Notes on the Boundary Conditions in Finite-Difference Algorithms

C.D. Clark III

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1 Implicit Algorithms

Any implicit finite difference algorithm is based on getting a matrix equation of the form

$$\mathbb{A}v = b \tag{1}$$

where, $\mathbb{A}$ is a known matrix, b is a known vector, and v is the vector of unknowns to be solved for. For most common Finite-Difference methods, the matrix $\mathbb{A}$ is tridiagonal, and so only three elements of v appear in each equation. The vector of knowns, b, must be calculated, and this to typically involves three elements of the "current" solution. In other words, in general we usually have something like this:

$$\mathbb{A}v^{n+1} = \mathbb{C}v^{n} + d \tag{2}$$

where $\mathbb{C}$ is a known matrix that operates on the current solution and gives a vector of constants, and d is a vector of constants that do not depend on the current solution.

This matrix equation represents a system of equation. One equation in this system can be written

$$a^{L}{}_{i}v^{n+1}{}_{i-1} + b^{L}{}_{i}v^{n+1}{}_{i} + c^{L}{}_{i}v^{n+1}{}_{i+1} = a^{R}{}_{i}v^{n}{}_{i-1} + b^{R}{}_{i}v^{n}{}_{i} + c^{R}{}_{i}v^{n}{}_{i+1} + d_i \tag{3}$$

There are two "boundaries" that have to be considered here. When $i = 0$, 3, refers to v_{-1}, which does not exist. At $i = N-1$, v_N is referred to, which also does not exist. These two equation, $i = 0$ and $i = N-1$, have to be replaced with equations that do not refer to the non-existent elements of v. Actually, these two equation are just modified to only refer to actual elements of v. To write the modification, a second equation relating the non-existent element of v to the existing elements is required. This equation is called the “boundary condition”. The boundary condition used is determined by the physics.

1.1 Dirichlet Boundary Conditions

The simplest boundary condition to implement is the “sink”. In this case, the solution is required to be zero at the boundary, so for example if the element v_i did exist, it would be zero. In this case, the terms in 3 referring to v_{-1} and v_N can just be ignored. The $i = 0$ equation is then

$$b^L{}_0 v^{n+1}{}_0 + c^L{}_0 v^{n+1}{}_1 = b^R{}_0 v^n{}_0 + c^R{}_0 v^n{}_1 + d_0 \tag{4}$$

and the $i = N - 1$ equation is similar,

$$a^L{}_0 v^{n+1}{}_{N-2} + b^L{}_0 v^{n+1}{}_{N-1} = a^R{}_0 v^n{}_{N-2} + b^R{}_0 v^n{}_{N-1} + d_0 \tag{5}$$

However, in general, we could allow the boundary be specified as an arbitrary constant,

$$v\,(x_0) = f \tag{6}$$

In which case we have

$$a^L{}_0 f + b^L{}_0 v^{n+1}{}_0 + c^L{}_0 v^{n+1}{}_1 = a^R{}_0 f + b^R{}_0 v^n{}_0 + c^R{}_0 v^n{}_1 + d_0 \tag{7}$$

The first term on the LHS side here is a constant, so it must be moved over the right right hand side,

$$b^L{}_0 v^{n+1}{}_0 + c^L{}_0 v^{n+1}{}_1 = b^R{}_0 v^n{}_0 + c^R{}_0 v^n{}_1 + d_0 + a^R{}_0 f - a^L{}_0 f \tag{8}$$

If we define a d'_0 as

$$d'_0 = a^R{}_0 f - a^L{}_0 f \tag{9}$$

then we can write the $i = 0$ equation as

$$b^L{}_0 v^{n+1}{}_0 + c^L{}_0 v^{n+1}{}_1 = b^R{}_0 v^n{}_0 + c^R{}_0 v^n{}_1 + d_0 + d'_0 \tag{10}$$

For the $i = N - 1$ equation, we have

$$d'_{N-1} = c^R{}_{N-1} f - c^L{}_{N-2} f \tag{11}$$

$$a^L{}_{N-1} v^{n+1}{}_{N-2} + b^L{}_{N-1} v^{n+1}{}_{N-1} = a^R{}_{N-1} v^n{}_{N-2} + b^R{}_{N-1} v^n{}_{N-1} + d_{N-1} + d'_{N-1} \tag{12}$$

