Appendix A. Cubic Spline

We can write the piece-wise continuous function for cubic spline in the following form:

$$f(x_k \le x \le x_{k+1}) = \frac{f(x_k)(x-x_{k+1})}{(x_k - x_{k+1})} + \frac{f(x_{k+1})(x-x_k)}{(x_{k+1}-x_k)} + [a_k \frac{(x-x_k)}{(x_{k+1}-x_k)} + b_k]\frac{(x-x_k)(x-x_{k+1})}{(x_{k+1}-x_k)^2} \quad \text{(A.1)}$$

The constants $\{a_k, b_k, \text{for } k = 1 \to n-1\}$ are chosen such that the matching conditions for cubic spline can be fulfilled, i.e.,

$$\left.\frac{df(x_{k-1} \le x \le x_k)}{dx}\right|_{x=x_k} = \left.\frac{df(x_k \le x \le x_{k+1})}{dx}\right|_{x=x_k}$$

and

$$\left.\frac{d^2 f(x_{k-1} \le x \le x_k)}{dx^2}\right|_{x=x_k} = \left.\frac{d^2 f(x_k \le x \le x_{k+1})}{dx^2}\right|_{x=x_k}$$

One can obtain the following two types of recursion formula:

$$f'(x_{k-1}) + f'(x_k)[2 + 2\frac{h_{k-1}}{h_k}] + f'(x_{k+1})\frac{h_{k-1}}{h_k} = 3f_0'(x_{k-1}) + 3f_0'(x_k)(\frac{h_{k-1}}{h_k}) \quad \text{(A.2)}$$

$$f''(x_{k-1}) + f''(x_k)[2 + 2\frac{h_k}{h_{k-1}}] + f''(x_{k+1})\frac{h_k}{h_{k-1}} = \frac{6}{h_{k-1}}[f_0'(x_k) - f_0'(x_{k-1})] \quad \text{(A.3)}$$

where $f_0'(x_k) = [f(x_{k+1}) - f(x_k)]/[x_{k+1} - x_k]$ and $h_k = x_{k+1} - x_k$.

As we can see from equations (A.2) and (A.3), the coefficients on the left-hand side depend only on the distribution of grids. For a given tabulate data set: $\{(x_k, f(x_k)), \text{for } k = 1 \to n\}$, we can solve equation (A.2) or (A.3), and evaluate the first and the second derivatives $f'(x_k)$ and $f''(x_k)$ at each grid x_k, as well as the constants $\{a_k, b_k, \text{for } k = 1 \to n-1\}$, based on given boundary conditions at x_1 and x_n. We can also evaluate the integration value, i.e., the area under the cubic-spline curve, $Area = \int_{x_1}^{x_n} f(x)dx$. This integration value is useful in kinetic plasma simulation to determine mass density, charge density, current density, and thermal pressure at each grid point.

Exercise A.1

Verify Equation (A.2) and Equation (A.3)

Verifying Equation (A.2)

Let

$$f(x_1 \le x \le x_2) = f_1 \frac{x - x_2}{x_1 - x_2} + f_2 \frac{x - x_1}{x_2 - x_1} + (x - x_1)(x - x_2)(ax + b) \tag{1}$$

where $f_1 = f(x_1)$ and $f_2 = f(x_2)$. To express the undetermined constants, a and b, in terms of the first derivative of $f(x)$ at $x = x_1$ and $x = x_2$, we take derivative of Eq. (1). It yields

$$f'(x_1 \le x \le x_2) = f_2 \frac{f_2 - f_1}{x_2 - x_1} + [(x - x_1) + (x - x_2)](ax + b) + (x - x_1)(x - x_2)a \tag{2}$$

Let $f_1' = f'(x_1)$ and $f_2' = f'(x_2)$. It yields

$$f_1' = f_2 \frac{f_2 - f_1}{x_2 - x_1} + (x_1 - x_2)(ax_1 + b) \tag{3}$$

and

$$f_2' = f_2 \frac{f_2 - f_1}{x_2 - x_1} + (x_2 - x_1)(ax_2 + b) \tag{4}$$

Solving Eqs. (3) and (4) for the unknown constants, a and b, it yields

$$a = \frac{f_1' + f_2'}{(x_2 - x_1)^2} - 2\frac{f_2 - f_1}{(x_2 - x_1)^3} \tag{5}$$

$$b = \frac{1}{2}\frac{f_2' - f_1'}{x_2 - x_1} - \frac{1}{2}\frac{f_1' + f_2'}{(x_2 - x_1)^2}(x_2 + x_1) + \frac{f_2 - f_1}{(x_2 - x_1)^3}(x_2 + x_1) \tag{6}$$

