

```
In[ ]:= Clear["Global`*"];
```

Comparison of FDMs with spectral methods - derivatives of a function

Periodic functions

Test function and its derivatives

```
In[ ]:= f[x_] = Exp[Sin[x]]  
df[x_] = D[f[x], x]  
ddf[x_] = D[f[x], x, x]  
Plot[{f[x], df[x], ddf[x]}, {x, -3 π, 3 π},  
PlotLegends → {"f(x)", "f'(x)", "f''(x)"}, AxesLabel → {"x", "f"}]
```

Out[]:=

$e^{\sin[x]}$

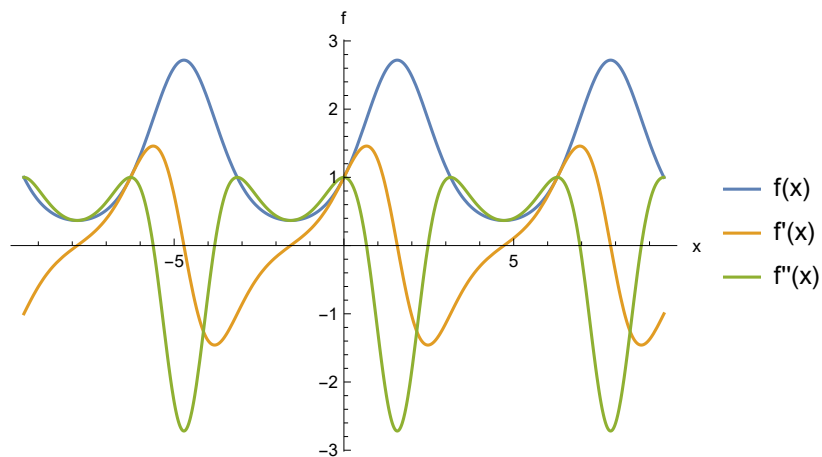
Out[]:=

$e^{\sin[x]} \cos[x]$

Out[]:=

$e^{\sin[x]} \cos[x]^2 - e^{\sin[x]} \sin[x]$

Out[]:=



Differentiation matrix for the finite-difference method

```

In[ ]:= Clear[h];
getSparseFDMatrix[n_, p_, h_] := Module[{v, pf2, matrix},
  v = ConstantArray[0, n];
  pf2 = Factorial[p]^2;
  Do[
    v[[s + 1]] = (-1)^(s + 1) * pf2 / (s * Factorial[p - s] * Factorial[p + s]);
    v[[n - s + 1]] = -v[[s + 1]],
    {s, 1, p}
  ];
  matrix = SparseArray[Flatten[{Table[Band[{1, i}] → v[[i]], {i, 1, n}],
    Table[Band[{i, 1}] → v[[n + 2 - i]], {i, 2, n}]}], {n, n}];
  Return[matrix / h];
n = 10;
getSparseFDMatrix[n, 3, h] // MatrixForm

```

Out[]:= //MatrixForm=

$$\begin{pmatrix} 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} \\ -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} \\ \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 & -\frac{1}{60h} \\ -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 \\ 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 \\ 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 \\ 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} \\ \frac{1}{60h} & 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} \\ -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} \\ \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 \end{pmatrix}$$

Differentiation matrix of the spectral method

Formula for even number of grid points

```
In[ ]:= Clear[h];
tmp = Flatten[{0, Table[(-1)^i * Cot[i * h / 2] / 2, {i, 1, n - 1}]}];
DM = ToeplitzMatrix[tmp, -tmp];
DM // MatrixForm
```

`Out[ ]//MatrixForm=`

[illegible]

Formula for odd number of grid points

```
In[ ] := Clear[h];
tmp = Flatten[{0, Table[(-1)^i * Csc[i * h / 2] / 2, {i, 1, n}]}];
DM = ToeplitzMatrix[tmp, -tmp];
DM // MatrixForm
```

Out[•]//MatrixForm=

[illegible]

