

An algorithm based on the Llewellyn Thomas algorithm for tridiagonal matrices for solving banded cyclic/periodic matrices:

Banded matrices can arise from finite difference methods, eg. :

$$a_j z_{j-1} + b_j z_j + c_j z_{j+1} = d_j$$

for a 3-point difference equation or

$$a_j z_{j-2} + b_j z_{j-1} + c_j z_j + d_j z_{j+1} + e_j z_{j+2} = f_j$$

for a 5-point formula.

A periodic version of a banded matrix can come from periodic boundary conditions. In these cases, none of the coefficients above are zero, whereas in a “regular” banded matrix, the boundary conditions make the off diagonal terms 0.

For the first example, the three (m=3) point equation $a_j z_{j-1} + b_j z_j + c_j z_{j+1} = d_j$ can be written as a cyclic or periodic version of the tridiagonal matrix with non-zero out of band elements:

$$\begin{bmatrix} b_1 & c_1 & . & . & . & 0 & a_1 \\ a_2 & b_2 & c_2 & . & . & . & 0 \\ . & . & . & . & a_{n-1} & b_{n-1} & c_{n-1} \\ c_n & 0 & . & . & 0 & a_n & b_n \end{bmatrix} \begin{bmatrix} z_1 \\ . \\ . \\ . \\ z_n \end{bmatrix} = \begin{bmatrix} d_1 \\ . \\ . \\ . \\ d_n \end{bmatrix} \quad \text{i.e. tridiagonal except for two off-diagonal terms.}$$

We will develop three versions of an inherently serial iterative algorithm for solving these systems. First, the system can be solved in $O[n]$ with what we shall call the forward algorithm.

Forward algorithm:

Starting with the 1st and nth equations and working inwards to the 2nd and n-1st and so on, for the jth pair of equations we can write, for the three point equations:

for $j: \{2, 3, 4, \dots\} \quad 1 < j < n/2$

$$\begin{bmatrix} b_j & 0 \\ 0 & b_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \begin{bmatrix} a_j & 0 \\ 0 & c_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j-1} \\ z_{n-j+2} \end{bmatrix} = \begin{bmatrix} d_j \\ d_{n-j+1} \end{bmatrix} - \begin{bmatrix} c_j & 0 \\ 0 & a_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j+1} \\ z_{n-j} \end{bmatrix}$$

which we rewrite as

$$\begin{bmatrix} b_j & 0 \\ 0 & b_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \begin{bmatrix} a_j & 0 \\ 0 & c_{n-j+1} \end{bmatrix} \left\{ \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \vec{v}_{j-1} \right\} = \begin{bmatrix} d_j \\ d_{n-j+1} \end{bmatrix} - \begin{bmatrix} c_j & 0 \\ 0 & a_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j+1} \\ z_{n-j} \end{bmatrix}$$

for $j: \{1, 2, 3, 4, \dots\} \quad 0 < j < n/2$

defining $\begin{bmatrix} z_{j-1} \\ z_{n-j+2} \end{bmatrix} = \left\{ \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \vec{v}_{j-1} \right\}$ for $j: \{2, 3, 4, \dots\} \quad 1 < j < n/2$

then we have

$$\begin{bmatrix} b_j & 0 \\ 0 & b_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \begin{bmatrix} a_j & 0 \\ 0 & c_{n-j+1} \end{bmatrix} \left\{ \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \vec{v}_{j-1} \right\} = \begin{bmatrix} d_j \\ d_{n-j+1} \end{bmatrix} - \begin{bmatrix} c_j & 0 \\ 0 & a_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j+1} \\ z_{n-j} \end{bmatrix}$$

and $\tilde{A}_0 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\vec{v}_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ for $j=1$ because at $j=1$:

$$\begin{bmatrix} b_1 & 0 \\ 0 & b_n \end{bmatrix} \begin{bmatrix} z_1 \\ z_n \end{bmatrix} + \begin{bmatrix} a_1 & 0 \\ 0 & c_n \end{bmatrix} \begin{bmatrix} z_n \\ z_1 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_n \end{bmatrix} - \begin{bmatrix} c_1 & 0 \\ 0 & a_n \end{bmatrix} \begin{bmatrix} z_2 \\ z_{n-1} \end{bmatrix}$$

Each pair is solved for in terms of the inner next pair of values. Using the first equation with $j=1$ yields the result for the second equation for $j=2$ by solving a 2x2 system of equations. Using the matrix \tilde{A}_1 and vector \vec{v}_1 the process is iterated repeatedly almost $n/2$ times, solving for all the \tilde{A}_j and \vec{v}_j