Substituting Eqs. (5) and (6) into Eqs. (3) and (4) to eliminate a and b, it yields

$$\begin{aligned} f(x_1 \le x \le x_2) &= f_1 \frac{x - x_2}{x_1 - x_2} + f_2 \frac{x - x_1}{x_2 - x_1} \\ &+ \frac{(x - x_1)(x - x_2)}{(x_2 - x_1)^2}\{(x - x_2)f_1' + (x - x_1)f_2' - \frac{f_2 - f_1}{x_2 - x_1}[(x - x_1) + (x - x_2)]\} \end{aligned} \tag{7}$$

Thus,

$$\begin{aligned} f'(x_1 \le x \le x_2) &= \frac{f_2 - f_1}{x_2 - x_1} + \frac{(x - x_1)(x - x_2)}{(x_2 - x_1)^2}(f_1' + f_2' - 2\frac{f_2 - f_1}{x_2 - x_1}) \\ &+ \frac{[(x - x_1) + (x - x_2)]}{(x_2 - x_1)^2}\{(x - x_2)f_1' + (x - x_1)f_2' - \frac{f_2 - f_1}{x_2 - x_1}[(x - x_1) + (x - x_2)]\} \end{aligned} \tag{8}$$

and

$$\begin{aligned} f''(x_1 \le x \le x_2) &= 2\frac{[(x - x_1) + (x - x_2)]}{(x_2 - x_1)^2}(f_1' + f_2' - 2\frac{f_2 - f_1}{x_2 - x_1}) \\ &+ \frac{2}{(x_2 - x_1)^2}\{(x - x_2)f_1' + (x - x_1)f_2' - \frac{f_2 - f_1}{x_2 - x_1}[(x - x_1) + (x - x_2)]\} \end{aligned} \tag{9}$$

Eq. (9) can be written as

$$f''(x_1 \le x \le x_2) = \frac{2}{(x_2 - x_1)^2}\{ f_1'[2(x-x_2)+(x-x_1)] + f_2'[2(x-x_1)+(x-x_2)] - 3\frac{f_2 - f_1}{x_2 - x_1}[(x-x_1)+(x-x_2)]\} \tag{10}$$

Let $f_1'' = f''(x_1)$ and $f_2'' = f''(x_2)$. Eq. (10) yields

$$f_1'' = \frac{-4 f_1' - 2 f_2'}{x_2 - x_1} + 6\frac{f_2 - f_1}{(x_2 - x_1)^2} \tag{11}$$

$$f_2'' = \frac{2 f_1' + 4 f_2'}{x_2 - x_1} - 6\frac{f_2 - f_1}{(x_2 - x_1)^2} \tag{12}$$

Likewise, for

$$f(x_0 \le x \le x_1) = f_0\frac{x - x_1}{x_0 - x_1} + f_1\frac{x - x_0}{x_1 - x_0} + \frac{(x-x_0)(x-x_1)}{(x_1 - x_0)^2}\{(x-x_1)f_0' + (x-x_0)f_1' - \frac{f_1 - f_0}{x_1 - x_0}[(x-x_0)+(x-x_1)]\}$$

it yields

$$f_0'' = \frac{-4 f_0' - 2 f_1'}{x_1 - x_0} + 6\frac{f_1 - f_0}{(x_1 - x_0)^2} \tag{13}$$

$$f_1'' = \frac{2 f_0' + 4 f_1'}{x_1 - x_0} - 6\frac{f_1 - f_0}{(x_1 - x_0)^2} \tag{14}$$

Eqs. (11) and (14) yields

$$\frac{f_0'}{x_1 - x_0} + 2\left(\frac{1}{x_2 - x_1} + \frac{1}{x_1 - x_0}\right) f_1' + \frac{f_2'}{x_2 - x_1} = 3\left[\frac{f_1 - f_0}{(x_1 - x_0)^2} + \frac{f_2 - f_1}{(x_2 - x_1)^2}\right] \tag{15}$$

Let $h_k = x_{k+1} - x_k$ and $(f_0')_k = (f_{k+1} - f_k)/(x_{k+1} - x_k)$. Eq. (15) yields

$$\frac{1}{h_{k-1}} f_{k-1}' + 2\left(\frac{1}{h_k} + \frac{1}{h_{k-1}}\right) f_k' + \frac{1}{h_k} f_{k+1}' = 3\left[\frac{(f_0')_{k-1}}{h_{k-1}} + \frac{(f_0')_k}{h_k}\right] \tag{16}$$

or

$$f_{k-1}' + 2\left(\frac{h_{k-1}}{h_k} + 1\right) f_k' + \frac{h_{k-1}}{h_k} f_{k+1}' = 3\left[(f_0')_{k-1} + \frac{h_{k-1}}{h_k}(f_0')_k\right] \tag{17}$$

Case 1:

Step 1: Determine $\{ f'(x_k), \text{for } k = 2 \to n-1 \}$ from a tabulate data set $\{ (x_k, f(x_k)), \text{for } k = 1 \to n \}$ with fixed boundary conditions of f' at $x = x_1$ and $x = x_n$.