Numerical derivative using differentiation matrices

```

ns = {15, 16, 19, 20, 23, 24, 28, 32, 40, 48, 56, 64, 72, 80, 96, 112, 128};
(* number of grid points *)
nm = 6; (* number of methods *)
ng = Length[ns]; (* number of grids *)
errorD1 = ConstantArray[0.0, {nm, ng}];
errorD2 = ConstantArray[0.0, {nm, ng}];
Do[ (* loop over grids *)
  n = ns[[i]];
  h = N[2  $\pi$  / n];
  xs = - $\pi$  + h * Range[n]; (* notice that point  $-\pi$  is not included *)
  fxs = N[f[xs]];
  eDfxs = N[df[xs]];
  eD2fxs = N[ddf[xs]];
  Do[ (* loop over methods - the first is spectral method,
    then FDMs of increasing even order *)
    If[m == 1, (* spectral method *)
      If[Mod[n, 2] == 0,
        tmp = Flatten[{0, Table[0.5 * (-1)^i * Cot[i * h / 2], {i, 1, n - 1}]}],
        (* even number of points *)
        tmp = Flatten[{0, Table[0.5 * (-1)^i * Csc[i * h / 2], {i, 1, n - 1}]}],
        (* odd number of points *)
      ];
      DM = ToeplitzMatrix[tmp, -tmp],
      (* finite-difference methods *)
      DM = getSparseFDMatrix[n, m - 1, h]
    ];
    Dfxs = DM.fxs;
    D2fxs = DM.Dfxs;
    errorD1[[m, i]] = Max[Abs[Dfxs - eDfxs]];
    errorD2[[m, i]] = Max[Abs[D2fxs - eD2fxs]],
    {m, 1, nm}
  ],
  {i, 1, Length[ns]}
];

```

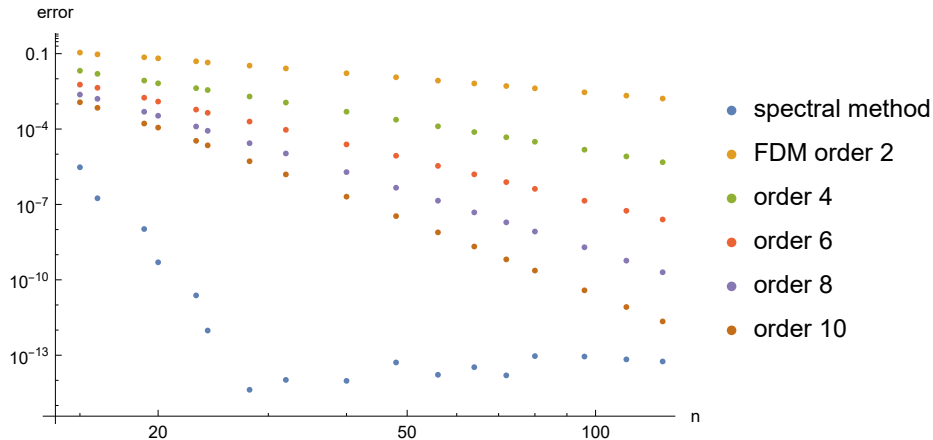
Error of the first derivative

```

In[ ]:= hs = N[2 π / ns] ;
ListLogLogPlot[Table[Transpose[{ns, errorD1[[i, All]]}], {i, 1, nm}],
  PlotLegends → {"spectral method", "FDM order 2", "order 4",
    "order 6", "order 8", "order 10"}, AxesLabel → {"n", "error"}]