At the center of the matrix we have to solve either a 2x2 system of equations if n is even or a 3x3 system if n is odd. If n is even the final equation becomes, with $j=n/2$:

$$\begin{bmatrix} b_{n/2} & 0 \\ 0 & b_{n/2+1} \end{bmatrix} \begin{bmatrix} z_{n/2} \\ z_{n/2+1} \end{bmatrix} + \begin{bmatrix} a_{n/2} & 0 \\ 0 & c_{n/2+1} \end{bmatrix} \left\{ \tilde{A}_{n/2-1} \begin{bmatrix} z_{n/2} \\ z_{n/2+1} \end{bmatrix} + \vec{v}_{n/2-1} \right\} = \begin{bmatrix} d_{n/2} \\ d_{n/2+1} \end{bmatrix} - \begin{bmatrix} c_{n/2} & 0 \\ 0 & a_{n/2+1} \end{bmatrix} \begin{bmatrix} z_{n/2+1} \\ z_{n/2} \end{bmatrix}$$

which is a 2x2 system solvable for the middle two values:

$$\begin{bmatrix} z_{n/2} \\ z_{n/2+1} \end{bmatrix} = \left(\begin{bmatrix} b_{n/2} & c_{n/2} \\ a_{n/2+1} & b_{n/2+1} \end{bmatrix} + \begin{bmatrix} a_{n/2} & 0 \\ 0 & c_{n/2+1} \end{bmatrix} \tilde{A}_{n/2-1} \right)^{-1} \left(\begin{bmatrix} d_{n/2} \\ d_{n/2+1} \end{bmatrix} - \begin{bmatrix} a_{n/2} & 0 \\ 0 & c_{n/2+1} \end{bmatrix} \vec{v}_{n/2-1} \right)$$

If n is odd, the middle term is included:

$$\begin{bmatrix} b_j & c_j & 0 \\ a_{j+1} & b_{j+1} & c_{j+1} \\ 0 & a_{j+2} & b_{j+2} \end{bmatrix} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{j+2} \end{bmatrix} = \begin{bmatrix} d_j \\ d_{j+1} \\ d_{j+2} \end{bmatrix} - \begin{bmatrix} a_j & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & c_{j+2} \end{bmatrix} \begin{bmatrix} z_{j-1} \\ 0 \\ z_{j+3} \end{bmatrix}$$

$$\begin{bmatrix} z_{j-1} \\ z_{j+3} \end{bmatrix} = \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{j+2} \end{bmatrix} + \vec{v}_{j-1}, j = \frac{(n-1)}{2}$$

With

$$\begin{bmatrix} z_{j-1} \\ 0 \\ z_{j+3} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} z_{j-1} \\ z_{j+3} \end{bmatrix} = \left(\begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{j+2} \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \vec{v}_{j-1} \right) \text{ then}$$

$$\begin{bmatrix} b_j & c_j & 0 \\ a_{j+1} & b_{j+1} & c_{j+1} \\ 0 & a_{j+2} & b_{j+2} \end{bmatrix} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{j+2} \end{bmatrix} = \begin{bmatrix} d_j \\ d_{j+1} \\ d_{j+2} \end{bmatrix} - \begin{bmatrix} a_j & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & c_{j+2} \end{bmatrix} \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{j+2} \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} \vec{v}_{j-1} \right\}$$

or, writing the components of \tilde{A}_{j-1} explicitly:

$$\begin{bmatrix} b_j + a_j A_{j-1}^{11} & c_j & a_j A_{j-1}^{12} \\ a_{j+1} & b_{j+1} & c_{j+1} \\ c_{j+2} A_{j-1}^{21} & a_{j+2} & b_{j+2} + c_{j+2} A_{j-1}^{22} \end{bmatrix} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{j+2} \end{bmatrix} = \begin{bmatrix} d_j - a_j v_{j-1}^1 \\ d_{j+1} \\ d_{j+2} - c_{j+2} v_{j-1}^2 \end{bmatrix}$$

We can then solve for all of the z_j by back substitution using $\begin{bmatrix} z_{j-1} \\ z_{n-j+2} \end{bmatrix} = \left\{ \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \vec{v}_{j-1} \right\}$

Similarly, the m=5 point scheme $a_j z_{j-2} + b_j z_{j-1} + c_j z_j + d_j z_{j+1} + e_j z_{j+2} = f_j$ results in

$$\begin{bmatrix} c_1 & d_1 & e_1 & \cdot & \cdot & \cdot & a_1 & b_1 \\ b_2 & c_2 & d_2 & e_2 & \cdot & \cdot & \cdot & a_2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ e_{n-1} & \cdot & \cdot & \cdot & a_{n-1} & b_{n-1} & c_{n-1} & d_{n-1} \\ d_n & e_n & \cdot & \cdot & \cdot & a_n & b_n & c_n \end{bmatrix} \begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ z_n \end{bmatrix} = \begin{bmatrix} f_1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ f_n \end{bmatrix} \quad \text{with 6 off-diagonal non-zero elements.}$$

