The boundary conditions in the Boundary Value Problems (BVP) in $[a, b]$ may come in the form of:

- Dirichlet : $u(a) = u_a \quad \& \quad u(b) = u_b$
- Neumann : $u'(a) = u_a \quad \& \quad u'(b) = u_b$
- Robin : $\alpha_1 u(a) + \beta_1 u'(a) = u_a \quad \& \quad \alpha_2 u(b) + \beta_2 u'(b) = u_b$.

There are two main approaches in the treatment of boundary conditions for spectral collocation methods in practice :

1. Restrict attention to interpolants that satisfy the boundary conditions (good for eigenproblems); or
2. Do not restrict the interpolants, but add additional equations to enforce the boundary conditions.

This chapter contains a collection of boundary value problems arising in ordinary (ODEs) and partial differential equations (PDEs). In each case, a different implementation aspects of the pseudospectral methods are demonstrated.

Case 1 : Homogeneous Dirichlet, Linear ODE (Keywords)

Consider the linear ODE boundary value problem

$$\Im[u] \equiv u_{xx} = \exp(4x), \qquad -1 < x < 1, \qquad u(\pm 1) = 0$$

whose exact solution is known to be

$$u(x) = \tfrac{1}{16}\left[\exp(4x) - x\sinh(4) - \cosh(4)\right].$$

To solve this problem numerically, we approximate the second derivative by a Chebyshev pseudospectral approach and impose the boundary conditions $u(\pm 1) = 0$ as follows :

- Let $u_N(x)$ be the unique polynomial of degree $\leq N$ such that

$$\left\{u_N(x_j)\right\}_{j=0}^{N} = \begin{bmatrix} 0 & u_1 & \cdots & u_{N-1} & 0 \end{bmatrix}^T \equiv U$$

  where $u_j \equiv u(x_j)$ over the grid $x_j = \cos(\pi j/N)$.

- Set $w_j = u_N''(x_j)$ at the interior grid for $j = 1, \ldots, N-1$.

This implies that the resulting discretization matrix $\widetilde{D}_N^{(2)}$ can be made to contain the boundary conditions built in as follows :

$$\begin{array}{r} \text{ignored} \rightarrow \\ \\ \\ \\ \text{ignored} \rightarrow \end{array} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{N-1} \\ w_N \end{bmatrix} = \underbrace{\begin{bmatrix} x & x & x & x & x \\ x & & & & x \\ x & & \widetilde{D}_N^{(2)} & & x \\ x & & & & x \\ x & x & x & x & x \end{bmatrix}}_{D_N^{(2)}} \begin{bmatrix} 0 \\ u_1 \\ \vdots \\ u_{N-1} \\ 0 \end{bmatrix} \begin{array}{l} \leftarrow \text{zeroed} \\ \\ \\ \\ \leftarrow \text{zeroed} \end{array}$$

Thus, we obtained the discretized version of the original BVP :

$$\Im[u] = \exp(4x) \quad \text{and} \quad u(\pm 1) = 0 \qquad \Rightarrow \qquad \tilde{D}_N^{(2)}\, U = F,$$

where $F = \left\{ \exp(4x_j) \right\}_{j=1}^{N-1}$.

