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WEST++

Allowed forms of PDEs and boundary conditions in WEST++ that can be solved using Orthogonal Collocation with matrices

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In this note, we describe the general form of the PDEs and boundary conditions which can be implemented and solved within WEST++ using orthogonal collocation, combined with matrices. Details of the orthogonal collocation method, and the use of corresponding matrices, have been presented in [1].

1 General form of the PDEs

Currently within WEST++, it is possible to handle second order one-dimensional PDEs defined over a certain spatial domain Ω. For simplicity, we consider a single PDE for the present discussion. Let $X(z,t)$ denote the physical quantity for which the PDE is written in the space co-ordinate z and time t. Then the following general form of the PDE can be discretized and solved within WEST++:

$$\frac{\partial X(z,t)}{\partial t} = A(X(z,t),z,t)\,\frac{\partial^2 X(z,t)}{\partial z^2} + B(X(z,t),z,t)\,\frac{\partial X(z,t)}{\partial z} + C(X(z,t),z,t) + D(z,t) + E\,. \tag{1}$$

As can be seen above, the PDE must be linear in the partial derivatives: that is, powers of derivatives higher than one are not allowed. But these linear derivatives can have non-linear coefficients, however: $\{A(X(z,t),z,t),\ B(X(z,t),z,t),\ C(X(z,t),z,t)\}$ can be any (non-linear) functions of $(X(z,t),z,t)$. $D(z,t)$ is any function of (z,t), and in particular can depend on only one of them. E is a constant independent of both z and t. We can write the above equation in a more compact form as follows, by writing the right hand side simply as a function F:

$$\frac{\partial X(z,t)}{\partial t} = F\left(\frac{\partial^2 X(z,t)}{\partial z^2}, \frac{\partial X(z,t)}{\partial z}, X(z,t), z, t\right)\,. \tag{2}$$

Now, instead of the single PDE (2) being defined over the entire domain Ω, the PDE could have different right hand sides over n different sub-domains $\{\Omega_1, \Omega_2, \ldots, \Omega_n\}$. We could therefore have:

$$\frac{\partial X(z,t)}{\partial t} = \begin{cases} F_1(\frac{\partial^2 X(z,t)}{\partial z^2}, \frac{\partial X(z,t)}{\partial z}, X(z,t), z, t), & z \in \ \Omega_1, \\ F_2(\frac{\partial^2 X(z,t)}{\partial z^2}, \frac{\partial X(z,t)}{\partial z}, X(z,t), z, t), & z \in \ \Omega_2, \\ \vdots & \\ F_n(\frac{\partial^2 X(z,t)}{\partial z^2}, \frac{\partial X(z,t)}{\partial z}, X(z,t), z, t) & z \in \ \Omega_n. \end{cases} \tag{3}$$

1.1 General form of the boundary conditions

In order to solve a given PDE, appropriate boundary conditions need to be specified. For second order PDEs, we need two boundary conditions. These boundary conditions are incorporated into the solution procedure within WEST++, along with the (linear) finite element boundary conditions, in matrix form.

As detailed in [1], we define U, a vector of the unknown quantity $X(z,t)$ evaluated at the (N_E+1) nodes (where N_E is the number of finite elements chosen for the discretization of the PDE) by $U \equiv (u_1, u_2, \ldots, u_{(N_E+1)})$. Similarly we define a vector $W \equiv (w_1, w_2, \ldots, w_{N_C})$, which is a vector of $X(z,t)$ evaluated at the N_C interior collocation points. In the matrix method, we can relate U and W through a matrix equation, whose general form is given by:

$$P\,W = Q\,U + C\,. \tag{4}$$

The elements of the first and last rows of the matrices (P,Q,C) are obtained from the boundary conditions specified for the PDE. The elements in the intermediate rows of (P,Q) are extracted from the element boundary conditions. The intermediate rows of C will contain zeroes.

Eq.(4) is solved for U:

$$U = Q^{-1}\, P\, W - Q^{-1}\, C\,. \tag{5}$$

Defining $R \equiv Q^{-1}\, P$ and $S \equiv Q^{-1}\, C$, we have:

$$U = R W - S. \tag{6}$$

Finding U from the above matrix equation, we can substitute for the $\{u_i\}$ in the DAE, and go on to solve it using an integrator. In order to use this method of matrices, however, it is obvious that the boundary conditions must be linear.

The most general linear form of the boundary conditions at either of the two boundaries z_B, which we denote by $\{z_{B_1},\, z_{B_2}\}$, is therefore given by:

$$\begin{aligned} a_1(z,t)\, X(z=z_{B_1},t) + b_1(z,t)\, \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=z_{B_1}} + c_1(z,t) + d_1 &= 0\;; \\ a_2(z,t)\, X(z=z_{B_2},t) + b_2(z,t)\, \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=z_{B_2}} + c_2(z,t) + d_2 &= 0\,. \end{aligned} \tag{7}$$

Here $\{a_1(z,t),\ a_2(z,t),\ b_1(z,t),\ b_2(z,t),\ c_1(z,t),\ c_2(z,t)\}$ are any functions of (z,t), and in particular can depend on only one of them. $\{d_1, d_2\}$ are constants independent of (z,t). Different kinds of boundary conditions are obtained by setting one or more of these coefficients to zero.