We can then write, for any set of 4 equations j:

$$\begin{bmatrix} c_j & d_j & 0 & 0 \\ b_{j+1} & c_{j+1} & 0 & 0 \\ 0 & 0 & c_{n-j} & d_{n-j} \\ 0 & 0 & b_{n-j+1} & c_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{n-j} \\ z_{n-j+1} \end{bmatrix} + \begin{bmatrix} a_j & b_j & 0 & 0 \\ 0 & a_{j+1} & 0 & 0 \\ 0 & 0 & e_{n-j} & 0 \\ 0 & 0 & d_{n-j} & e_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j-2} \\ z_{j-1} \\ z_{n-j+2} \\ z_{n-j+3} \end{bmatrix} = \begin{bmatrix} f_j \\ f_{j+1} \\ f_{n-j} \\ f_{n-j+1} \end{bmatrix} - \begin{bmatrix} e_j & 0 & 0 & 0 \\ d_{j+1} & e_{j+1} & 0 & 0 \\ 0 & 0 & a_{n-j} & b_{n-j} \\ 0 & 0 & 0 & a_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j+2} \\ z_{j+3} \\ z_{n-j-2} \\ z_{n-j-1} \end{bmatrix}$$

where we can define

$$\begin{bmatrix} z_{j-2} \\ z_{j-1} \\ z_{n-j+2} \\ z_{n-j+3} \end{bmatrix} = \tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{n-j} \\ z_{n-j+1} \end{bmatrix} + \vec{v}_{j-1} \quad \text{as before for } j: \{3, 5, 7, \dots\} \quad j > 1 \quad \text{and} \quad \tilde{A}_0 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \quad \vec{v}_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{for } j=1.$$

and then

$$\begin{aligned}
& \begin{bmatrix} c_j & d_j & 0 & 0 \\ b_{j+1} & c_{j+1} & 0 & 0 \\ 0 & 0 & c_{n-j} & d_{n-j} \\ 0 & 0 & b_{n-j+1} & c_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{n-j} \\ z_{n-j+1} \end{bmatrix} + \begin{bmatrix} a_j & b_j & 0 & 0 \\ 0 & a_{j+1} & 0 & 0 \\ 0 & 0 & e_{n-j} & 0 \\ 0 & 0 & d_{n-j} & e_{n-j+1} \end{bmatrix} \left(\tilde{A}_j \begin{bmatrix} z_j \\ z_{j+1} \\ z_{n-j} \\ z_{n-j+1} \end{bmatrix} + \vec{v}_j \right) \\
&= \begin{bmatrix} f_j \\ f_{j+1} \\ f_{n-j} \\ f_{n-j+1} \end{bmatrix} - \begin{bmatrix} e_j & 0 & 0 & 0 \\ d_{j+1} & e_{j+1} & 0 & 0 \\ 0 & 0 & a_{n-j} & b_{n-j} \\ 0 & 0 & 0 & a_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j+2} \\ z_{j+3} \\ z_{n-j-2} \\ z_{n-j-1} \end{bmatrix}
\end{aligned}$$

We then have either 5,6 or 7 rows left after iterating the recurrence relations: for example with 6 rows, we have:

$$\begin{bmatrix} c_j & d_j & e_j & 0 & 0 & 0 \\ b_{j+1} & c_{j+1} & d_{j+1} & e_{j+1} & 0 & 0 \\ a_{j+2} & b_{j+2} & c_{j+2} & d_{j+2} & e_{j+2} & 0 \\ 0 & a_{n-j-1} & b_{n-j-1} & c_{n-j-1} & d_{n-j-1} & e_{n-j-1} \\ 0 & 0 & a_{n-j} & b_{n-j} & c_{n-j} & d_{n-j} \\ 0 & 0 & 0 & a_{n-j+1} & b_{n-j+1} & c_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{j+2} \\ z_{j+3} \\ z_{j+4} \\ z_{j+5} \end{bmatrix} = \begin{bmatrix} f_j \\ f_{j+1} \\ f_{j+2} \\ f_{j+3} \\ f_{j+4} \\ f_{j+5} \end{bmatrix} - \begin{bmatrix} a_j & b_j & 0 & 0 & 0 & 0 \\ 0 & a_{j+1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{n-j} & 0 \\ 0 & 0 & 0 & 0 & d_{n-j} & e_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j-2} \\ z_{j-1} \\ 0 \\ 0 \\ z_{n-j+2} \\ z_{n-j+3} \end{bmatrix}$$

but

$$\begin{bmatrix} z_{j-2} \\ z_{j-1} \\ 0 \\ 0 \\ z_{n-j+2} \\ z_{n-j+3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} z_{j-2} \\ z_{j-1} \\ z_{n-j+2} \\ z_{n-j+3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \left(\tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{j+4} \\ z_{j+5} \end{bmatrix} + \vec{v}_{j-1} \right)$$

and so

$$= \begin{bmatrix} f_j \\ f_{j+1} \\ f_{j+2} \\ f_{j+3} \\ f_{j+4} \\ f_{j+5} \end{bmatrix} - \begin{bmatrix} a_j & b_j & 0 & 0 & 0 & 0 \\ 0 & a_{j+1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{n-j} & 0 \\ 0 & 0 & 0 & 0 & d_{n-j} & e_{n-j+1} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \left(\tilde{A}_{j-1} \begin{bmatrix} z_j \\ z_{j+1} \\ z_{j+4} \\ z_{j+5} \end{bmatrix} + \tilde{v}_{j-1} \right)$$