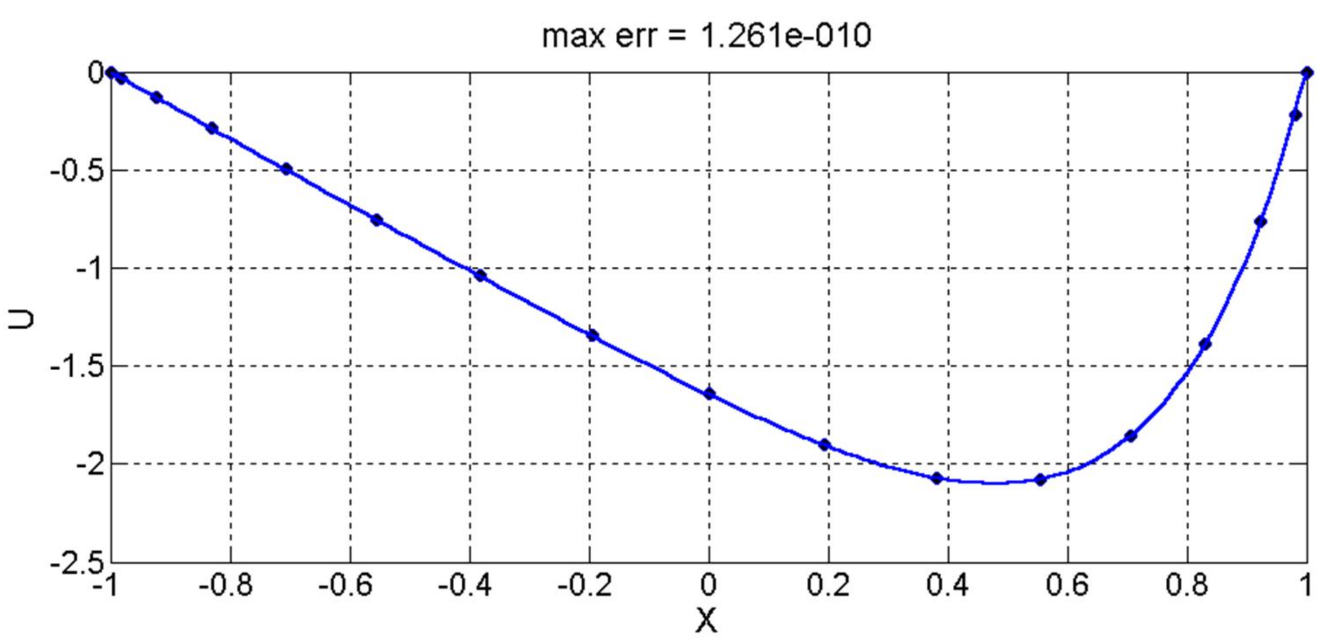
This is implemented in **p13.m** in which the discretized operator is constructed by the steps

```
[D,x] = cheb(N);
D2 = D^2;
D2 = D2(2:N,2:N);    % boundary conditions
```

and the resulting is solved at the steps

```
u = D2\f;       % Poisson eq. solved here
u = [0;u;0];
```

The result is accurate to nine digits for the resolution of $N = 16$.



Case 6 : Non-homogeneous Dirichlet, Linear ODE

Consider the linear ODE boundary value problem

$$\Im[u] \equiv u_{xx} = \exp(4x), \quad -1 < x < 1, \quad u(-1) = 0, \quad u(+1) = 1$$

which we have solved subject to homogeneous Dirichlet conditions in Case 1.

To solve this problem numerically, we approximate the second derivative by a Chebyshev pseudospectral approach and add additional equation to enforce the boundary conditions $u(+1) = 1$ as follows :

- Let $u_N(x)$ be the unique polynomial of degree $\le N$ such that
$$\left\{ u_N(x_j) \right\}_{j=0}^{N} = \begin{bmatrix} u_0 & u_1 & \cdots & u_{N-1} & 0 \end{bmatrix}^T \equiv U$$
where $u_j \equiv u(x_j)$ over the grid $x_j = \cos(\pi j / N)$.

- Set $w_j = u_N''(x_j)$ at the interior grid for $j = 1, \ldots, N-1$.

- Add the additional equation $u_0 = 1$.

This implies that the resulting discretized operator can be constructed as follows :

$$\text{ignored} \rightarrow \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{N-1} \\ w_N \end{bmatrix} = \underbrace{\left[\begin{array}{ccccc} \multicolumn{4}{c}{\overbrace{1 \quad 0 \quad \dots \quad 0}^{\Im_N}} & x \\ & & & & x \\ & & & & x \\ & & & & x \\ x & x & x & x & x \end{array}\right]}_{D^{(2)}} \begin{bmatrix} u_0 \\ u_1 \\ \vdots \\ u_{N-1} \\ 0 \end{bmatrix} \leftarrow \text{zeroed}$$

The right-hand side, F, of the discretized version of the BVP, $\Im_N U = F$, is then modified to complete the additional equation as follows :

$$F = \begin{bmatrix} 1 & \exp(4x_1) & \cdots & \exp(4x_{N-1}) \end{bmatrix}^T.$$

