Supporting textbook chapters: §§ 9.3.3, 9.3.4

Lecture 9, topics:

- Stability,
- Implicit and Crank-Nicolson methods,
- Spectral methods.

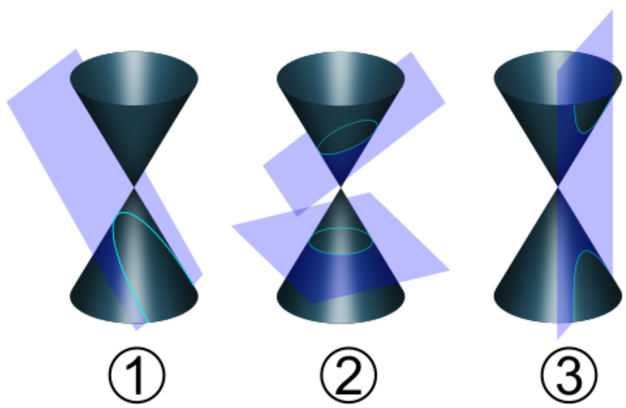
Recall...

$$\alpha\frac{\partial^2\phi}{\partial x^2} + \beta\frac{\partial^2\phi}{\partial x\partial y} + \gamma\frac{\partial^2\phi}{\partial y^2} + \delta\frac{\partial\phi}{\partial x} + \varepsilon\frac{\partial\phi}{\partial y} = f.$$

Classification based on

$$\Delta = \beta^2 - 4\alpha\gamma.$$

1. $\Delta = 0$: parabolic PDE,
2. $\Delta < 0$: elliptic PDE,
3. $\Delta > 0$: hyperbolic PDE.



1. Canonical parabolic PDE: the diffusion equation, $\kappa\nabla^2\phi - \dfrac{\partial T}{\partial t} = 0$,
2. Canonical elliptic PDE: the Poisson equation, $\nabla^2\phi = \rho$,
3. Canonical hyperbolic PDE: the wave equation, $c^2\nabla^2\phi - \dfrac{\partial^2 T}{\partial t^2} = 0$.

- Discretize system spatially and temporally. Can use finite differences, spectral coefficients, etc.
- Elliptical equations (e.g., Poisson eqn.):
  - Jacobi relaxation (always stable),
  - Speed-up with overrelaxation (not always stable),
  - Gauss-Seidel (overrelaxed or not): replace on the fly; more stable than Jacobi when overrelaxing.
- Parabolic PDEs (e.g., heat eqn):
  - FTCS (Forward Time, Centred Space) scheme: centred finite-diff. in space, forward Euler in time
  - Stable if sufficient spatial resolution.

- Hyperbolic PDEs (e.g., wave eqn.):
  - Von Neumann analysis says FTCS never stable.
  - This week: better schemes for hyperbolic PDEs.
- Von Neumann stability analysis: plug a Fourier mode, see if it grows or not.

Today: stable and accurate schemes for Hyperbolic PDEs?

The implicit method

We have choices on how to discretize in time the set of ODEs

$$\frac{\partial\phi_m}{\partial t} = \psi_m, \quad \text{and} \quad \frac{\partial\psi_m}{\partial t} = \frac{c^2}{a^2}(\phi_{m+1} - 2\phi_m + \phi_{m-1})$$

"Explicit" method we saw last time was

$$\begin{bmatrix}\phi_m^{n+1}\\ \psi_m^{n+1}\end{bmatrix} = \begin{bmatrix}1 & +h\\ -\frac{2hc^2}{a^2} & 1\end{bmatrix}\begin{bmatrix}\phi_m^n\\ \psi_m^n\end{bmatrix} + \begin{bmatrix}0\\ \frac{c^2h}{a^2}\left(\phi_{m+1}^n + \phi_{m-1}^n\right)\end{bmatrix}$$

But what if we evaluate the RHS at time $t+h$ instead of t?

To compute with the "implicit method"

- first do $h \to -h$ (from the current time step, compute the *previous* one):

$$\phi_m^{n-1} = \phi_m^n - h\psi_m^n,$$
$$\psi_m^{n-1} = \psi_m^n - h\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right),$$

- Then, $n \to n+1$ (one shift forward in time):

$$\phi_m^n = \phi_m^{n+1} - h\psi_m^{n+1},$$
$$\psi_m^n = \psi_m^{n+1} - h\frac{c^2}{a^2}\left(\phi_{m-1}^{n+1} + \phi_{m+1}^{n+1} - 2\phi_m^{n+1}\right),$$

or

$$\begin{bmatrix}\phi_m^n \\ \psi_m^n\end{bmatrix} = \begin{bmatrix}1 & -h \\ +\frac{2hc^2}{a^2} & 1\end{bmatrix}\begin{bmatrix}\phi_m^{n+1} \\ \psi_m^{n+1}\end{bmatrix} - \begin{bmatrix}0 \\ \frac{c^2h}{a^2}\left(\phi_{m+1}^{n+1} + \phi_{m-1}^{n+1}\right)\end{bmatrix}$$

"Implicit": we now have a set of simultaneous equations relating the values of $\phi,\ \psi$ at t to their values at $t+h$.

Why bother solving these simultaneous equations, rather than using an "explicit" expression for the values of $\phi,\ \psi$ at $t+h$ given their values at t ?

Because of stability.