$$\text{and} \begin{bmatrix} a_j & b_j & 0 & 0 & 0 & 0 \\ 0 & a_{j+1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{n-j} & 0 \\ 0 & 0 & 0 & 0 & d_{n-j} & e_{n-j+1} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_j & b_j & 0 & 0 \\ 0 & a_{j+1} & 0 & 0 \\ 0 & 0 & e_{n-j} & 0 \\ 0 & 0 & d_{n-j} & e_{n-j+1} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

We can workout similar formulae for 5 and 7 rows left, with:

$$\begin{bmatrix} c_j & d_j & e_j & 0 & 0 \\ b_{j+1} & c_{j+1} & d_{j+1} & e_{j+1} & 0 \\ a_{(n+1)/2} & b_{(n+1)/2} & c_{(n+1)/2} & d_{(n+1)/2} & e_{(n+1)/2} \\ 0 & a_{n-j} & b_{n-j} & c_{n-j} & d_{n-j} \\ 0 & 0 & a_{n-j+1} & b_{n-j+1} & c_{n-j+1} \end{bmatrix} \quad \text{with 5 rows}$$

$$\text{and} \begin{bmatrix} c_j & d_j & e_j & 0 & 0 & 0 & 0 \\ b_{j+1} & c_{j+1} & d_{j+1} & e_{j+1} & 0 & 0 & 0 \\ a_{j+2} & b_{j+2} & c_{j+2} & d_{j+2} & e_{j+2} & 0 & 0 \\ 0 & a_{(n+1)/2} & b_{(n+1)/2} & c_{(n+1)/2} & d_{(n+1)/2} & e_{(n+1)/2} & 0 \\ 0 & 0 & a_{n-j-1} & b_{n-j-1} & c_{n-j-1} & d_{n-j-1} & e_{n-j-1} \\ 0 & 0 & 0 & a_{n-j} & b_{n-j} & c_{n-j} & d_{n-j} \\ 0 & 0 & 0 & 0 & a_{n-j+1} & b_{n-j+1} & c_{n-j+1} \end{bmatrix} \quad \text{with 7 rows}$$

Writing more generally, if we write the first equation corresponding to the 3 point formula

$$\begin{bmatrix} b_j & 0 \\ 0 & b_{n-j+1} \end{bmatrix} \begin{bmatrix} z_j \\ z_{n-j+1} \end{bmatrix} + \begin{bmatrix} a_j & 0 \\ 0 & c_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j-1} \\ z_{n-j+2} \end{bmatrix} = \begin{bmatrix} d_j \\ d_{n-j+1} \end{bmatrix} - \begin{bmatrix} c_j & 0 \\ 0 & a_{n-j+1} \end{bmatrix} \begin{bmatrix} z_{j+1} \\ z_{n-j} \end{bmatrix}$$

as

$$\tilde{C}_{jj} \vec{z}_{jj} + \tilde{S}_{jj} \vec{z}_{jj-1} = \vec{b}_{jj} - \tilde{P}_{jj} \vec{z}_{jj+1} \quad \text{and defining} \quad KU = \frac{(m-1)}{2}$$

where \vec{z}_{jj} is understood to be the corresponding vector with length $2 KU$ (or $m-1$) defined as

$$(z_j, z_{j+1} \dots z_{j+(m-3)/2}, z_{n-j+1-(m-3)/2} \dots z_{n-j}, z_{n-j+1}) = (z_j, z_{j+1} \dots z_{j+KU-1}, z_{n-j+2-KU} \dots z_{n-j}, z_{n-j+1})$$

with \vec{b}_{jj} defined similarly so that $\tilde{C}_{jj}, \tilde{S}_{jj}, \tilde{P}_{jj}, \vec{b}_{jj}, \vec{z}_{jj}$ are defined (see Appendix) for jj every $j KU$ apart.

Substituting \tilde{A}_{jj} and \vec{v}_{jj} defined as:

$$\vec{z}_{jj-1} = \tilde{A}_{jj-1} \vec{z}_{jj} + \vec{v}_{jj-1}$$

results in the second equation as

$$(\tilde{C}_{jj} + \tilde{S}_{jj} \tilde{A}_{jj-1}) \vec{z}_{jj} + \tilde{S}_{jj} \vec{v}_{jj-1} = \vec{b}_{jj} - \tilde{P}_{jj} \vec{z}_{jj+1}$$

Using the definition of \tilde{A}_{jj} and \vec{v}_{jj} and the second equation we can recognize the recurrence relations:

$$\tilde{A}_{jj} = -(\tilde{C}_{jj} + \tilde{S}_{jj} \tilde{A}_{jj-1})^{-1} \tilde{P}_{jj}$$

$$\vec{v}_{jj} = (\tilde{C}_{jj} + \tilde{S}_{jj} \tilde{A}_{jj-1})^{-1} (\vec{b}_{jj} - \tilde{S}_{jj} \vec{v}_{jj-1})$$

which are solved every jj , reducing the number of equations by $(m-1)$ each iteration with

$\tilde{A}_0 = \begin{bmatrix} 0 & I_{(m-1)/2} \\ I_{(m-1)/2} & 0 \end{bmatrix}$ an $(m-1) \times (m-1)$ orthogonal matrix and $I_{(m-1)/2}$ the $(m-1)/2 \times (m-1)/2$ identity matrix.