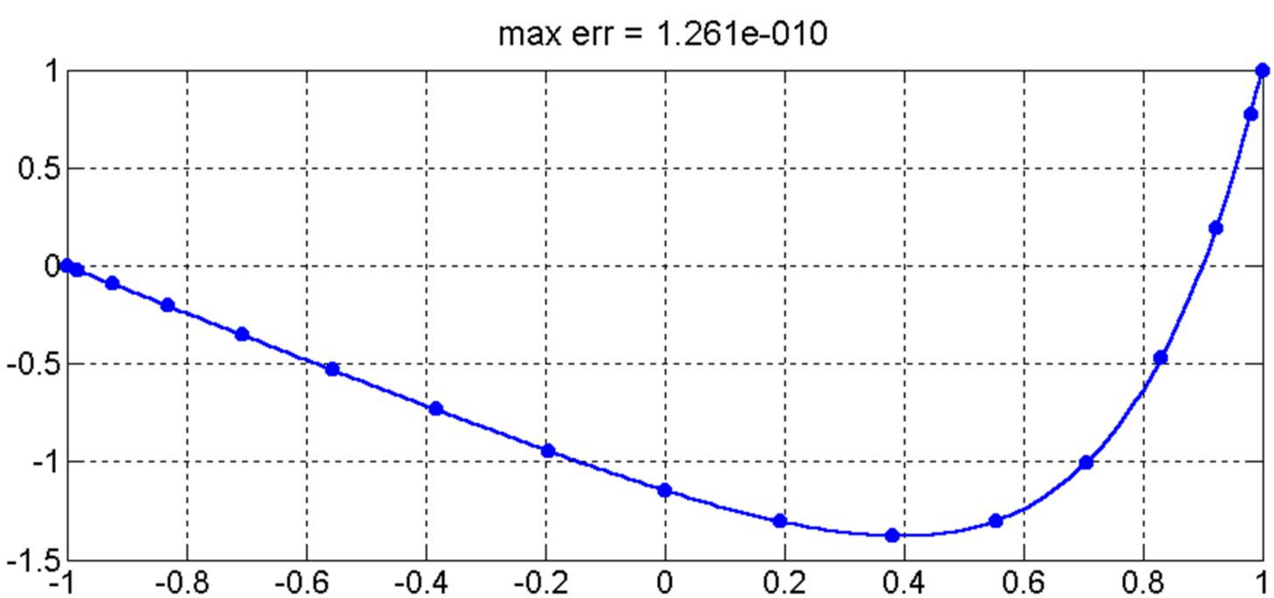
This is implemented in **p32.m** in which the discretized operator is constructed by the steps

```
[D,x] = cheb(N); D2 = D^2;
D2(1,:) = zeros(1,N); D2(1,1) = 1; % add equation
D2 = D2(1:N,1:N);    % boundary conditions
```

and the resulting linear system is solved at the steps

```
F = exp(4*x(2:N));
u = D2\[0;F];      % Poisson eq. solved here
u = [u;0];
```

The result is shown below for $N = 16$.



Case 7 : Homogeneous Neumann/Dirichlet, Linear ODE

Now, consider the same equation as in Cases 1 & 6, but with a Neumann condition at the left endpoint

$$\Im[u] \equiv u_{xx} = \exp(4x), \quad -1 < x < 1, \quad u_x(-1) = u(+1) = 0.$$

This problem will be discretized as before, except that, an additional equation will be added to enforce the Neumann condition as follows :

- Let $u_N(x)$ be the unique polynomial of degree $\le N$ such that $\left\{ u_N(x_j) \right\}_{j=0}^{N} = \begin{bmatrix} 0 & u_1 & \cdots & u_{N-1} & u_N \end{bmatrix}^T \equiv U$.
- Set $w_j = u_N''(x_j)$ at the interior grid for $j = 1, \ldots, N-1$.
- Add $u_N'(-1) = D_{N,1}u_1 + \cdots + D_{N,N}u_N = 0$ where D is the first order Chebyshev differentiation matrix.

