\frac{h^2}{12}\left.\left(\frac{\partial^4\Phi}{\partial x^4}+\frac{\partial^4\Phi}{\partial y^4}\right)\right\|_c$
2-D, $w_{cf} = 1$	$\frac{h^2}{12}\left.\left(\frac{\partial^4\Phi}{\partial x^4}+\frac{\partial^4\Phi}{\partial y^4}\right)\right\|_c + \frac{2h^2}{3}\left.\frac{\partial^4\Phi}{\partial x^2\partial y^2}\right\|_c$
2-D, $w_{cf} = 1/d_{cf}^2$	$\frac{h^2}{12}\left.\left(\frac{\partial^4\Phi}{\partial x^4}+\frac{\partial^4\Phi}{\partial y^4}\right)\right\|_c + \frac{2h^2}{7}\left.\frac{\partial^4\Phi}{\partial x^2\partial y^2}\right\|_c$
3-D, Standard	$\frac{h^2}{12}\left.\left(\frac{\partial^4\Phi}{\partial x^4}+\frac{\partial^4\Phi}{\partial y^4}+\frac{\partial^4\Phi}{\partial z^4}\right)\right\|_c$
3-D, $w_{cf} = 1$	$\frac{h^2}{12}\left.\left(\frac{\partial^4\Phi}{\partial x^4}+\frac{\partial^4\Phi}{\partial y^4}+\frac{\partial^4\Phi}{\partial z^4}\right)\right\|_c +$ $\frac{2h^2}{3}\left.\left(\frac{\partial^4\Phi}{\partial x^2\partial y^2}+\frac{\partial^4\Phi}{\partial x^2\partial z^2}+\frac{\partial^4\Phi}{\partial y^2\partial z^2}\right)\right\|_c$
3-D, $w_{cf} = 1/d_{cf}^2$	$\frac{h^2}{12}\left.\left(\frac{\partial^4\Phi}{\partial x^4}+\frac{\partial^4\Phi}{\partial y^4}+\frac{\partial^4\Phi}{\partial z^4}\right)\right\|_c +$ $\frac{38h^2}{101}\left.\left(\frac{\partial^4\Phi}{\partial x^2\partial y^2}+\frac{\partial^4\Phi}{\partial x^2\partial z^2}+\frac{\partial^4\Phi}{\partial y^2\partial z^2}\right)\right\|_c$

Telluride LSLR Method - Orthogonal Accuracy Order

In general, expansion terms must consist of only even exponents to give non-zero sums. This means that the fifth-order (h^3) terms for all discretizations sum to zero.

So, all of the discretizations expand to this form:

$$\nabla^2 \Phi\big|_c + \{\text{Leading Error Terms}\} + \mathcal{O}\left(h^4\right)$$

The leading error terms for the Standard Discretization derived here agree exactly with the 1-D and 2-D results reported in *Numerical Solution of Partial Differential Equations: Finite Difference Methods*, by G. D. Smith, pgs. 98 and 221.

We can't really compare the errors between the discretizations in an absolute sense, because the derivatives are all independent and may even include opposite signs causing cancellations.

However, to get a rough feel for the relative difference in error between the discretizations, we assume that all the fourth-order derivatives are unity, and then divide by the result for the Standard Discretization to get a very loose estimate of relative error:

Dimension	$w_{cf} = 1$	$w_{cf} = 1/d_{cf}^2$	Standard Discretization
1-D	1	1	1
2-D	5	2.714	1
3-D	9	5.515	1

Telluride LSLR Method Properties

Good:

- The method is linear and a matrix may be formed.
- It has a local stencil.
- It consists of only cell-centered unknowns. Or, with some changes, node-centered unknowns. Very pliable.
- It is conservative, if a single D is used at each face.
- The method will work on polyhedra.
- The method is second-order on uniform meshes. The method is likely to be second order in general if there are not strong material discontinuities (gut instinct plus comparison with the paper by Ollivier-Gooch and Van Altena, which is a slightly different method).
- The accuracy of the method can be increased easily by simply increasing the stencil and adding terms to the Taylor series expansion in the χ^2 function. This would, however, exacerbate the material discontinuity issue.
- The $w_{cf} = 1/d_{cf}^2$ version probably generates a positive definite matrix. Proving so would be difficult.

Telluride LSLR Method Properties

Bad:

- The method does not treat material discontinuities rigorously (this is less of a problem for small discontinuities in the diffusion coefficient, but it is a show-stopper for radiation transport calculations). The error order probably degrades to first or zeroth order for strong material discontinuities.
- The method generates an asymmetric matrix.
- It is not exact for linear functions, unless there is a constant diffusion coefficient.
- The method does not reduce to the standard differencing scheme in 2-D (5-pt) or 3-D (7-pt) if the mesh is orthogonal and uniform. It reduces to a 9-pt (2-D) or 27-pt (3-D) stencil, with unusual values. The stencil is second-order, but has additional terms compared to the standard discretization scheme.
- The $w_{cf} = 1$ version is probably not positive definite, and not an M-matrix (it has negative off-diagonal entries for the uniform mesh case).

Indifferent:

- The method generates a "ragged right" matrix (i.e. a non-constant number of nonzeros per row).