At the center of the system matrix, if $p = \text{modulo}(n, m-1) = 0$, then $\vec{z}_{jj+1} = \tilde{A}_0 \vec{z}_{jj}$ (recognizing that the final $\tilde{A}_{j-1} = \{\tilde{A}_0\}^{-1}$)

so that the final inner values are given by

$$\vec{z}_{jj} = (\tilde{C}_{jj} + \tilde{P}_{jj} \tilde{A}_0 + \tilde{S}_{jj} \tilde{A}_{jj-1})^{-1} (\vec{b}_{jj} - \tilde{S}_{jj} \vec{v}_{jj-1}) \quad \text{for the last } 2*(m-1) \text{ values at } jj=n/2$$

More generally, if $p = \text{modulo}(n, m-1)$ and $p \neq 0$, we have $m-1+p$ rows left. The central rows can be written

$$\vec{z}_L = \{ z_j, z_{j+1}, \dots, z_{m-1+p} \}$$

We can then state that these central values are given by:

$$\vec{z}_L = [\tilde{C}_L + \tilde{P}_L \tilde{A}_0 + \tilde{I}_0^* S_{jj} \tilde{A}_{jj-1} \tilde{I}_0^{*T}]^{-1} \left\{ \vec{b}_L - \tilde{I}_0^* \tilde{S}_{jj} \vec{v}_{jj-1} \right\} \quad \text{or}$$

$$\vec{z}_L = [\tilde{C}_{jL} + \tilde{I}_0^* S_{jj} \tilde{A}_{jj-1} \tilde{I}_0^{*T}]^{-1} \left\{ \vec{b}_L - \tilde{I}_0^* \tilde{S}_{jj} \vec{v}_{jj-1} \right\}$$

where $\tilde{C}_{jL} = \tilde{C}_L + \tilde{P}_L \tilde{A}_0$ and \vec{b}_L consists of the last $2*KU+p$ inner values.

\tilde{I}_0^* is an $(m-1) \times (m-1+p)$ orthonormal matrix composed of the $(m-1) \times (m-1)$ identity matrix with $p = \text{modulo}(n, m-1)$ extra zero rows. Note we use the fact that $\tilde{I}_0^* \tilde{I}_0^{*T} = \tilde{I}_{m-1+p}$ that for the central rows

where :
$$\tilde{I}_0^* \vec{z}_L = \tilde{I}_0^* \{ z_j, z_{j+1}, \dots, z_{j+m-1+p} \}^T = \tilde{I}_0^* \vec{z}_j = \tilde{I}_0^* \{ z_j, z_{j+1}, \dots, z_{j+(m-3)/2}, 0, 0, \dots, 0, z_{n-j+1-(m-3)/2}, \dots, z_{n-j}, z_{n-j+1} \}^T$$

In summary, the forward algorithm consists of computing the matrix and vector every $(m-1)$ sets of rows with

$$\tilde{A}_{jj} = -[\tilde{C}_{jj} + \tilde{S}_{jj} \tilde{A}_{jj-1}]^{-1} \tilde{P}_{jj}$$

$$\vec{v}_{jj} = [\tilde{C}_{jj} + \tilde{S}_{jj} \tilde{A}_{jj-1}]^{-1} \left\{ \vec{b}_{jj} - \tilde{S}_{jj} \vec{v}_{jj-1} \right\}$$

for $n/(m-1)$ number of times. (integer division)

then computing the $m-1+p$ central values needing only \tilde{A}_{jj-1} and \vec{v}_{jj-1}

$$\vec{z}_L = [\tilde{C}_L + \tilde{P}_L \tilde{A}_0 + \tilde{I}_0^* S_{jj} \tilde{A}_{jj-1} \tilde{I}_0^{*T}]^{-1} \left\{ \vec{b}_L - \tilde{I}_0^* \tilde{S}_{jj} \vec{v}_{jj-1} \right\}$$

or

$$\vec{z}_L = [\tilde{C}_{jL} + \tilde{I}_0^* S_{jj} \tilde{A}_{jj-1} \tilde{I}_0^{*T}]^{-1} \left\{ \vec{b}_L - \tilde{I}_0^* \tilde{S}_{jj} \vec{v}_{jj-1} \right\}$$

where $\tilde{C}_{jL} = \tilde{C}_L + \tilde{P}_L \tilde{A}_0$ and \vec{b}_L consists of the last $2*KU+p$ inner values.

where \tilde{I}_0^* is an $(m-1) \times (m-1+p)$ matrix composed of the $(m-1) \times (m-1)$ identity matrix with $p = \text{modulo}(n, m-1)$ extra central zero rows, and \tilde{A}_0 is the $(m-1) \times (m-1)$ circular permutation matrix composed of the identity matrix from above.