Given $f'(x_1)$ and $f'(x_n)$, equation (A.2) can be rewritten as

$$
\begin{aligned}
& f'(x_k)B_k + f'(x_{k+1})C_k = 3f_0'(x_{k-1}) + 3f_0'(x_k)C_k - f'(x_{k-1}) && \text{for } k = 2 \\
& f'(x_{k-1}) + f'(x_k)B_k + f'(x_{k+1})C_k = 3f_0'(x_{k-1}) + 3f_0'(x_k)C_k && \text{for } k = 3 \to n-2 \\
& f'(x_{k-1}) + f'(x_k)B_k = 3f_0'(x_{k-1}) + 3f_0'(x_k)C_k - f'(x_{k+1})C_k && \text{for } k = n-1
\end{aligned}
\tag{A.4}
$$

or

$$
\begin{pmatrix}
B_2 & C_2 & 0 & \cdots & 0 \\
1 & B_3 & C_3 & \ddots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & 1 & B_{n-2} & C_{n-2} \\
0 & \cdots & 0 & 1 & B_{n-1}
\end{pmatrix}
\begin{pmatrix}
f'(x_2) \\ f'(x_3) \\ \vdots \\ f'(x_{n-2}) \\ f'(x_{n-1})
\end{pmatrix}
=
\begin{pmatrix}
3f_0'(x_1) + 3f_0'(x_2)C_2 - f'(x_1) \\
3f_0'(x_2) + 3f_0'(x_3)C_3 \\
\vdots \\
3f_0'(x_{n-3}) + 3f_0'(x_{n-2})C_{n-2} \\
3f_0'(x_{n-2}) + 3f_0'(x_{n-1})C_{n-1} - f'(x_n)C_{n-1}
\end{pmatrix}
\tag{A.4'}
$$

where $B_k = (2 + 2\dfrac{h_{k-1}}{h_k})$, $C_k = \dfrac{h_{k-1}}{h_k}$, for $k = 2 \to n-1$

Equation (A.4) or (A.4') is the governing equation of $\{ f'(x_k), \text{for } k = 2 \to n-1 \}$ with a fixed boundary condition of f' at $x = x_1$ and $x = x_n$.

Step 2: Evaluate $\{ f''(x_k), \text{for } k = 1 \to n \}$, $\{ a_k, b_k, \text{for } k = 1 \to n-1 \}$, and $Area = \int_{x_1}^{x_n} f(x)\,dx$ from the results obtained in step 1.

Using the matching conditions for the cubic spline, we can show that for $k = 1 \to n-1$, we have

$$a_k = [f'(x_{k+1}) + f'(x_k) - 2f_0'(x_k)]h_k \tag{A.5}$$

$$b_k = [f_0'(x_k) - f'(x_k)]h_k \tag{A.6}$$

$$f''(x_k) = (2/h_k)[3f_0'(x_k) - 2f'(x_k) - f'(x_{k+1})] \tag{A.7}$$

for $k = n$, we have

$$f''(x_n) = (2/h_{n-1})[f'(x_{n-1}) + 2f'(x_n) - 3f_0'(x_{n-1})] \tag{A.8}$$

The area under the cubic spline curve between $x_k \le x \le x_{k+1}$, is given by

$$\int_{x_k}^{x_{k+1}} f(x_k \le x \le x_{k+1})\,dx = (x_{k+1} - x_k)[\frac{f(x_k) + f(x_{k+1})}{2} - \frac{a_k}{12} - \frac{b_k}{6}] \tag{A.9}$$

The $Area = \int_{x_1}^{x_n} f(x)\,dx$ can be obtained by summation of equation (A.9) over all intervals.

Case 2:

Step 1: Determine $\{ f'(x_k), \text{for } k = 1 \to n-1 \}$ from a tabulate data set $\{ (x_k, f(x_k)), \text{for } k = 1 \to n \}$ with periodic boundary conditions: $f(x_1) = f(x_n)$, $f'(x_1) = f'(x_n)$, and $f''(x_1) = f''(x_n)$.

