Implicit approach to heat equation: recall **A · T=b.** What is **A**?

E.g. Euler implicit:

$$T_{i,j}^{n+1} = T_{i,j}^{n} + \alpha_x(T_{i+1,j}^{n+1} - 2T_{i,j}^{n+1} + T_{i-1,j}^{n+1}) + \alpha_y(T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j-1}^{n+1})$$

1. Set-up: T(i,j) stored in computer as 1-D. In Fortran ordering

   T(1,1),T(2,1),T(3,1)...T(I,1); T(1,2),T(2,2)...T(I,2); .....T(I,J) = vector of length I*J

   ↑ row 1 ↑ row 2

   That is i,j ⇔ i+(j-1)*I

   For understanding but not how it will be solved

$$\boldsymbol{T} = \begin{pmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \\ \cdot \\ \cdot \\ \cdot \\ T_{1,2} \\ T_{2,2} \\ T_{3,2} \\ \cdot \\ \cdot \\ \cdot \\ T_{I-2,J} \\ T_{I-1,J} \\ T_{I,J} \end{pmatrix}$$

   $\delta T/\delta y|_{3,2}$ = (T(3,2)-T(3,1))/Δy

$$\delta_y T = \frac{T_{i,j+1} - T_{i,j}}{\Delta y}$$

   The 2-point stencil is separated by I locations:

   i+j*I - [i+(j-1)*I] = I

   (i,j+1) (i,j)

   T(i,j) stored at location i+(j-1)*I. Length of **T** is M= I*J = number of grid points.

2. Implicit form is still **A*T=b**, but **A** is no longer tridiagonal. What does it look like?

3. Start with $\delta^2T/\delta y^2$ as row times column

$$\frac{\delta^2 T}{\delta y^2} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} = \boldsymbol{R} \cdot \boldsymbol{T}$$

   In **T** vector $T_{i,j-1}$ is at i+(j-2)*I and $T_{i,j}$ is at i+(j-1)*I; so there are i+(j-1)*I - [i+(j-2)*I]-1 entries in between them: **I-1** elements. These must be 0's in **R** so that they don't add to the dot product. Specifically,

← - - - - - - - - - - 2I+1 - - - - - - - - - - →

$$\mathbf{R\cdot T} = \left(0,\ldots,0,\frac{1}{\Delta y^2},\underbrace{0,\ldots\ldots,0}_{I-1\ \ 0's}\ \underbrace{\frac{-2}{\Delta y^2}}_{i+(j-1)I},\underbrace{0,\ldots\ldots,0}_{I-1\ \ 0's}\ \frac{1}{\Delta y^2},0,\ldots,0\right)\bullet\begin{pmatrix}T_{1,2}\\ T_{2,1}\\ \cdot\\ \cdot\\ \cdot\\ T_{I,J}\end{pmatrix}$$

i+(j-2) I   i+(j-1)I   i+j I

Along the row,

the (i,j-1) element is at i+(j-2) I so it multiplies the i,j-1 element of the T vector

the (i,j) element is at i+(j-1)I

the (i,j+1) element is at i+j I

In between are zeros, so the corresponding $T_{n,m}$ does not contribute.

Along the row: i+(j-2) I-1 zeros, then an element, then i+j I - [i+(j-1) I] -1 = I -1 more zeros, then an element... The total row length is I*J

Counting zeros is not essential, since only the non-zero elements need be stored: just be aware of the sparse structure.

4. Denoting just the fill:

$$\mathbf{R} = \ (0,0,\ldots,\bullet,0,0,\ldots,0,\bullet,0,0,\ldots,0,\bullet,0,\ldots)$$

and filling the matrix: $\delta^2(\bullet)/\delta y^2$ (i.e. $\delta^2 T/\delta y^2 = \mathbf{A}_{\delta y^2} * \mathbf{T}$)

$$\begin{array}{cc} A_{\delta^2 y} = \begin{pmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ 0,\ldots,\bullet,0,0,\ldots,0,\bullet,0,0,\ldots,0,\bullet,0,0,\ldots \\ 0,\ldots,0,\bullet,0,\ldots,0,0,\bullet,0,\ldots,0,0,\bullet,0,\ldots \\ 0,\ldots,0,0,\bullet,\ldots,0,0,0,\bullet,\ldots,0,0,0,\bullet,\ldots \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \end{pmatrix} & \text{I*J rows} \end{array}$$

M=I*J is number of grid points. **A** is MxM matrix.
Only the 3 non-zero elements need be stored: A(i,j ; 3). i,j run from 1 to I and J along a column: in each row of the column 3 elements are filled.