```

Out[]:=



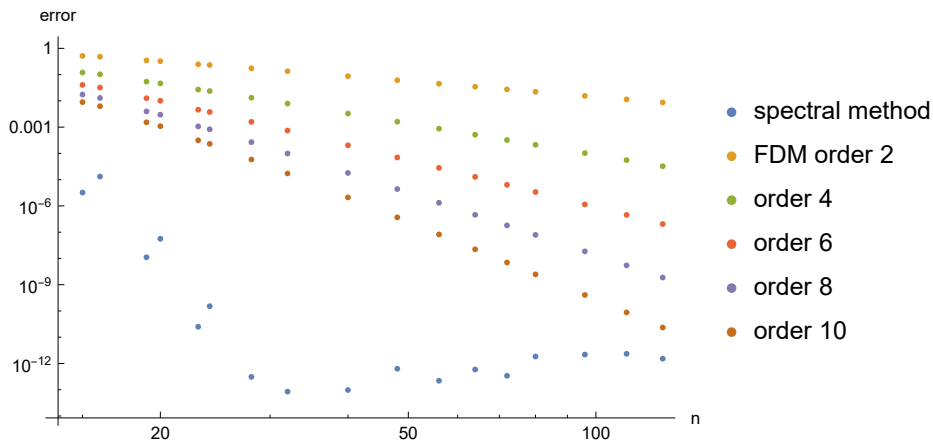
Error of the second derivative

```

In[ ]:= hs = N[2 π / ns] ;
ListLogLogPlot[Table[Transpose[{ns, errorD2[[i, All]]}], {i, 1, nm}],
  PlotLegends → {"spectral method", "FDM order 2", "order 4",
    "order 6", "order 8", "order 10"}, AxesLabel → {"n", "error"}]

```

Out[]:=



Non-Periodic functions

Problem

Calculate approximate derivatives of a function

$$f(x) = e^{-x^2} \sin(3x)$$

(1)

using differentiation matrices and study convergence with respect to space grid parameter h .

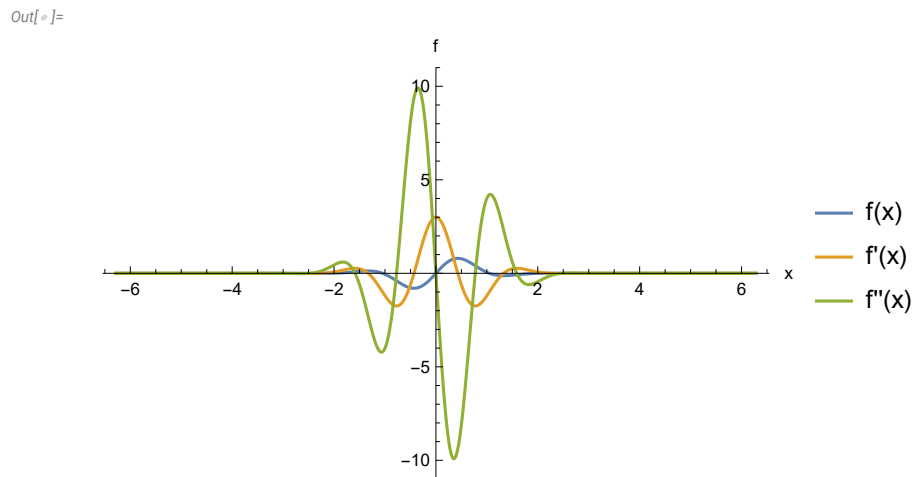
Test function and its derivatives

```
In[ ]:= f[x_] = Exp[-x^2] × Sin[3 x]
df[x_] = D[f[x], x]
ddf[x_] = D[f[x], x, x]
Plot[{f[x], df[x], ddf[x]}, {x, -2 π, 2 π}, PlotRange → All,
  PlotLegends → {"f(x)", "f'(x)", "f''(x)"}, AxesLabel → {"x", "f"}]
```

```
Out[ ]:= e-x2 Sin[3 x]
```

```
Out[ ]:= 3 e-x2 Cos[3 x] - 2 e-x2 x Sin[3 x]
```

```
Out[ ]:= -12 e-x2 x Cos[3 x] - 11 e-x2 Sin[3 x] + 4 e-x2 x2 Sin[3 x]
```