This can be summarized as follows :

$$\text{ignored} \rightarrow \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_{N-1} \\ w_N \end{bmatrix} = \overbrace{\begin{bmatrix} x & x & x & x & x \\ x & & & & \\ x & & & & \\ x & & & & \\ x & \underbrace{D_{N,1} & \cdots & D_{N,N-1} & D_{N,N}}_{\Im_N} \end{bmatrix}}^{D_N^{(2)}} \begin{bmatrix} 0 \\ u_1 \\ \vdots \\ u_{N-1} \\ u_N \end{bmatrix} \leftarrow \text{zeroed}$$

Thus, we obtained the discretized version of the BVP,

$$\mathfrak{I}_N U = F,$$

where

$$F = \left[\exp(4x_1) \quad \cdots \quad \exp(4x_{N-1}) \quad 0\right]^T.$$

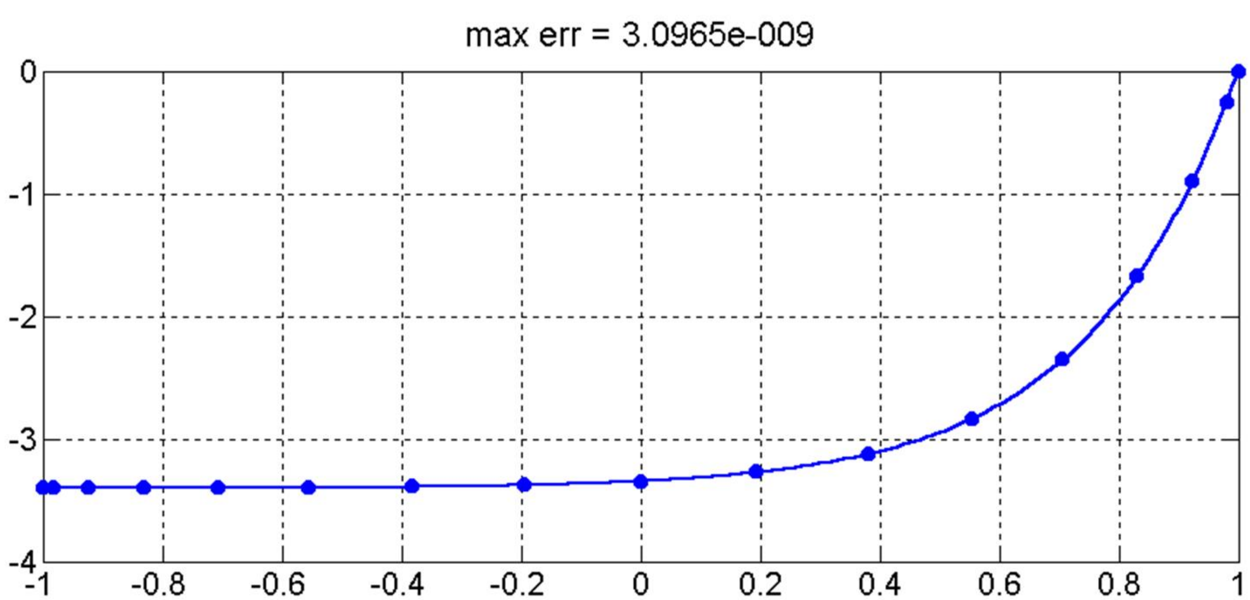
This is implemented in **p33.m** in which the discretized operator is constructed by the steps

```
[D,x] = cheb(N); D2 = D^2;
D2(N+1,:) = D(N+1,:); % Neumann condition at x = -1
D2 = D2(2:N+1,2:N+1);
```

and the resulting linear system is solved at the steps

```
F = exp(4*x(2:N));
u = D2\[F;0];      % Poisson eq. solved here
u = [0;u];
```

The Neumann condition is successfully implanted into the discrete operator as shown by the highly accurate result for just $N = 16$.



Case 10 : Higher-order derivatives

Suppose that we wish to solve the biharmonic problem

$$\Im[u] \equiv u_{xxxx} = f(x), \quad -1 < x < 1, \quad u(\pm 1) = u_x(\pm 1) = 0.$$

Physically, $u(x)$ might represent the tranverse displacement of a beam subject to a force $f(x)$. The conditions at $x = \pm 1$ are known as clamped boundary conditions, corresponding to holding both the position and the slope of a beam fixed at the ends.