Once the center values are known the stored matrices \tilde{A}_{jj} and vectors \vec{v}_{jj} are used for back substitution using $\vec{z}_{jj-1} = \tilde{A}_{jj-1} \vec{z}_{jj} + \vec{v}_{jj-1}$.

Reverse algorithm:

We can also solve the equations in reverse. Defining $\vec{z}_{jj+1} = \bar{A}_{jj+1} \vec{z}_{jj} + \bar{v}_{jj+1}$ then our equations are

$$\{\tilde{C}_{jj} + \tilde{P}_{jj} A_{jj+1}^{-}\} \vec{z}_{jj} + \tilde{P}_{jj} \vec{v}_{jj+1} = \vec{b}_{jj} - \tilde{S}_{jj} \vec{z}_{jj-1} \quad \text{leading to}$$

$$\bar{A}_{jj} = -\{\tilde{C}_{jj} + \tilde{P}_{jj} A_{jj+1}^{-}\}^{-1} \tilde{S}_{jj}$$

$$\bar{v}_{jj} = \{\tilde{C}_{jj} + \tilde{P}_{jj} A_{jj+1}^{-}\}^{-1} \{\vec{b}_{jj} - \tilde{P}_{jj} \vec{v}_{jj+1}\}$$

Instead of starting at $jj=0$, we start at $jj=(n-p)/2$, and calculate each decreasing jj starting with $A_{(n-p)/2+1}^{-}$ and $v_{(n-p)/2+1}$, which we will define shortly.

At the beginning and end, or edges, of the system matrix, $\vec{z}_{jj-1} = \bar{A}_0 \vec{z}_{jj}$ (recognizing that the final $\bar{A}_j = \{\bar{A}_0\}^{-1}$) so that the last $2*(m-1)$ values at $jj=1$ are solved for in terms of $jj=2$ by

$$\vec{z}_1 = \{\tilde{C}_1 + \tilde{S}_1 \bar{A}_0 + \tilde{P}_1 \bar{A}_2\}^{-1} \{\vec{b}_1 - \tilde{P}_1 \vec{v}_2\}$$

The 2 x 2 version is given below as an example:

$$\begin{bmatrix} z_1 \\ z_n \end{bmatrix} = \begin{bmatrix} b_1 & a_1 \\ c_n & b_n \end{bmatrix}^{-1} \left\{ \begin{bmatrix} d_1 \\ d_n \end{bmatrix} - \begin{bmatrix} c_1 & 0 \\ 0 & a_n \end{bmatrix} \begin{bmatrix} z_2 \\ z_{n-1} \end{bmatrix} \right\}$$

The rest of the values are then solved by back substitution with $\vec{z}_{jj+1} = \bar{A}_{jj+1} \vec{z}_{jj} + \bar{v}_{jj+1}$.

Here we have implicitly decided to start the iterative solution at $jj=(n-p)/2$. If $p = \text{modulo}(n, m-1) = 0$, then we have the 2KU x 2KU matrix:

$$\bar{A}_{(n/2+1)} = \begin{bmatrix} 0 & \tilde{I}_{KU} \\ \tilde{I}_{KU} & 0 \end{bmatrix}, \bar{v}_{(n/2+1)} = \vec{0} \quad \text{because} \quad \vec{z}_{n/2+1} = \tilde{A}_0 \vec{z}_{n/2}$$

If $p \neq 0$, we have p additional values of \vec{z}_{jj} to solve for, and the definitions of $A_{(n-p)/2+1}^{-}$ and $v_{(n-p)/2+1}$ are more complex. There are two cases, $p > KU$ or $p < KU$, with both reducing to the same solution at $p=KU$. Consider the central rows:

$$\vec{z}_p = \{ z_{(n-p)/2+1}, z_{(n-p)/2+2}, \dots, z_{(n-p)/2+p} \} \quad \text{a vector } p \text{ in length vs the definition of } \vec{z}_j \text{ at } j=(n-p)/2+1:$$

$$\vec{z}_{(n-p)/2+1} = (\vec{z}_{(n-p)/2+1}, \vec{z}_{(n-p)/2+2} \dots \vec{z}_{(n-p)/2+KU}, \vec{z}_{(n+p)/2+3-KU} \dots \vec{z}_{(n+p)/2+1}, \vec{z}_{(n+p)/2+2})$$

If $p > KU$, then vector \vec{z}_p is longer than each half of vector $\vec{z}_{(n-p)/2+1}$ so that there is a duplication of the middle $2KU-p$ rows.