Differentiation matrix for the finite-difference method

```

In[ ]:= Clear[h];
getSparseFDBandMatrix[n_, p_, h_] := Module[{v, pf2, matrix},
  v = ConstantArray[0, n];
  pf2 = Factorial[p]^2;
  Do[
    v[[s + 1]] = (-1)^(s + 1) * pf2 / (s * Factorial[p - s] * Factorial[p + s]),
    {s, 1, p}
  ];
  matrix = SparseArray[Flatten[{Table[Band[{1, i}] → v[[i]], {i, 1, n}],
    Table[Band[{i, 1}] → -v[[i]], {i, 2, n}]}], {n, n}];
  Return[matrix / h];
n = 8;
getSparseFDBandMatrix[n, 3, h] // MatrixForm

```

Out[]:= //MatrixForm=

$$\begin{pmatrix} 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 & 0 \\ -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 & 0 \\ \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 & 0 \\ -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} & 0 \\ 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} & \frac{1}{60h} \\ 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} & -\frac{3}{20h} \\ 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 & \frac{3}{4h} \\ 0 & 0 & 0 & 0 & -\frac{1}{60h} & \frac{3}{20h} & -\frac{3}{4h} & 0 \end{pmatrix}$$

Differentiation matrix of the spectral method

```

In[ ]:= getSpectralDiffMatrix[x_] := Module[{dist, matrix, n},
  n = Length[x];
  dist = ConstantArray[0, {n, n}];
  matrix = ConstantArray[0, {n, n}];
  (* precompute distances of points *)
  Do[Do[ dist[[i, j]] = x[[i]] - x[[j]], {j, 1, n}], {i, 1, n}];
  (* diagonal elements *)
  Do[ matrix[[j, j]] = Sum[If[k == j, 0, 1 / dist[[j, k]]], {k, 1, n}], {j, 1, n}];
  (* off-diagonal elements *)
  Do[
    If[i != j,
      matrix[[i, j]] =
        Product[If[k != j && k != i, dist[[i, k]] / dist[[j, k]], 1], {k, 1, n}] / dist[[j, i]]
    ],
    {j, 1, n}, {i, 1, n}
  ];
  Return[matrix]
];
getSpectralDiffMatrix[{1, 1 / 2, 0, -1 / 2, -1}] // MatrixForm

```

Out[]:= //MatrixForm=

$$\begin{pmatrix} \frac{25}{6} & -8 & 6 & -\frac{8}{3} & \frac{1}{2} \\ \frac{1}{2} & \frac{5}{3} & -3 & 1 & -\frac{1}{6} \\ -\frac{1}{6} & \frac{4}{3} & 0 & -\frac{4}{3} & \frac{1}{6} \\ \frac{1}{6} & -1 & 3 & -\frac{5}{3} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{8}{3} & -6 & 8 & -\frac{25}{6} \end{pmatrix}$$

Numerical derivative using differentiation matrices on the equidistant grid
 => large error similar to error of an interpolating polynomial of high order on the equidistant grid

```
In[ ]:= ns = {8, 10, 12, 14, 16, 20, 24, 32, 40, 48, 56}; (* number of grid points *)
nm = 4; (* number of methods *)
ng = Length[ns]; (* number of grids *)
errorD1 = ConstantArray[0.0, {nm, ng}];
errorD2 = ConstantArray[0.0, {nm, ng}];
xmin = -2  $\pi$ ; xmax = -xmin;
Do[ (* loop over grids *)
  n = ns[[i]];
  h = N[(xmax - xmin) / n];
  xs = xmin + h * Range[n];
  fxs = N[f[xs]];
  eDfxs = N[df[xs]];
  eD2fxs = N[ddf[xs]];
  Do[ (* loop over methods - the first is spectral method,
    then FDMs of increasing even order *)
    If[m == 1, (* spectral method *)
      DM = getSpectralDiffMatrix[xs],
      (* finite-difference methods *)
      DM = getSparseFDBandMatrix[n, m - 1, h]
    ];
    Dfxs = DM.fxs;
    D2fxs = DM.Dfxs;
    errorD1[[m, i]] = Max[Abs[Dfxs - eDfxs]];
    errorD2[[m, i]] = Max[Abs[D2fxs - eD2fxs]],
    {m, 1, nm}
  ],
  {i, 1, Length[ns]}
];
```

