1.1 Derivative (Neumann) boundary conditions. Consider model problem (1.1) subject to the *Neumann boundary conditions* $u'(0) = u'(1) = 0$. Find the system of linear equations that results when second-order differences are used to discretize this problem at the grid points $x_0, \ldots, x_n$. At the endpoints, x_0 and x_n, one of the many ways to incorporate the boundary conditions is to let $v_1 = v_0$ and $v_{n-1} = v_n$. How many equations and how many unknowns are there in this problem? Give the matrix that corresponds to this boundary value problem.

The new set of equations we wish to discretize is

$$\left\{ \begin{array}{rcl} -u''(x) + \sigma u(x) & = & f(x), \qquad 0 < x < 1, \quad \sigma \geq 0 \\ u'(0) & = & 0 \\ u'(1) & = & 0 \end{array} \right\}. \tag{1}$$

The differential equation can be discretized the same way it was for Dirichlet boundaries. Let $x_i = ih$, $v_i = u(x_i)$, for $i = 0, \ldots, n$ and $h = \frac{1}{n}$, where n is the number of sub-intervals in the domain. Using Taylor's theorem, we have

$$u(x_{i-1}) = u(x_i) - hu'(x_i) + \frac{h^2}{2}u''(x_i) - \frac{h^3}{6}u'''(x_i) + \mathcal{O}(h^4), \tag{2}$$

and

$$u(x_{i+1}) = u(x_i) + hu'(x_i) + \frac{h^2}{2}u''(x_i) + \frac{h^3}{6}u'''(x_i) + \mathcal{O}(h^4). \tag{3}$$

Adding these two Taylor expansions together and solving for $u''(x_i)$ gives

$$u''(x_i) = \frac{-u(x_{i-1}) + 2u(x_i) - u(x_{i+1})}{h^2} + \mathcal{O}(h^2), \tag{4}$$

a second order approximation to the second derivative at x_i. Now substituting v_i for $u(x_i)$, we get the following discretized equations:

$$\frac{-v_{j-1} + 2v_j - v_{j+1}}{h^2} + \sigma v_j = f(x_j), \qquad 1 \leq j \leq n-1. \tag{5}$$

The Neumann boundary conditions can be handled in many ways, but we choose to satisfy them by setting a forward difference to zero for the left end-point, and a backward difference to zero for the right end-point:

$$u'(0) = \frac{v_1 - v_0}{h} = 0, \qquad \text{and} \qquad u'(1) = \frac{v_n - v_{n-1}}{h} = 0. \tag{6}$$

Solving each of these equations gives $v_1 = v_0$ and $v_n = v_{n-1}$. This reduces the amount of unknowns by 2. The finite difference equations for $j = 1$ and $j = n-1$ may be rewritten as

$$\frac{v_1 - v_2}{h^2} + \sigma v_1 = f(x_1), \qquad \text{and} \qquad \frac{v_{n-1} - v_{n-2}}{h^2} + \sigma v_{n-1} = f(x_{n-1}). \tag{7}$$

$$\frac{1}{h^2}\begin{bmatrix} 1+\sigma h^2 & -1 & & \\ -1 & 2+\sigma h^2 & -1 & \\ & & \ddots & \ddots \\ & & -1 & 1+\sigma h^2 \end{bmatrix}\begin{bmatrix} v_1 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{bmatrix} = \begin{bmatrix} f(x_1) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) \end{bmatrix}, \tag{8}$$

a system with $n-1$ equations and $n-1$ unknowns. For your convenience only, here is an example of `MATLAB` code that produces the matrix A for this system:

```
% number of intervals
n = 8;

%reaction coeffecient
sigma = 1;

%interval size
h = 1/n;

%make second derivative Dirichlet matrix
DIFF = 2*diag(sparse(ones(n-1,1))) ...
-1*diag(sparse(ones(n-2,1)),-1) ...
-1*diag(sparse(ones(n-2,1)), 1);

%change upper-left entry for left Neumann b.c.
DIFF(1,1) = 1;

%change lower-right entry for right Neumann b.c.
DIFF(n-1,n-1) = 1;

%build the dicrete system
A=(1/h^2)*DIFF + sigma*diag(sparse(ones(n-1,1)));

%display matrix
full(A)
```

1.3 Periodic boundary conditions. Consider model problem (1.1) subject to the *periodic boundary conditions* $u(0) = u(1)$ and $u'(0) = u'(1)$. Find the system of linear equations that results when second-order finite differences are used to discretize this problem at the grid points $x_0, \ldots, x_{n-1}$. How many equations and unknowns are there in this problem?