In order to compute spectral approximation to u_{xxxx}, let $\{u_j\}$ be the vector of values of u sampled at $x_1, \ldots, x_{N-1}$. The polynomial interpolant, $p(x)$, satisfying the boundary conditions can be constructed as follows :

- Let p be the unique polynomial of degree $\leq N+2$ with $p(\pm 1) = p_x(\pm 1) = 0$ and $p(x_j) = u_j$ for $j = 1, \ldots, N-1$.
- Set $w_j = p_{xxxx}(x_j)$.

If we set

$$p(x) = (1 - x^2) q(x),$$

from which after four differentiation, we obtain

$$p_{xxxx}(x) = (1 - x^2)\, q_{xxxx}(x) - 8x\, q_{xxx}(x) - 12\, q_{xx}(x).$$

Thus, a polynomial q of degree $\leq N$ with $q(\pm 1) = 0$ corresponds to a polynomial p of degree $\leq N+2$ with $p(\pm 1) = p_x(\pm 1) = 0$.

Now, we can carry out the required spectral differentiation as follows :

- Let q be the unique polynomial of degree $\leq N$ with $q(\pm 1) = 0$ and $q(x_j) = u_j / (1 - x_j^2)$ for $j = 1, \ldots, N-1$.
- Set $w_j = (1 - x_j^2) q_{xxxx}(x_j) - 8 x_j q_{xxx}(x_j) - 12 q_{xx}(x_j)$.

Then, our spectrally discretized biharmonic operator is

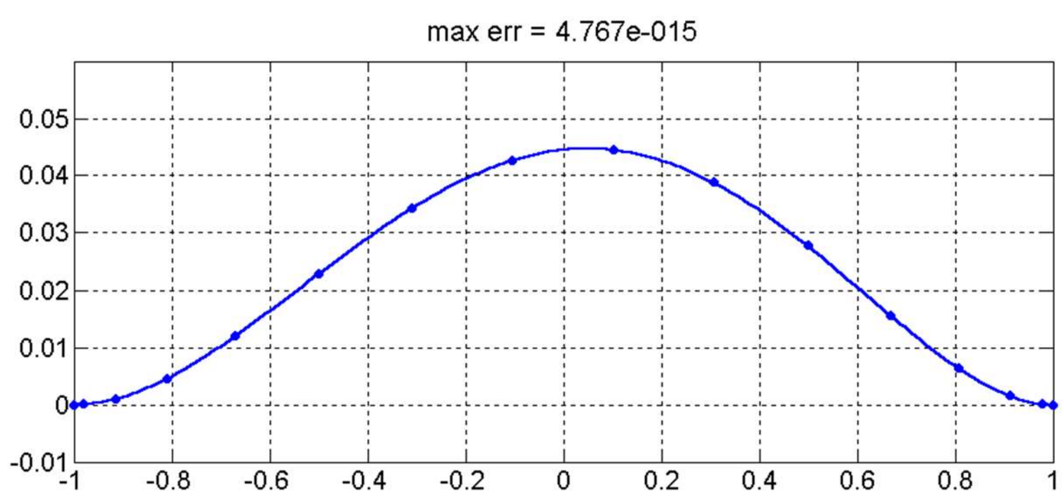
$$\mathfrak{I}_N \equiv \left[\mathrm{diag}(1 - x_j^2) \widetilde{D}_N^{(4)} - 8 \mathrm{diag}(x_j) \widetilde{D}_N^{(3)} - 12 \widetilde{D}_N^{(2)} \right] \times \mathrm{diag}\left(\frac{1}{1 - x_j^2} \right)$$

for $j = 1, \ldots, N-1$, where $\widetilde{D}_N^{(2)}$, $\widetilde{D}_N^{(3)}$, $\widetilde{D}_N^{(4)}$ are the higher-order differentiation matrices obtained by taking the indicated powers 2, 3, and 4 of D_N, respectively, and stripping away the first and last rows and columns.

__Example__ : Set $f(x) = \exp(x)$. The procedure above is implemented in **p38.m** in the following steps :

```
% Construct discrete biharmonic operator:
  [D,x] = cheb(N);
  S = diag([0; 1 ./(1-x(2:N).^2); 0]);
  D4 = (diag(1-x.^2)*D^4 - 8*diag(x)*D^3 - 12*D^2)*S;
  D4 = D4(2:N,2:N);

% Solve boundary-value problem and plot result:
  f = exp(x(2:N)); u = D4\f; u = [0;u;0];
```



Case 11 : Differential eigenvalue problems

Differential eigenvalue problems with high order derivatives often arise in hydrodynamic stability calculations. The pseudospectral approximation to such eigenvalue problems is found to produce spurious (unphysical) eigenvalues if the interpolating polynomial is not chosen properly.