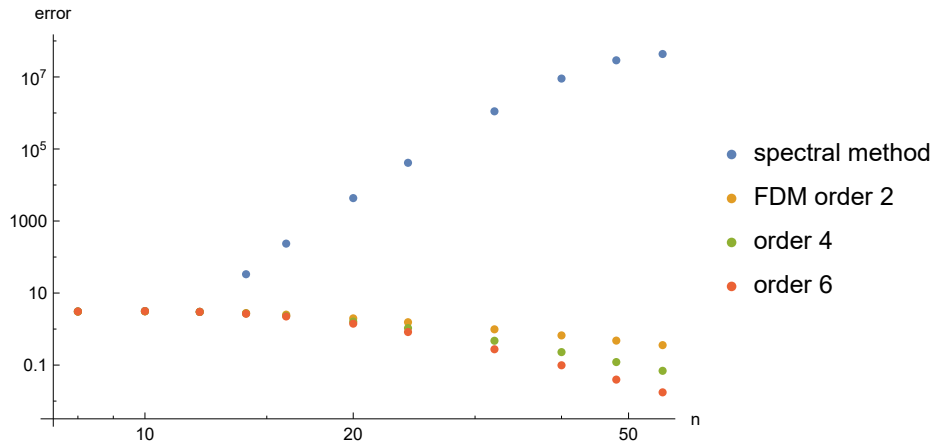
Error of the first derivative

```

In[ ]:= hs = N[2  $\pi$  / ns];
ListLogLogPlot[Table[Transpose[{ns, errorD1[[i, All]]}], {i, 1, nm}], PlotRange -> All,
  PlotLegends -> {"spectral method", "FDM order 2", "order 4", "order 6"},
  AxesLabel -> {"n", "error"}]

```

Out[]:=



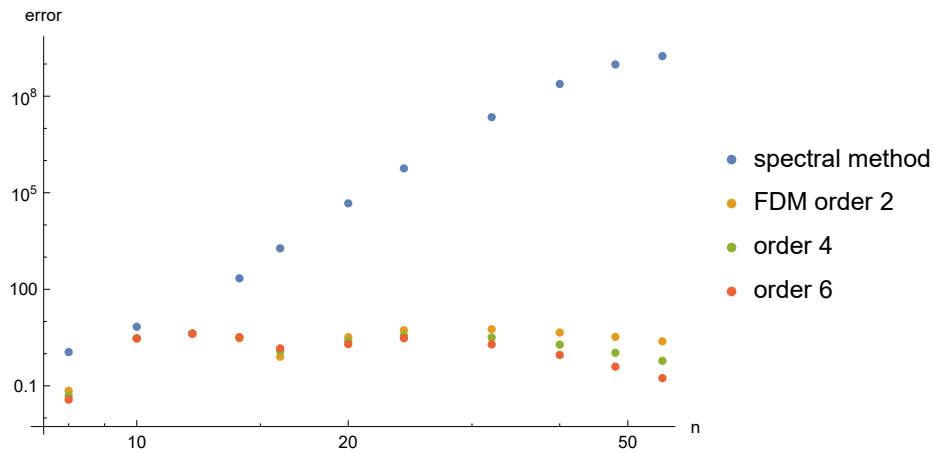
Error of the second derivative

```

In[ ]:= hs = N[2  $\pi$  / ns];
ListLogLogPlot[Table[Transpose[{ns, errorD2[[i, All]]}], {i, 1, nm}], PlotRange -> All,
  PlotLegends -> {"spectral method", "FDM order 2", "order 4", "order 6"},
  AxesLabel -> {"n", "error"}]

```

Out[]:=



Numerical derivative using differentiation matrices for FDM on the equidistant grid and for the Chebyshev spectral method