1.2 Nuemann Boundary Conditions

The other type of boundary condition that can be specified involves the derivative of v (with respect to x) at the boundary. This is the type of boundary condition is required to model surfaces where the material loses energy to the environment through convection, radiation, and evaporation. It is also the boundary condition used to model an insulator. In general, any boundary condition can be written as

$$\left.\frac{\partial v}{\partial x}\right|_{x=boundary} = f(v) \tag{13}$$

By finite differencing the derivative, we obtain a relationship for the non-existent element of x.

$$\frac{v_{i+1} - v_{i-1}}{x_{i+1} - x_{i-1}} = f(v_i) \tag{14}$$

Let us only consider the $i = 0$ case for now. Later, the $i = N - 1$ case can be derived in a very similar manner. For $i = 0$, equation 14 gives

$$v_{-1} = v_1 - \Delta x f(v_0) \tag{15}$$

For the RHS of 3, this can be incorporated directly,

$$a^R{}_0 v_{-1}{}^n + b^R{}_0 v_0{}^n + c^R{}_0 v_1{}^n + d_0 = a^R{}_0 \left[v^n{}_1 - \Delta x f(v^n{}_0)\right] + b^R{}_0 v_0{}^n + c^R{}_0 v_1{}^n + d_0 \tag{16}$$

For the LHS however, $f(v)$ needs to be evaluated at $v_0{}^{n+1}$, which isn't known. We approximate this by expanding $f(v)$ in a Taylor series, and only keeping the first two terms.

$$f(v_0{}^{n+1}) \approx f(v_0{}^n) + f'(v_0{}^n)\left(v_0{}^{n+1} - v_0{}^n\right) \tag{17}$$

Now the LHS of 3 can be written as

$$\begin{aligned} a^L{}_0 v_{-1}{}^{n+1} + b^L{}_0 v_0{}^{n+1} + c^L{}_0 v_1{}^{n+1} &= a^L{}_0 \left[v_1{}^{n+1} - \Delta x\left(f(v_0{}^n) + f'(v_0{}^n)\left(v_0{}^{n+1} - v_0{}^n\right)\right)\right] \\ &\quad + b^L{}_0 v_0{}^{n+1} + c^L{}_0 v_1{}^{n+1} \end{aligned} \tag{18}$$

Note that any terms that are constant (i.e. do not contain a v^{n+1}) must be moved over to the RHS, so after some rearranging,

$$LHS : \left[b^L{}_0 - a^L{}_0 \Delta x f'(v_0{}^n)\right] v_0{}^{n+1} + \left[c^L{}_0 + a^L{}_0\right] v_1{}^{n+1} \tag{19}$$

$$\begin{aligned} RHS :\ & b^R{}_0 v_0{}^n + c^R{}_0 v_1{}^n + d_0 \\ & + \left[-a^L{}_0 \Delta x f'(v_0{}^n) v^n{}_0 + a^R{}_0 v_1{}^n - a^R{}_0 \Delta x f(v_0{}^n) + a^L{}_0 \Delta x f(v_0{}^n)\right] \end{aligned} \tag{20}$$

Comparing these to 4, we see that in fact they just contain 4 plus some extra terms. Therefore, in general, we can *assume* that we have a sink boundary condition when we create the representation for the first and last equations, and then add an arbitrary boundary condition on by adding on to the right terms. All the extra information we need is the boundary condition function and its derivative with respect to v.

Let

$$\begin{aligned} b'^{L}{}_{0} &\equiv -a^{L}{}_{0}\Delta x f'(v_0{}^{n}) && (21)\\ c'^{L}{}_{0} &\equiv \quad a^{L}{}_{0} && (22)\\ b'^{R}{}_{0} &\equiv -a^{L}{}_{0}\Delta x f'(v_0{}^{n}) && (23)\\ c'^{R}{}_{0} &\equiv \quad a^{R}{}_{0} && (24)\\ d'_{0} &\equiv \quad a^{L}{}_{0}\Delta x f(v_0{}^{n}) - a^{R}{}_{0}\Delta x f(v_0{}^{n}) && (25) \end{aligned}$$