The new set of equations we wish to discretize is

$$\left\{ \begin{array}{rcll} -u''(x) + \sigma u(x) & = & f(x), & 0 < x < 1, \quad \sigma \geq 0 \\ u(0) & = & u(1) & \\ u'(0) & = & u'(1) & \end{array} \right\}. \tag{9}$$

Again, the differential equation can be discretized the same way it was for Dirichlet boundaries. Let $v_i = u(ih)$, for $i = 0, \ldots, n$ and $h = \frac{1}{n}$, where n is the number of sub-intervals in the domain. Then, the discretization of the PDE in the interior is given by

$$\frac{-v_{j-1} + 2v_j - v_{j+1}}{h^2} + \sigma v_j = f(x_j), \qquad 1 \leq j \leq n-1. \tag{10}$$

For details about the PDE discretization, see the solutions to problem 1.1 or chapter 1 in the book. The boundary condition $u(0) = u(1)$ is discretized simply as $v_0 = v_n$. This reduces our amount of unknowns by 1. The finite difference equation for $j = n-1$ can be rewritten as

$$\frac{-v_{n-2} + 2v_{n-1} - v_0}{h^2} + \sigma v_{n-1} = f(x_{n-1}). \tag{11}$$

The boundary condition on the derivative can be handled in many ways. The first method we consider handles this boundary condition implicitly. If we think of the domain being inscribed on a circle, we have that $v_{-1} = v_{n-1}$, $v_0 = v_n$, $v_1 = v_{n+1}$. Note that this automatically satisfies the boundary condition $u'(0) = u'(1)$ by making the central difference approximation to the first derivative at each endpoint v_0 and v_n equal:

$$\frac{v_1 - v_{-1}}{2h} = \frac{v_{n+1} - v_{n-1}}{2h}. \tag{12}$$

Now we have the following finite difference equation, which could be posed on either endpoint v_0 or v_n:

$$\frac{-v_{n-1} + 2v_0 - v_1}{h^2} + \sigma v_{n-1} = f(x_{n-1}). \tag{13}$$

We choose to pose it on the left endpoint or x_0. Putting all these equations together, we get the following:

$$\frac{1}{h^2}\begin{bmatrix} 2+\sigma h^2 & -1 & & & -1 \\ -1 & 2+\sigma h^2 & -1 & & \\ & -1 & 2+\sigma h^2 & -1 & \\ & & \ddots & \ddots & \ddots \\ -1 & & & -1 & 2+\sigma h^2 \end{bmatrix}\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) \end{bmatrix}, \quad (14)$$

a system with n equations and n unknowns. Here is some more `MATLAB` code for forming the matrix in this system:

```
% number of intervals
n = 8;

%reaction coeffecient
sigma = 1;

%interval size
h = 1/n;

%make second derivative Dirichlet matrix
DIFF = 2*diag(sparse(ones(n,1))) ...
-1*diag(sparse(ones(n-1,1)),-1) ...
-1*diag(sparse(ones(n-1,1)), 1);

%put upper-right entry for Periodic b.c.
DIFF(1,n) = -1;

%put lower-right entry for Periodic b.c.
DIFF(n,1) = -1;

%build the dicrete system
A=(1/h^2)*DIFF + sigma*diag(sparse(ones(n,1)));

%display matrix
full(A)
```

Another method we consider is to directly discretize the derivative boundary conditions. We discretize the first derivative at the left end-point with a forward difference and discrectize the first derivative at the right end-point with a backwards difference:

$$u'(0) = \frac{v_1 - v_0}{h}, \qquad \text{and} \qquad u'(1) = \frac{v_n - v_{n-1}}{h}. \tag{15}$$

Using $u'(0) = u'(1)$ and $v_0 = v_n$, we can set these two difference equations equal to each other and move all the unknowns to one side to get the equation

$$2v_0 - v_1 - v_{n-1} = 0. \tag{16}$$

Using equation (16) instead of equation (13) gives

$$\frac{1}{h^2}\begin{bmatrix} 2h^2 & -h^2 & & & -h^2 \\ -1 & 2+\sigma h^2 & -1 & & \\ & -1 & 2+\sigma h^2 & -1 & \\ & & \ddots & \ddots & \ddots \\ -1 & & & -1 & 2+\sigma h^2 \end{bmatrix} \begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{bmatrix} = \begin{bmatrix} 0 \\ f(x_1) \\ \vdots \\ f(x_{n-2}) \\ f(x_{n-1}) \end{bmatrix}, \tag{17}$$

another system with n equations and n unknowns.

1.4 Convection terms in two dimensions. A convection term can be added (*instead of the reaction term*) to the two-dimensional model problem in the form

$$-\epsilon(u_{xx} + u_y y) + au_x = f(x), \tag{18}$$

(*with Dirichlet boundary conditions.*) Using the grid described in the text and second-order central finite difference approximations, find the system of linear equations associated with this problem. What conditions must be met by a and ϵ for the associated matrix to be diagonally dominant?