=> works because an interpolating polynomial on the Chebyshev grid also works

```
In[ ]:= ns = {16, 20, 24, 32, 40, 48, 56, 64, 72, 80, 96, 112, 128}; (* number of grid points *)
nm = 4; (* number of methods *)
ng = Length[ns]; (* number of grids *)
errorD1 = ConstantArray[0.0, {nm, ng}];
errorD2 = ConstantArray[0.0, {nm, ng}];
xmin = -π; xmax = -xmin;
Do[ (* loop over methods - the first is spectral method,
    then FDMs of increasing even order *)
  Do[ (* loop over grids *)
    n = ns[[i]];
    If[m == 1,
      (* Chebyshev extreme grid *)
      xs = N[(xmin + xmax) - (xmax - xmin) * Cos[(Range[n] - 1) * π / (n - 1)]] / 2,
      (* equidistant grid *)
      h = N[(xmax - xmin) / n];
      xs = xmin + h * Range[n]
    ];
    fxs = N[f[xs]];
    eDfxs = N[df[xs]];
    eD2fxs = N[ddf[xs]];
    If[m == 1, (* spectral method *)
      DM = getSpectralDiffMatrix[xs],
      (* finite-difference methods *)
      DM = getSparseFDBandMatrix[n, m - 1, h]
    ];
    Dfxs = DM.fxs;
    D2fxs = DM.Dfxs;
    errorD1[[m, i]] = Max[Abs[Dfxs[[6 ;; n - 6]] - eDfxs[[6 ;; n - 6]]]];
    errorD2[[m, i]] = Max[Abs[D2fxs[[6 ;; n - 6]] - eD2fxs[[6 ;; n - 6]]],
      {i, 1, Length[ns]}
    ],
  {m, 1, nm}
];
```

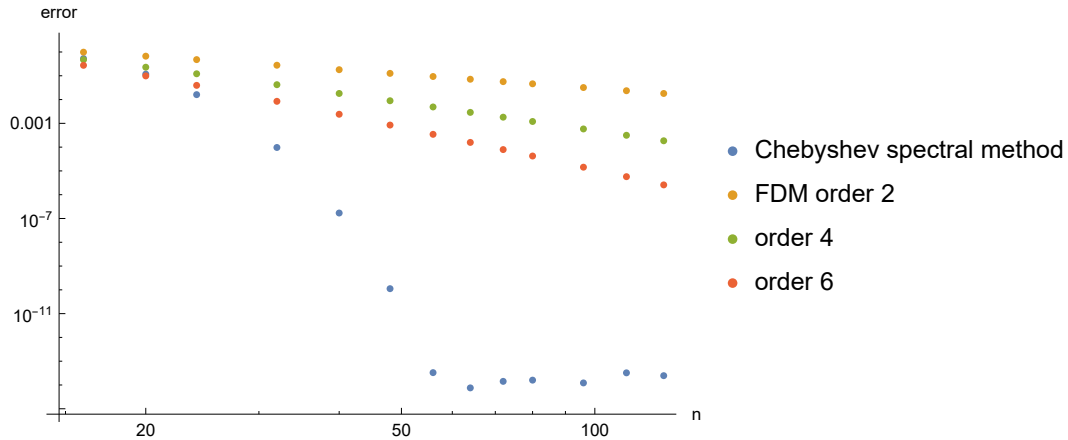
Error of the first derivative

```

In[ ]:= hs = N[2  $\pi$  / ns];
ListLogLogPlot[Table[Transpose[{ns, errorD1[[i, All]]}], {i, 1, nm}],
  PlotLegends -> {"Chebyshev spectral method", "FDM order 2", "order 4", "order 6"},
  AxesLabel -> {"n", "error"}]

```

Out[]:=



Error of the second derivative

```

In[ ]:= hs = N[2  $\pi$  / ns];
ListLogLogPlot[Table[Transpose[{ns, errorD2[[i, All]]}], {i, 1, nm}],
  PlotLegends -> {"Chebyshev spectral method", "FDM order 2", "order 4", "order 6"},
  AxesLabel -> {"n", "error"}]

```

Out[]:=