5. We are developing a matrix representation for

$$\alpha_x = \kappa\Delta t/\Delta x^2, \alpha_y = \kappa\Delta t/\Delta y^2$$

$$T_{i,j}^{n+1} \quad -\alpha_x(T_{i+1,j}^{n+1} - 2T_{i,j}^{n+1} + T_{i-1,j}^{n+1}) - \alpha_y(T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j-1}^{n+1}) = T_{i,j}^{n}$$

representing **T** as a 1-D vector (i,j)→ (j-1)*I+i:

$$\boldsymbol{T} = \begin{pmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \\ . \\ . \\ . \\ T_{1,2} \\ T_{2,2} \\ T_{3,2} \\ . \\ . \\ . \\ T_{I-2,J} \\ T_{I-1,J} \\ T_{I,J} \end{pmatrix}$$

or, there is an equivalence between T(I,J) and TT(I*J):

$$\begin{pmatrix} T_{1,1} \\ T_{2,1} \\ T_{3,1} \\ . \\ . \\ . \\ T_{I-2,J} \\ T_{I-1,J} \\ T_{I,J} \end{pmatrix} = \begin{pmatrix} TT_1 \\ TT_2 \\ TT_3 \\ . \\ . \\ . \\ TT_{I*J-2} \\ TT_{I*J-1} \\ TT_{I*J} \end{pmatrix}$$

That is T(i,j) → T(i+(j-1)I). So T(i+1,j), T(i,j) and T(i-1,j) are adjacent in the vector. Then the dot product of the row vector

$$\boldsymbol{R} = (\underbrace{0, \ldots\ldots ,0}_{i-2+(j-1)I}, \frac{1}{\Delta x^2}, \underbrace{\frac{-2}{\Delta x^2}}_{i+(j-1)I}, \frac{1}{\Delta x^2}, \underbrace{0, \ldots\ldots ,0}_{IJ-[i+1+(j-1)I]} \;)$$

with the $\boldsymbol{T}$-vector gives

$$\frac{\delta^2 T}{\delta x^2} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} = \boldsymbol{R} \cdot \boldsymbol{T}$$

In the y-direction

$$\frac{\delta^2 T}{\delta y^2} = \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} = \boldsymbol{R} \cdot \boldsymbol{T}$$

where (using i,j → i+(j-1)I) corresponds to the row vector

$$\boldsymbol{R} = \left(\underbrace{0,\ldots,0,\frac{1}{\Delta y^2}}_{i+(j-2)I}, \underbrace{0,\ldots\ldots,0}_{I-1\ \ 0's}\ \underbrace{\frac{-2}{\Delta y^2}}_{i+(j-1)I}, \underbrace{0,\ldots\ldots,0}_{I-1\ \ 0's} \frac{1}{\Delta y^2}, 0,\ldots,0 \right)$$

6. Filling in the rows, the second order, central difference for δ²(●)/δx² is tridiagonal. Adding the x and y contributions, schematically, the implicit matrix has the pentadiagonal form

Matrix operator for Laplacian

$\delta_x^2(\bullet)+\delta_y^2(\bullet) =$ **A**

=

$$\begin{pmatrix}
\bullet & \bullet & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
0 & \cdots & 0 & \frac{1}{\Delta y^2} & \cdots & \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2}-\frac{2}{\Delta y^2} & \frac{1}{\Delta x^2} & \cdots & \frac{1}{\Delta y^2} & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & \frac{1}{\Delta y^2} & \cdots & \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2}-\frac{2}{\Delta y^2} & \frac{1}{\Delta x^2} & \cdots & \frac{1}{\Delta y^2} & \cdots & 0 \\
0 & \cdots & & & 0 & \frac{1}{\Delta y^2} & \cdots & \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2}-\frac{2}{\Delta y^2} & \frac{1}{\Delta x^2} & \cdots & \frac{1}{\Delta y^2}\cdots & 0 \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bullet & \bullet
\end{pmatrix}$$

Some are b.c. rows (i=1,I or j=1,J): assume they fit penta-diagonal structure. For Euler implicit

$$\begin{pmatrix}
\bullet & \bullet & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
0 & \cdots & 0 & -\frac{1}{\Delta y^2} & \cdots & -\frac{1}{\Delta x^2} & 1+\frac{2}{\Delta x^2}+\frac{2}{\Delta y^2} & -\frac{1}{\Delta x^2} & I-2\,0's & -\frac{1}{\Delta y^2} & 0 & \cdots & 0 \\
0 & \cdots & 0 & 0 & -\frac{1}{\Delta y^2} & \cdots & -\frac{1}{\Delta x^2} & 1+\frac{2}{\Delta x^2}+\frac{2}{\Delta y^2} & -\frac{1}{\Delta x^2} & \cdots & -\frac{1}{\Delta y^2} & \cdots & 0 \\
0 & \cdots & & & 0 & -\frac{1}{\Delta y^2} & \cdots & -\frac{1}{\Delta x^2} & 1+\frac{2}{\Delta x^2}+\frac{2}{\Delta y^2} & -\frac{1}{\Delta x^2} & \cdots & -\frac{1}{\Delta y^2}\cdots & 0 \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots & & \cdots & & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \bullet & \bullet
\end{pmatrix}$$

Note that diagonal contains $-2/\Delta x^2$ $-2/\Delta y^2$. Adjacent elements are $1/\Delta x^2$ and distant diagonals are $1/\Delta y^2$.