If $p < KU$, vector \vec{z}_p is contained within each half of vector $\vec{z}_{(n-p)/2+1}$ and an additional $2KU-2p$ rows are required.

If $p=0$, the $2KU$ rows (and columns) are generated by $\bar{A}_{(n)/2+1} = \bar{A}_0$ given above.

The p rows are generated by the central p equations given by $\tilde{C}_p \vec{z}_p + \tilde{S}_p \vec{z}_{(n-p)/2} = \vec{b}_p$ where \vec{z}_p, \vec{b}_p consists of the middle p inner values and \tilde{C}_p, \tilde{S}_p are $p \times p$ and $p \times 2KU$ matrices.

Using the relationship between vector \vec{z}_p and vector $\vec{z}_{(n-p)/2+1}$, and $\vec{z}_{(n-p)/2+1} = \bar{A}_{(n-p)/2+1} \vec{z}_{(n-p)/2} + \bar{v}_{(n-p)/2+1}$, we can define $\bar{A}_{(n-p)/2+1}$ and $\bar{v}_{(n-p)/2+1}$.

If $p < KU$, the first p rows of $\bar{A}_{(n-p)/2+1}$ are given by the first p rows of $-C_p^{-1} S_p$ and the last p rows of $\bar{A}_{(n-p)/2+1}$ are given by the last p rows of $-C_p^{-1} S_p$. The center of the matrix is a $2KU-2p$ version of \bar{A}_0 .

If $p > KU$, then first KU rows of $\bar{A}_{(n-p)/2+1}$ are given by the first KU rows of $-C_p^{-1} S_p$ and the last KU rows of $\bar{A}_{(n-p)/2+1}$ are given by the last KU rows of $-C_p^{-1} S_p$, resulting in a duplication of the middle $2KU-p$ rows. $\bar{v}_{(n-p)/2+1}$ is similarly defined, using $C_p^{-1} b_p$ and $\bar{v}_{(n)/2}$.

Parallel algorithm:

Although the algorithms developed are iterative and inherently serial, we can solve both forward and back algorithms in parallel, theoretically cutting down the computation time.

Note that by definition $\vec{z}_{jj+1} = \bar{A}_{jj+1} \vec{z}_{jj} + \bar{v}_{jj+1}$

Now, recalling that $\vec{z}_{jj-1} = \tilde{A}_{jj-1} \vec{z}_{jj} + \tilde{v}_{jj-1}$ which is also $\vec{z}_{jj} = \tilde{A}_{jj} \vec{z}_{jj+1} + \tilde{v}_{jj}$, then inverting leads to $\vec{z}_{jj+1} = \tilde{A}_{jj}^{-1} \vec{z}_{jj} - \tilde{A}_{jj}^{-1} \tilde{v}_{jj}$

Note however despite that:

$$\tilde{A}_{jj}^{-1} \neq \bar{A}_{jj+1} \quad \text{and} \quad \tilde{A}_{jj}^{-1} \tilde{v}_{jj} \neq \bar{v}_{jj+1}.$$

We can use this lack of equality to solve the iteration equations simultaneously forward and backward, starting from the first and last set of z at the edges, $jj=1$ and also starting from the middle of the matrix at $kk=(n-p)/2$. Proceeding iteratively from either direction eventually we will be at some value $jj=kk+1$, and we can solve for the values of z there, then back substitute simultaneously in both directions to solve for the all the values. It is straightforward to show that at some value jj :

$$\vec{z}_{jj} = \left(\tilde{I} - \bar{A}_{jj} \tilde{A}_{jj-1} \right)^{-1} \left(\bar{A}_{jj} \bar{v}_{jj-1} + \tilde{v}_{jj} \right)$$

and

$$\vec{z}_{jj-1} = \left[\tilde{I} - A_{jj-1}^{-1} \bar{A}_{jj} \right]^{-1} \left\{ A_{jj-1}^{-1} \vec{v}_{jj} + \vec{v}_{jj-1} \right\}$$

at the common point if $A_{jj-1}^{-1} \neq \bar{A}_{jj}$. We can pick $jj=(n/4)$ so that each iterative series takes half as many steps as either the usual forward or backward algorithm. Since each iterative series is independent, the computation can be done in parallel.