Then we can write the boundary equation as

$$\left(b^{L}{}_{0} + b'^{L}{}_{0}\right) v^{n+1}{}_{0} + \left(c^{L}{}_{0} + c'^{L}{}_{0}\right) v^{n+1}{}_{1} = \left(b^{R}{}_{0} + b'^{R}{}_{0}\right) v^{n}{}_{0} + \left(c^{R}{}_{0} + c'^{R}{}_{0}\right) v^{n}{}_{1} + d_0 + d'_{0} \tag{26}$$

For the other boundary, $i = N - 1$, equation 3 gives

$$v_N = v_{N-2} + \Delta x f(v_0). \tag{27}$$

Again, the boundary condition can be incorporated directly into the RHS, but a Taylor Series approximation must be used for the LHS. The left and right sides will look like this

$$\begin{aligned} LHS\ &: a^{L}{}_{N-1} v_{N-2}{}^{n+1} + b^{L}{}_{N-1} v_{N-1}{}^{n+1} \\ &\quad + \left[c^{L}{}_{N-1} v_{N-2}{}^{n+1} + c^{L}{}_{N-1}\Delta x f(v_{N-1}{}^{n}) + c^{L}{}_{N-1}\Delta x f'(v_{N-1}{}^{n})\left(v_{N-1}{}^{n+1} - v_{N-1}{}^{n}\right)\right] \\ RHS\ &: a^{R}{}_{N-1} v_{N-2}{}^{n} + b^{R}{}_{N-1} v_{N-1}{}^{n} + d_{N-1} \\ &\quad + \left[c^{R}{}_{N-1} v_{N-2}{}^{n} + c^{R}{}_{N-1}\Delta x f(v_{N-1}{}^{n})\right] \end{aligned}$$

and then we have to move the constant terms from the LHS to the RHS

$$\begin{aligned} LHS\ &: a^{L}{}_{N-1} v_{N-2}{}^{n+1} + b^{L}{}_{N-1} v_{N-1}{}^{n+1} \\ &\quad + \left[c^{L}{}_{N-1} v_{N-2}{}^{n+1} + c^{L}{}_{N-1}\Delta x f'(v_{N-1}{}^{n}) v_{N-1}{}^{n+1}\right] && (28)\\ RHS\ &: a^{R}{}_{N-1} v_{N-2}{}^{n} + b^{R}{}_{N-1} v_{N-1}{}^{n} + d_{N-1} \\ &\quad + \left[c^{R}{}_{N-1} v_{N-2}{}^{n} + c^{R}{}_{N-1}\Delta x f(v_{N-1}{}^{n}) - c^{L}{}_{N-1}\Delta x f(v_{N-1}{}^{n}) + c^{L}{}_{N-1}\Delta x f'(v_{N-1}{}^{n}) v_{N-1}{}^{n}\right] && (29) \end{aligned}$$

Now, defining a set of prime constants again,

$$
\begin{aligned}
a'^{L}_{N-1} &\equiv c^{L}_{N-1} && (30)\\
b'^{L}_{N-1} &\equiv c^{L}_{N-1}\Delta x f'({\nu_0}^{n}) && (31)\\
a'^{R}_{N-1} &\equiv c^{R}_{N-1} && (32)\\
b'^{R}_{N-1} &\equiv c^{L}_{N-1}\Delta x f'({\nu_0}^{n}) && (33)\\
d'_{N-1} &\equiv c^{R}_{N-1}\Delta x f({\nu_{N-1}}^{n}) - c^{L}_{N-1}\Delta x f({\nu_{N-1}}^{n}) && (34)
\end{aligned}
$$

Then we can write the boundary equation as

$$
\begin{aligned}
&\left(a^{L}_{N-1} + a'^{L}_{N-1}\right)\nu^{n+1}_{N-2} + \left(b^{L}_{N-1} + b'^{L}_{N-1}\right)\nu^{n+1}_{N-1}\\
&= \left(a^{R}_{N-1} + a'^{R}_{N-1}\right)\nu^{n}_{N-2} + \left(b^{R}_{N-1} + b'^{R}_{N-1}\right)\nu^{n}_{N-1} + d_{N-1} + d'_{N-1} \qquad (35)
\end{aligned}
$$