7. The Euler-implicit diffusion equation

$$T_{i,j}^{n+1} - \alpha_x (T_{i+1,j}^{n+1} - 2T_{i,j}^{n+1} + T_{i-1,j}^{n+1}) - \alpha_y (T_{i,j+1}^{n+1} - 2T_{i,j}^{n+1} + T_{i,j-1}^{n+1}) = T_{i,j}^{n}$$

becomes the matrix equation

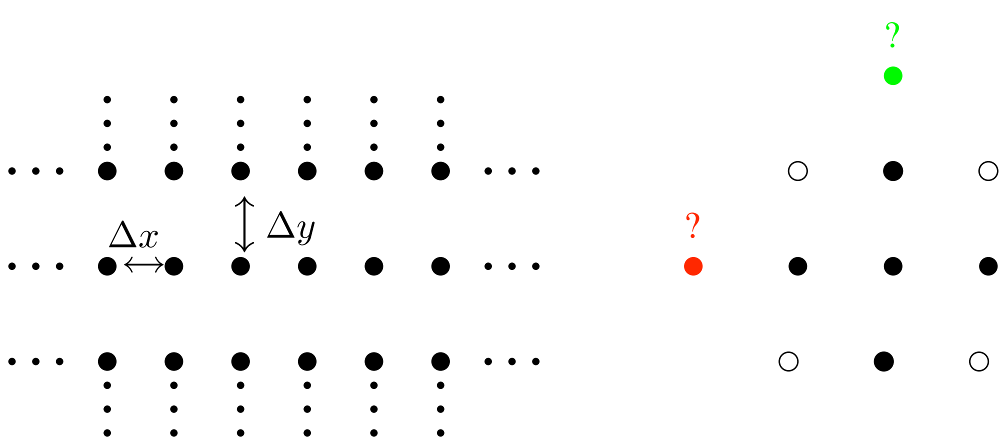
$$\mathbf{A} \cdot \mathbf{T}^{n+1} = \mathbf{T}^{n}$$

in which **A** is penta-diagonal with $1+2\alpha_x + 2\alpha_y$ on the diagonal, $-\alpha_x$ and $-\alpha_y$ on the lower and lower-lower diagonals.

The matrix, ignoring zeros has

```
  DO i=2,I-1; j=2,J-1
     A(i,j,1) = -alp_y
     A(i,j,2) = -alp_x
     A(i,j,3) = 1+2*alp_x+2*alp_y
     A(i,j,4) = -alp_x
     A(i,j,5) = -alp_y
     b(i,j)   = T(i,j)   !Crank-Nicholson involves Laplacian
 ENDDO
A(1,:,3) = 1 ; b(1,:) = Twall
```

8. Question: what is structure of matrix for red and green?



9. Computational complexity

   a. Bandwidth = number of elements between first and last fill on each line, inclusive:
      (i,j+1) - (i,j-1) +1 = i+j*I - i+(j-2)*I +1 = 2*I +1

   b. 1-D NxN matrix, 3 non-zero diagonals --- BW=3

   c. 2-D, M = I*J = # of grid points; or if I = J=N, $M=N^2$. MxM= $N^2 x N^2$ matrix, 5 non-zero diagonals. BW= 2*I +1 = 2N+1.

   d. #operations ~ M x BW^2 ~ M x N^2 ~ M^2. Say N~100 then M~10^4 , M^2~10^8
      or N~1,000 then M~10^6 , M^2~10^{12}

      Tridiag ~ M ops (M x BW^2 = 9M)

      3-D M= I*J*K, BW~2I*J+1. ops ~ $I^2*J^2*I*J*K$ = I^3*J^3*K; say I,J,K~200
      ops ~ $2^7\ 10^6\ 10^6\ 10^2 \sim 10^{16}$ Peta = 10^{15}

Gauss Elimination: across I+1 columns
down I rows
for each ~N diagonal element
~ I^2N operations

$\delta^2(\bullet)/\delta x^2 + \delta^2(\bullet)/\delta y^2 \longleftrightarrow$ **A** =