Appendix: Definition of matrices

In general, an m-point equation, with m-odd, can be written:

in contrast with $\sum_{i=1}^n a_{ij} z_j = b_j$ letting i, j run from 1 to N

$$\sum_{i=1}^{1+2KU} AB(i, j) * z(1 + \text{mod}(N+i+j-2, N)) = b_j$$

where the AB matrix is m x N, with N the number of points, similar to the general LAPACK band matrix (which we shall call CD) (<https://www.netlib.org/lapack/lug/node124.html>) notation, again letting i, j run from 1 to N:

$CD(KU+1+i-j, j) = a_{ij}$ with $KU = (m-1)/2$ where the **columns** of A are the columns of CD and the diagonals of A are the rows of CD,

except that we allow wrapping the periodic coefficients and have the **rows** of A as the columns of AB and the diagonals of A are the rows of AB:

$$AB(2KU+2-\text{mod}(N+KU+1+i-j), i) = a_{ij} \text{ with } KU = (m-1)/2$$

However, letting i run from 1 to $1+2*KU$ (or 1 to m), with j from 1 to N, AB can efficiently be generated by

$$AB(i, j) = a_{ij}(j, 1 + \text{mod}(N+i+j-2-KU, N))$$

contrasted with the LAPACK “CD” form:

$$CD(i+KL, j) = a_{ij}(1 + \text{mod}(N+i+j-2-KU, N), j)$$

from which we can also derive a conversion formula:

$$CD(i+KL, j) = AB(m-i+1, 1 + \text{mod}(N+i+j+KU-m-1, N))$$

Note that in the non-periodic banded matrix, the coefficients $CD(i,j)=0$ when $i+j-(m+1)/2$ is < 1 or $> N$.

Then the m-point equation, with m-odd, can be written:

$$\tilde{C}_{jj}\vec{z}_{jj} + \tilde{S}_{jj}z_{jj-1} = \vec{b}_{jj} - \tilde{P}_{jj}z_{jj+1} \quad \text{and defining} \quad KU = \frac{(m-1)}{2}$$

where \vec{z}_{jj} is understood to be the corresponding vector with length $2KU$ (or $m-1$) defined as

$$(z_j, z_{j+1} \dots z_{j+(m-3)/2}, z_{n-j+1-(m-3)/2} \dots z_{n-j}, z_{n-j+1}) = (z_j, z_{j+1} \dots z_{j+KU-1}, z_{n-j+2-KU} \dots z_{n-j}, z_{n-j+1})$$

with \vec{b}_{jj} defined similarly so that $\tilde{C}_{jj}, \tilde{S}_{jj}, \tilde{P}_{jj}, \vec{b}_{jj}$ are defined below for jj every jKU apart.

With the above definition of $AB[i,j]$ we have the square $(i \times k)$ for each j matrices:

$$\tilde{C}_{jj} = \begin{cases} AB[KU+k-i+1, j+i-1] & \forall i, k \{1, 2 \dots KU\} \\ AB[KU+k-i+1, n-2*KU+i-j+1] & \forall i, k \{KU+1 \dots 2*KU\} \\ else \ 0 \end{cases}$$

$$\tilde{S}_{jj} = \begin{cases} AB[1+k-i, j+i-1] & \forall i, k \{1, 2 \dots KU\} \\ AB[2*KU+1+k-i, n-2*KU+i-j] & \forall i, k \{KU+1 \dots 2*KU\} \\ else \ 0 \end{cases}$$

$$\tilde{P}_{jj} = \begin{cases} AB[2*KU+1+k-i, j+i-1] & \forall i, k \{1, 2 \dots KU\} \\ AB[1+k-i, n-2*KU+i-j] & \forall i, k \{KU+1 \dots 2*KU\} \\ else \ 0 \end{cases}$$

For the forward algorithm, the last C_{jj} and P_{jj} are $(m-1+p) \times (m-1+p)$, in combination we define C_{jL} generally even if $p \neq 0$

$$\tilde{C}_{jL} = \tilde{C}_L + \tilde{P}_L \tilde{A}_0 = \begin{cases} AB[KU+1+k-i, j+i-1] & \forall i, k \{1, 2 \dots 2*KU+p\} \\ else \ 0 \end{cases}$$

if $p=0$, there are no extra rows:

$$\tilde{C}_{jL} = \tilde{C}_L + \tilde{P}_L \tilde{A}_0 = C_{N/(2KU)} + P_{N/(2KU)} \tilde{A}_0 \quad \text{using the above definitions at the last } j=(n-m+2)/2=(n+1)/2-KU$$

For the reverse algorithm, the middle p equations can be written in the following format:

$\tilde{C}_p \vec{z}_p + \tilde{S}_p z_{(n-p)/2} = \vec{b}_p$ where \vec{z}_p, \vec{b}_p consists of the last p inner values and \tilde{C}_p, \tilde{S}_p are the matrices given below with dimensions $p \times p$ and $p \times 2KU$.

$$\tilde{C}_p = \begin{cases} AB[KU+1+k-i, j+i-1] & \forall i, k \{1, 2 \dots p\} \\ else \ 0 \end{cases} \quad j=(N-p)/2+1$$

and

$$\tilde{S}_p = \begin{cases} AB[1+k-i, j+i-1] & \forall k \geq i \quad k: \{1, 2, \dots, KU\} \forall i: \{1, 2, \dots, p\} \\ AB[k+p-i+1, j+i-1] & \forall k: \{KU+1, \dots, 2*KU-p+i\} \forall i: \{1, 2, \dots, p\} \\ else \ 0 & j - (N-p)/2 + 1 \end{cases}$$

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