Huang & Sloan (1994) suggested a new differentiation matrix approach in which two distinct interpolating polynomials are used.

This approach is presented below using various eigenvalue problems.

Example :

Consider the fourth-order eigenvalue problem

$$u_{xxxx} + Ru_{xxx} = \lambda u_{xx}, \quad -1 < x < 1, \quad u(\pm 1) = u_x(\pm 1) = 0,$$

where R is a real parameter and λ is the eigenparameter.

In pseudospectral approximation of this problem, two interpolation problems are posed :

1. Find the unique polynomial p of degree $N+2$ such that $p(x_j) = u(x_j), \quad j = 1, \ldots, N\text{-}1 \quad \text{with} \quad p(\pm 1) = p_x(\pm 1) = 0$.

2. Find the unique polynomial $\hat{p}$ of degree N such that $\hat{p}(x_j) = u(x_j), \quad j = 1, \ldots, N\text{-}1 \quad \text{with} \quad \hat{p}(\pm 1) = 0$.

In this approach, $\hat{p}$ is used for spectral approximation to the second-order derivative operator, while p is used for the higher-order derivative terms in the equation.

The spectral approximation to the problem becomes

$$p_{xxxx}(x_j) + Rp_{xxx}(x_j) = \lambda \hat{p}_{xx}(x_j), \quad j = 1, \ldots, N-1.$$

These interpolating polynomials are constructed by setting

$$p(x) = (1 - x^2)q(x), \quad \text{and} \quad \hat{p}(x) = q(x),$$

where q is a polynomial of degree $\le N$ with $q(\pm 1) = 0$, as before.

The derivatives are then discretized to get :

$$p_{xxxx} \;\Rightarrow\; D4 \equiv \left[\mathrm{diag}(1 - x_j^2)\widetilde{D}_N^{(4)} - 8\,\mathrm{diag}(x_j)\widetilde{D}_N^{(3)} - 12\widetilde{D}_N^{(2)}\right] \times \mathrm{diag}\left(\frac{1}{1 - x_j^2}\right)$$

$$p_{xxx} \;\Rightarrow\; D3 \equiv \left[\mathrm{diag}(1 - x_j^2)\widetilde{D}_N^{(3)} - 6\,\mathrm{diag}(x_j)\widetilde{D}_N^{(2)} - 6\widetilde{D}_N^{(1)}\right] \times \mathrm{diag}\left(\frac{1}{1 - x_j^2}\right)$$

$$\hat{p}_{xx} \;\Rightarrow\; \hat{D}2 \equiv \widetilde{D}_N^{(2)}$$

At the matrix level, by introducing the spectral differentiation matrices D4, D3 and $\hat{D}2$ in the equation, we obtain the $(N-1)\times(N-1)$ generalized eigenvalue problem :

$$\left(D4 + R\,D3\right)U = \lambda\,(\hat{D}2)\,U.$$

This is implemented in **fourth.m** for $R = 4$ in the following steps :

```
% Construct spectral approximation to the operator:
[x,D] = chebdif(N,4); D2 = D(:,:,2); D2 = D2(2:N-1,2:N-1);
S = diag([0; 1 ./(1-x(2:N-1).^2); 0]);
D3 = (diag(1-x.^2)*D(:,:,3)-6*diag(x)*D(:,:,2)-6*D(:,:,1))*S;
D3 = D3(2:N-1,2:N-1);
D4 =(diag(1-x.^2)*D(:,:,4)-8*diag(x)*D(:,:,3)-12*D(:,:,2))*S;
D4 = D4(2:N-1,2:N-1);
A = D4 + R*D3; B = D2;

% Find the eigenparameters:
Lam = eig(A,B); Lam = sort(Lam);
```

N	λ_1
9	**-17.91**1150290177738
14	**-17.9129218**7679245
19	**-17.9129218001**4924
Exact	**-17.91292180018440**

Example :

Consider the incompressible flow in a straight channel (plane Poiseuille flow). The governing equations are