Since $f(x_1) = f(x_n)$, we have $f_0'(x_0) = f_0'(x_{n-1})$. Given periodic boundary conditions: $f'(x_1) = f'(x_n)$ and $f''(x_1) = f''(x_n)$, equation (A.2) can be rewritten as

$$\begin{aligned}
f'(x_{n-1}) + f'(x_k)B_k + f'(x_{k+1})C_k &= 3f_0'(x_{n-1}) + 3f_0'(x_k)C_k && \text{for } k = 1 \\
f'(x_{k-1}) + f'(x_k)B_k + f'(x_{k+1})C_k &= 3f_0'(x_{k-1}) + 3f_0'(x_k)C_k && \text{for } k = 2 \to n-2 \\
f'(x_{k-1}) + f'(x_k)B_k + f'(x_1)C_k &= 3f_0'(x_{k-1}) + 3f_0'(x_k)C_k && \text{for } k = n-1
\end{aligned} \tag{A.10}$$

or

$$\begin{pmatrix} B_1 & C_1 & 0 & 0 & 1 \\ 1 & B_2 & C_2 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & 1 & B_{n-2} & C_{n-2} \\ C_{n-1} & 0 & 0 & 1 & B_{n-1} \end{pmatrix} \begin{pmatrix} f'(x_1) \\ f'(x_2) \\ \vdots \\ f'(x_{n-2}) \\ f'(x_{n-1}) \end{pmatrix} = \begin{pmatrix} 3f_0'(x_{n-1}) + 3f_0'(x_1)C_1 \\ 3f_0'(x_1) + 3f_0'(x_2)C_2 \\ \vdots \\ 3f_0'(x_{n-3}) + 3f_0'(x_{n-2})C_{n-2} \\ 3f_0'(x_{n-2}) + 3f_0'(x_{n-1})C_{n-1} \end{pmatrix} \tag{A.10'}$$

where $B_k = (2 + 2\frac{h_{k-1}}{h_k})$, $C_k = \frac{h_{k-1}}{h_k}$, for $k = 1 \to n-1$

Equation (A.10) or (A.10') is the governing equation of $\{ f'(x_k), \text{for } k = 1 \to n-1 \}$ with periodic boundary conditions: $f'(x_1) = f'(x_n)$ and $f''(x_1) = f''(x_n)$.

Step 2: Step 2 in Case 2 is the same as Step 2 in Case 1.

Case 3:

Step 1: Determine $\{ f''(x_k), \text{ for } k = 2 \rightarrow n-1 \}$ from a tabulate data set $\{ (x_k, f(x_k)), \text{for } k = 1 \rightarrow n \}$ with fixed boundary conditions of f'' at $x = x_1$ and $x = x_n$.

Given $f''(x_1)$ and $f''(x_n)$, equation (A.3) can be rewritten as

$$\begin{aligned} f''(x_k)B_k + f''(x_{k+1})C_k &= (6/h_{k-1})[f_0'(x_k) - f_0'(x_{k-1})] - f''(x_1) && \text{for } k = 2 \\ f''(x_{k-1}) + f''(x_k)B_k + f''(x_{k+1})C_k &= (6/h_{k-1})[f_0'(x_k) - f_0'(x_{k-1})] && \text{for } k = 3 \rightarrow n-2 \\ f''(x_{k-1}) + f''(x_k)B_k &= (6/h_{k-1})[f_0'(x_k) - f_0'(x_{k-1})] - f''(x_n)C_k && \text{for } k = n-1 \end{aligned} \tag{A.11}$$

or

$$\begin{pmatrix} B_2 & C_2 & 0 & \cdots & 0 \\ 1 & B_3 & C_3 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1 & B_{n-2} & C_{n-2} \\ 0 & \cdots & 0 & 1 & B_{n-1} \end{pmatrix} \begin{pmatrix} f''(x_2) \\ f''(x_3) \\ \vdots \\ f''(x_{n-2}) \\ f''(x_{n-1}) \end{pmatrix} = \begin{pmatrix} (6/h_1)[f_0'(x_2) - f_0'(x_1)] - f''(x_1) \\ (6/h_2)[f_0'(x_3) - f_0'(x_2)] \\ \vdots \\ (6/h_{n-3})[f_0'(x_{n-2}) - f_0'(x_{n-3})] \\ (6/h_{n-2})[f_0'(x_{n-1}) - f_0'(x_{n-2})] - C_{n-1}f''(x_n) \end{pmatrix}$$

(A.11')

where $B_k = (2 + 2\dfrac{h_k}{h_{k-1}})$, $C_k = \dfrac{h_k}{h_{k-1}}$, for $k = 2 \rightarrow n-1$

Equation (A.11) or (A.11') is the governing equation of $\{ f''(x_k), \text{for } k = 2 \rightarrow n-1 \}$ with a fixed boundary condition of f'' at $x = x_1$ and $x = x_n$.