So, we now have a general, concise method for implementing any type of Nuemann boundary condition. Note that, while in general the method relies on an approximation involving the Taylor Series expansion of the boundary condition function, it gives the same equations as directly implementing a boundary condition that is linear in ν. Meaning, the boundary condition used to model energy loss due surface convection,

$$
\kappa \left.\frac{\partial \nu}{\partial x}\right|_{x=0} = h_e\left(\nu - \nu_\infty\right) \qquad (36)
$$

can be directly implemented without the use of a Taylor Series expansion, because there are no non-linear terms. However, doing so leads to the exact same equations as 19, 20, 28, and 29 with $f({\nu_i}^{n}) = \frac{h_e}{\kappa}\left({\nu_i}^{n} - \nu_\infty\right)$ and $f'({\nu_i}^{n}) = \frac{h_e}{\kappa}$. The same is true for the insulating boundary conditions. Therefore, there is no reason to implement linear boundary conditions separatly, this general method will give the exact same results.

1.3 Time-Dependent Boundary Conditions

If the boundary condition is time dependent, for example if the ambient temperature is a function of time, then the boundary conditions will be

$$
\nu\left(x_0\right) = f(t) \qquad (37)
$$

or

$$\left.\frac{\partial v}{\partial x}\right|_{x=boundary} = f(v,t) \tag{38}$$

, then the primed coefficients need to be updated. Any factors of f or f' that start out on the left hand side should be evaluated at the next timestep. So, for the sink boundary condition, we have

$$d'_0 = a^R{}_0 f(t) - a^L{}_0 f(t+\Delta t) \tag{39}$$

and

$$d'_{N-1} = c^R{}_{N-1} f(t) - c^L{}_{N-2} f(t+\Delta t) \tag{40}$$

For the heat flux boundary conditions we have

$$b'^L{}_0 \equiv -a^L{}_0 \Delta x f'(v_0{}^n, t+\Delta t) \tag{41}$$
$$c'^L{}_0 \equiv \quad a^L{}_0 \tag{42}$$
$$b'^R{}_0 \equiv -a^L{}_0 \Delta x f'(v_0{}^n, t+\Delta t) \tag{43}$$
$$c'^R{}_0 \equiv \quad a^R{}_0 \tag{44}$$
$$d'{}_0 \equiv \quad a^L{}_0 \Delta x f(v_0{}^n, t+\Delta t) - a^R{}_0 \Delta x f(v_0{}^n, t) \tag{45}$$

and

$$a'^L{}_{N-1} \equiv c^L{}_{N-1} \tag{46}$$
$$b'^L{}_{N-1} \equiv c^L{}_{N-1} \Delta x f'(v_0{}^n, t+\Delta t) \tag{47}$$
$$a'^R{}_{N-1} \equiv c^R{}_{N-1} \tag{48}$$
$$b'^R{}_{N-1} \equiv c^L{}_{N-1} \Delta x f'(v_0{}^n, t+\Delta t) \tag{49}$$
$$d'{}_{N-1} \equiv c^R{}_{N-1} \Delta x f(v_{N-1}{}^n, t) - c^L{}_{N-1} \Delta x f(v_{N-1}{}^n, t+\Delta t) \tag{50}$$

If the boundary conditions are constant in time, these primed coefficients reduce to the same as before. So the only terms that must be evaluated for the current and next time time are the d''s. In fact, all of the primed coefficients can be evaluated for the next time step *except* the d''s.

1.4 Heat Flux Boundaries

For the heat equation, the heat flux at the boundary is usually specified, rather than the temperature derivative.

$$k\frac{\mathrm{d}v}{\mathrm{d}x} = f(x,t) \tag{51}$$

If the heat flux, $k\frac{\mathrm{d}v}{\mathrm{d}x}$ is positive, it means that thermal energy flows to the "left". If it is negative, the thermal energy flows to the "right". Because of this, there is a sign difference between the upper and lower boundaries from the point of view of energy leaving the system or entering the system. At the lower boundary, a positive heat flux corresponds to energy leaving the system as heat,

$$k\frac{\mathrm{d}v}{\mathrm{d}x} = f(x,t). \tag{52}$$

At the upper boundary, a negative heat flux corresponds to energy leaving the system as heat,

$$k\frac{\mathrm{d}v}{\mathrm{d}x} = -f(x,t). \tag{53}$$

If we adopt the convention that a positive function corresponds to heat entering the system, regardless of which boundary it is applied to, then we need to account for this sign difference in the derivation of our primed coefficients above. This leads to all references of f and f' being replaced with $-f$ and $-f'$ for the $i = 0$ primed coefficients.