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{\partial p}{\partial x}+\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right),$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{\partial p}{\partial y}+\nu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right),$$

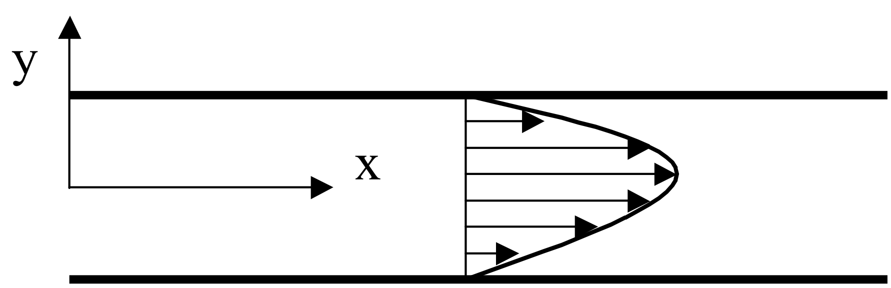
$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0.$$

The boundary conditions at the impermeable and no-slip walls are

$$u(x,+1,t)=v(x,+1,t)=0,$$

$$u(x,-1,t)=v(x,-1,t)=0,$$

where the upper and lower boundaries in the direction normal to the walls are normalized to $y=\pm 1$.



An equilibrium (time-independent) solution is

$$u(x,y,t)=1-y^2,$$

$$v(x,y,t)=0,$$

$$p(x,y,t)=-2\nu x.$$

The stability of this flow is assessed by studying the perturbations of the form :

$$u(x,y,t) = \left(1-y^2\right) + u'(x,y,t),$$
$$v(x,y,t) = 0 + v'(x,y,t),$$
$$p(x,y,t) = -2\nu x + p'(x,y,t),$$

where

$$[u', v', p'](x,y,t) = [\ \hat{u}, \hat{v}, \hat{p}\ ](y)\exp(\imath\sigma x + \lambda t).$$

The temporal frequency λ come from solutions to the Orr-Sommerfeld eigenvalue problem,

$$-\frac{1}{\sigma R}\left[\hat{v}_{yyyy} - 2\sigma^2\hat{v}_{yy} + \sigma^4\hat{v}\right] + \imath\left[U(\hat{v}_{yy} - \sigma^2\hat{v}) - U''\,\hat{v}\right] = \lambda\left[\hat{v}_{yy} - \sigma^2\hat{v}\right]$$

in $-1 < y < 1$ subject to

$$\hat{v}(\pm 1) = \hat{v}_y(\pm 1) = 0,$$

where R is the Reynolds number and $U(y) = 1 - y^2$ is the mean flow.

Discretizing as in the previous example, we obtain the $(N-1)\times(N-1)$ generalized eigenvalue problem $AU = \lambda BU$ where

$$A = R^{-1}\left((D4) - 2\,(\hat{D}2) + I\right) - 2\imath\, I - \imath\,\mathrm{diag}(1-x^2)\left((\hat{D}2) - I\right),$$
$$B = (\hat{D}2) - I.$$

It is known that the most sensitive longitudinal structure (perturbation) has a dependence on x closer to $\exp(1.02\imath x)$, i.e. $\sigma = 1.02 \approx 1$.

To test for the instability of this structure, we look for values of R, which give eigenvalues λ with positive real part. In that case, the flow is linearly unstable.

p40.m implements these formulas to calculate eigenvalues corresponding to $R = 5772$, the critical Reynolds number determined by *Orszag* (1971) in the following steps :

```
% 2nd- and 4th-order differentiation matrices:
    [D,x] = cheb(N); D2 = D^2; D2 = D2(2:N,2:N);
    S = diag([0; 1 ./(1-x(2:N).^2); 0]);
    D4 = (diag(1-x.^2)*D^4 - 8*diag(x)*D^3 - 12*D^2)*S;
    D4 = D4(2:N,2:N);

% Orr-Sommerfeld operators A,B and generalized eigenvalues:
    I = eye(N-1);
    A = (D4-2*D2+I)/R - 2i*I - 1i*diag(1-x(2:N).^2)*(D2-I);
    B = D2-I; Lam = eig(A,B);
```

As expected, the rightmost eigenvalue is nearly on the imaginary axis.