Step 2: Evaluate $\{ f'(x_k), \text{for } k = 1 \rightarrow n \}$, $\{ a_k, b_k, \text{for } k = 1 \rightarrow n-1 \}$, and $Area = \int_{x_1}^{x_n} f(x)\,dx$ from the results obtained in step 1.

Using the matching conditions for the cubic spline, we can show that for $k = 1 \rightarrow n-1$, we have

$$a_k = (h_k^2 / 6)[f''(x_{k+1}) - f''(x_k)] \tag{A12}$$

$$b_k = (h_k^2 / 6)[f''(x_{k+1}) + 2f''(x_k)] \tag{A.13}$$

$$f'(x_k) = f_0'(x_k) - (h_k / 6)[2f''(x_k) + f''(x_{k+1})] \tag{A.14}$$

for $k = n$, we have

$$f'(x_n) = f_0'(x_{n-1}) + (h_{n-1} / 6)[f''(x_{n-1}) + 2f''(x_n)] \tag{A.15}$$

Substituting equations (A.12) and (A.13) into equation (A.9), one can obtain the area under the cubic-spline curve between $x_k \le x \le x_{k+1}$. The $Area = \int_{x_1}^{x_n} f(x)\,dx$ can be obtained by summation of equation (A.9) over all intervals.

Case 4:

Step 1: Determine $\{ f''(x_k), \text{for } k = 1 \to n-1 \}$ from a tabulate data set $\{ (x_k, f(x_k)), \text{for } k = 1 \to n \}$ with periodic boundary conditions: $f(x_1) = f(x_n)$, $f'(x_1) = f'(x_n)$, and $f''(x_1) = f''(x_n)$.

Since $f(x_1) = f(x_n)$, we have $f_0'(x_0) = f_0'(x_{n-1})$. Given periodic boundary conditions: $f'(x_1) = f'(x_n)$, and $f''(x_1) = f''(x_n)$, equation (A.3) can be rewritten as

$$
\begin{aligned}
f''(x_{n-1}) + f''(x_k)B_k + f''(x_{k+1})C_k &= (6/h_{n-1})[f_0'(x_k) - f_0'(x_{n-1})] && \text{for } k = 1 \\
f''(x_{k-1}) + f''(x_k)B_k + f''(x_{k+1})C_k &= (6/h_{k-1})[f_0'(x_k) - f_0'(x_{k-1})] && \text{for } k = 2 \to n-2 \\
f''(x_{k-1}) + f''(x_k)B_k + f''(x_1)C_k &= (6/h_{k-1})[f_0'(x_k) - f_0'(x_{k-1})] && \text{for } k = n-1
\end{aligned}
\tag{A.16}
$$

or

$$
\begin{pmatrix}
B_1 & C_1 & 0 & 0 & 1 \\
1 & B_2 & C_2 & \ddots & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & \ddots & 1 & B_{n-2} & C_{n-2} \\
C_{n-1} & 0 & 0 & 1 & B_{n-1}
\end{pmatrix}
\begin{pmatrix}
f''(x_1) \\ f''(x_2) \\ \vdots \\ f''(x_{n-2}) \\ f''(x_{n-1})
\end{pmatrix}
=
\begin{pmatrix}
(6/h_{n-1})[f_0'(x_1) - f_0'(x_{n-1})] \\
(6/h_1)[f_0'(x_2) - f_0'(x_1)] \\
\vdots \\
(6/h_{n-3})[f_0'(x_{n-2}) - f_0'(x_{n-3})] \\
(6/h_{n-2})[f_0'(x_{n-1}) - f_0'(x_{n-2})]
\end{pmatrix}
\tag{A.16'}
$$

where $B_k = (2 + 2\dfrac{h_k}{h_{k-1}})$, $C_k = \dfrac{h_k}{h_{k-1}}$, for $k = 1 \to n-1$.

Equation (A.16) or (A.16') is the governing equation of $\{ f''(x_k), \text{for } k = 1 \to n-1 \}$ with periodic boundary conditions: $f'(x_1) = f'(x_n)$ and $f''(x_1) = f''(x_n)$.

Step 2: Step 2 in Case 4 is the same as Step 2 in Case 3.