If there are non-linear functions in the boundary conditions, for example:

$$\left.\frac{\partial X(z,t)}{\partial z}\right|_{z=z_B} = G(X(z=z_B,t), z_B, t)\,, \tag{8}$$

where $G(X(z,t),z,t)$ is a non-linear function of $X(z,t)$, then, as a first approximation, the function can be linearized (by retaining the first term in its Taylor expansion). However, this may not be such a good approximation always. In order to determine the usefulness of Taylor expanding $G(X,z,t)$, it is a good idea to plot the function $G(X)$ and $G_T(X)$, the first term in its Taylor series, *vs.* X, treating (z,t) as fixed parameters. One can then accept or reject this simple linearization procedure, depending on how well both curves agree.

If Taylor expansion indeed proves unsatisfactory, it might be a better idea to select a suitable piecewise-linear approximation scheme to render $G(X)$ as a curve made up of several polygons. Therefore, if there are m such polygons corresponding to m linear segments $\{L_i\}$, we have:

$$G(X) = \begin{cases} c_1\, X + d_1, & X \in\ L_1, \\ c_2\, X + d_2, & X \in\ L_2, \\ \vdots & \\ c_m\, X + d_m, & X \in\ L_m. \end{cases} \tag{9}$$

where $\{c_1, c_2, \ldots, c_m\}$ and $\{d_1, d_2, \ldots d_m\}$ are all constants. In this way, the constraint of linear boundary conditions can still be maintained, and the matrix method can be used.

2 Specification of PDEs and boundary conditions in MSL-USER

The PDEs can be coded in MSL-USER directly in the form presented in Eqns.(1, 3), and the boundary conditions in Eq.(7) above. As an example, consider the two test case PDEs discussed in [1], which describe batch and continuous sedimentation of suspended solids in a 1-D clarifier.

The PDE describing the concentration of suspended solids during batch sedimentation in a 1-D clarifier has a form similar to that in Eq.(1), and is defined over the domain $[0, L]$:

$$\frac{\partial X(z,t)}{\partial t} = - \left((1 - n\, X(z,t))\, v_0\, e^{-n\, X(z,t)} \right) \frac{\partial X(z,t)}{\partial z} + D_0 \frac{\partial^2 X(z,t)}{\partial z^2}. \tag{10}$$

where $\{v_0, n, D_0\}$ are constants. This can be coded directly as it is, in MSL-USER.

The corresponding boundary conditions at the boundaries $(z = 0, z = L)$ are given by:

$$\begin{aligned} v_o e^{-n\, X(z=0,t)} - D_0 \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=0} &= 0 \\ v_o e^{-n\, X(z=L,t)} - D_0 \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=L} &= 0. \end{aligned} \tag{11}$$

These nonlinear boundary conditions are linearized to a first approximation, by replacing the exponential functions by 1, the first term in their Taylor expansions. We then have:

$$\begin{aligned} v_o - D_0 \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=0} &= 0 \\ v_o - D_0 \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=L} &= 0. \end{aligned} \tag{12}$$

In this form, the boundary conditions can be coded directly as they are given above.

As a second example, we consider the PDE for continuous sedimentation in a 1-D clarifier, to illustrate the form of the PDE in Eq.(2). We consider the case when the effluent overflows. The domain $[0, L]$ is divided into three sub-domains, with corresponding PDEs. These are given by:

1. for $\{\, 0 \;\le\; z \;\le\; z_f - \sigma \,\}$:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= - \left[(\, 1 - n\, X(z,t) \,) \;\; v_0 \;\; e^{-n\, X(z,t)} + q_1(t) \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad + D_0 \frac{\partial^2 X(z,t)}{\partial z^2}\,; \end{aligned} \tag{13}$$

2. for $\{\, z_f - \sigma \;<\; z \;<\; z_f + \sigma \,\}$:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= - \left[(\, 1 - n\, X(z,t) \,) \;\; v_0 \;\; e^{-n\, X(z,t)} + q_2(t) \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad + X_f(t)\;\; q_2(t)\, \frac{1}{2\,\sigma} \\ &\quad + D_0 \frac{\partial^2 X(z,t)}{\partial z^2}\,; \end{aligned} \tag{14}$$

3. for $\{\, z_f + \sigma \;\le\; z \;\le\; L \,\}$:

$$\begin{aligned} \frac{\partial X(z,t)}{\partial t} &= - \left[(\, 1 - n\, X(z,t) \,) \;\; v_0 \;\; e^{-n\, X(z,t)} + q_1(t) \right] \frac{\partial X(z,t)}{\partial z} \\ &\quad + D_0 \frac{\partial^2 X(z,t)}{\partial z^2}\,. \end{aligned} \tag{15}$$

In the above, $\{q_1(t), q_2(t), X_f(t)\}$ are functions only of time, or they can be constants. $\{z_f, \sigma\}$ are parameters which define the three subdomains.

The PDE can also be specified in MSL-USER directly as above, by defining it as a set of three PDEs.

As for boundary conditions, they can also be specified in their original form:

$$\begin{aligned} \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=0} &= 0 \\ \left.\frac{\partial X(z,t)}{\partial z}\right|_{z=L} &= 0. \end{aligned} \tag{16}$$

References

[1] Indrani A.V., *WEST++: Transformation of a given PDE to a DAE using the Orthogonal Collocation Method on Finite Elements*, BIOMATH Technical Report (1998).