The grid (found on pg. 2 in the text) has points $(x_i, y_j) = (ih_x, jh_y)$ for $h_x = \frac{1}{m}$ and $h_y = \frac{1}{n}$, where m and n are the number of grid intervals in the x and y directions, respectively. Let $v_{i,j} = u(x_i, y_j)$. Here are the 2D finite difference discretizations we require for this grid:

$$\begin{aligned} -\epsilon u_{xx}(x_i, y_j) &\rightarrow \frac{-\epsilon v_{i-1,j} + 2\epsilon v_{i,j} - \epsilon v_{i+1,j}}{h_x^2} \\ -\epsilon u_{yy}(x_i, y_j) &\rightarrow \frac{-\epsilon v_{i,j-1} + 2\epsilon v_{i,j} - \epsilon v_{i,j+1}}{h_y^2} \\ au_x(x_i, y_j) &\rightarrow \frac{-av_{i-1,j} + av_{i+1,j}}{2h_x} \end{aligned}$$

The Dirichlet boundary gives:

$$v_{i0} = v_{in} = v_{0j} = v_{mj} = 0, \quad 0 \le i \le m, \quad 0 \le j \le n. \tag{19}$$

Setting $h_x = h_y = h$, we have the following stencil:

$$\frac{1}{h^2}\begin{bmatrix} & -\epsilon & \\ (-\epsilon - \frac{ah}{2}) & 4\epsilon & (-\epsilon + \frac{ah}{2}) \\ & -\epsilon & \end{bmatrix}.$$

Using ordering by lines of constant i, we turn this stencil into a linear system by forming a matrix B that stands for the vertical part of of the stencil:

$$B := \frac{1}{h^2}\begin{bmatrix} 4\epsilon & -\epsilon & & \\ -\epsilon & 4\epsilon & -\epsilon & \\ & \ddots & \ddots & \ddots \\ & & -\epsilon & 4\epsilon \end{bmatrix} \tag{20}$$

Then we form a block diagonal matrix A, whose off-diagonal blocks represent the horizontal part of the stencil:

$$A := \begin{bmatrix} B & \frac{-2\epsilon+ah}{2h^2}I & & \\ \frac{-2\epsilon-ah}{2h^2}I & B & \frac{-2\epsilon+ah}{2h^2}I & \\ & \ddots & \ddots & \ddots \\ & & \frac{-2\epsilon-ah}{2h^2}I & B \end{bmatrix}, \quad \mathbf{v} = \begin{bmatrix} v_{11} \\ \vdots \\ v_{1,n-1} \\ v_{21} \\ \vdots \\ v_{m-1,n-1} \end{bmatrix},$$

$$\mathbf{f} = \begin{bmatrix} f(x_1, y_1) \\ \vdots \\ f(x_1, y_{n-1}) \\ f(x_2, y_1) \\ \vdots \\ f(x_{m-1}, y_{n-1}) \end{bmatrix}.$$

The discretization is then given by $A\mathbf{v} = \mathbf{f}$, a linear system of $(m-1)(n-1)$ equations with $(m-1)(n-1)$ unknowns. Here is some example `MATLAB` code that will form the matrix for this system.

```
% number of intervals
n = 4;
```

```
%diffusion coeffecient
epsilon = 1;

%convection coeffecient
a = 1;

%interval width
h = 1/n;

%make second derivative Dirichlet matrix for u_xx
DIFF_X = 2*diag(sparse(ones(n,1))) ...
-1*diag(sparse(ones(n-1,1)),-1) ...
-1*diag(sparse(ones(n-1,1)), 1);

%make second derivative Dirichlet matrix for u_yy
DIFF_Y = DIFF_X;

%make first derivative Convection matrix for u_x
CONV_X = -1*diag(sparse(ones(n-2,1)),-1) ...
+1*diag(sparse(ones(n-2,1)), 1);

%create (n-1)x(n-1) identity matrix
IDEN = diag(sparse(ones(n-1,1)));

%build the dicrete system using tensor products
A = kron((epsilon/h^2)*DIFF_X + a*CONV_X, IDEN) + ...
kron(IDEN, (epsilon/h^2)*DIFF_Y);

%display matrix
full(A)
```

To test the matrix A for being diagonally dominant, pick any full line of the matrix (from an unknown in the interior), and then compare the absolute value of diagonal entry to the sum of the absolute values of the off-diagonal entries. Note that this guarantees diagonal dominance near the boundary due to the Dirichlet boundary condition.

$$\frac{4\epsilon}{h^2} \geq \left| \frac{-2\epsilon - ah}{2h^2} \right| + \left| \frac{-2\epsilon + ah}{2h^2} \right| + \frac{2\epsilon}{h^2} \tag{21}$$

Note that $|2\epsilon + ah| + |2\epsilon - ah| = \max\{|4\epsilon|, |2ah|\}$, so either

$$|2\epsilon| \geq |ah| \tag{22}$$

or

$$\frac{4\epsilon}{h^2} \geq \left|\frac{2ah}{2h^2}\right| + \frac{2\epsilon}{h^2}. \tag{23}$$

In either case, each of these inequalities simplify to

$$\epsilon \geq \left|\frac{ah}{2}\right|, \tag{24}$$

which is our criteria for weak diagonal dominance.