Stability

Examine implicit step

$$\begin{bmatrix}\phi_m^n \\ \psi_m^n\end{bmatrix} = \begin{bmatrix}1 & -h \\ +\frac{2hc^2}{a^2} & 1\end{bmatrix}\begin{bmatrix}\phi_m^{n+1} \\ \psi_m^{n+1}\end{bmatrix} - \begin{bmatrix}0 \\ \frac{c^2h}{a^2}\left(\phi_{m+1}^{n+1} + \phi_{m-1}^{n+1}\right)\end{bmatrix}$$

If we do the Von Neumann substitution, $(\phi_m^n, \psi_m^n) = \left(\widehat{\phi}_k^n, \widehat{\psi}_k^n\right)\exp(ikma)$, we get

$$\mathbf{B}\begin{bmatrix}\widehat{\phi}_k^{n+1} \\ \widehat{\psi}_k^{n+1}\end{bmatrix} = \begin{bmatrix}\widehat{\phi}_k^n \\ \widehat{\psi}_k^n\end{bmatrix} \Rightarrow \begin{bmatrix}\widehat{\phi}_k^{n+1} \\ \widehat{\psi}_k^{n+1}\end{bmatrix} = \mathbf{B}^{-1}\begin{bmatrix}\widehat{\phi}_k^n \\ \widehat{\psi}_k^n\end{bmatrix}.$$

with:

$$\mathbf{B} = \begin{bmatrix}1 & -h \\ hr^2 & 1\end{bmatrix}, r = \frac{2c}{a}\sin\frac{ka}{2}$$

In [14]:
```
from sympy import *
init_printing()
h, r = symbols('h, r', positive=True)
B = Matrix([[1, -h], [h*r**2, 1]])
B
```

Out[14]:

$$\begin{bmatrix}1 & -h \\ hr^2 & 1\end{bmatrix}$$

In [15]:
```
# inverse of B
B**-1
```

Out[15]:

$$\begin{bmatrix}\frac{1}{h^2r^2+1} & \frac{h}{h^2r^2+1} \\ -\frac{hr^2}{h^2r^2+1} & \frac{1}{h^2r^2+1}\end{bmatrix}$$

In [16]:
```
# eigenvalues as a list
L = list((B**-1).eigenvals().keys())
```

In [17]:
```
# First eigenvalue
L[0].factor()
```

Out[17]:

$$-\frac{i(hr+i)}{h^2r^2+1}$$

In [18]:
```
# Magnitude of first eigenvalue
abs(L[0].factor())
```

Out[18]:

$$\frac{1}{\sqrt{h^2r^2+1}}$$

In [19]:
```
# Magnitude of 2nd eigenvalue
abs(L[1].factor())
```

Out[19]:

$$\frac{1}{\sqrt{h^2r^2+1}}$$

$$\text{Recall} \quad \begin{bmatrix} \widehat{\phi}_k^{m+1} \\ \widehat{\psi}_k^{m+1} \end{bmatrix} = \mathbf{B}^{-1} \begin{bmatrix} \widehat{\phi}_k^{m} \\ \widehat{\psi}_k^{m} \end{bmatrix}.$$

The eigenvalues of $\mathbf{B}^{-1}$ are

$$\lambda_\pm = \frac{1 \pm ihr}{1 + h^2 r^2}, \qquad |\lambda_\pm| = \frac{1}{\sqrt{1 + h^2 r^2}} \leq 1.$$

- The eigenvalues are the growth factors and these are less than one.
- So the implicit method is unconditionally stable.
- But solutions decay exponentially! This is a big problem e.g. for the wave equation (all Fourier components of our solution, except k=0, die away... meaning a wave cannot propagate)

Crank-Nicolson

Crank-Nicolson: average of explicit (fwd Euler) and implicit methods.

Forward Euler, Explicit:

$$\phi_m^{n+1} = \phi_m^n + h\psi_m^n, \qquad \psi_m^{n+1} = \psi_m^n + h\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right).$$

Backward Euler, Implicit:

$$\phi_m^{n+1} - h\psi_m^{n+1} = \phi_m^n, \qquad \psi_m^n = \psi_m^{n+1} - h\frac{c^2}{a^2}\left(\phi_{m-1}^{n+1} + \phi_{m+1}^{n+1} - 2\phi_m^{n+1}\right).$$

Crank-Nicholson (C-N):

$$\phi_m^{n+1} - \frac{h}{2}\psi_m^{n+1} = \phi_m^n + \frac{h}{2}\psi_m^n$$
$$\psi_m^{n+1} - \frac{h}{2}\frac{c^2}{a^2}\left(\phi_{m-1}^{n+1} + \phi_{m+1}^{n+1} - 2\phi_m^{n+1}\right) = \psi_m^n + \frac{h}{2}\frac{c^2}{a^2}\left(\phi_{m-1}^n + \phi_{m+1}^n - 2\phi_m^n\right).$$

If we do the Von Neumann substitution, $(\phi_m^n, \psi_m^n) = \left(\widehat{\phi}_k^n, \widehat{\psi}_k^n\right)\exp(ikma)$, we get

$$\mathbf{B}' \begin{bmatrix} \widehat{\phi}_m^{n+1} \\ \widehat{\psi}_m^{n+1} \end{bmatrix} = \mathbf{A}' \begin{bmatrix} \widehat{\phi}_m^{n} \\ \widehat{\psi}_m^{n} \end{bmatrix},$$

or

$$\begin{bmatrix} \widehat{\phi}_m^{n+1} \\ \widehat{\psi}_m^{n+1} \end{bmatrix} = \mathbf{B}'^{-1}\mathbf{A}' \begin{bmatrix} \widehat{\phi}_m^{n} \\ \widehat{\psi}_m^{n}, \end{bmatrix}$$

with

$$\mathbf{B}'^{-1}\mathbf{A}' = \frac{a}{1 + h^2 r'^2}\begin{bmatrix} 1 - h^2 r'^2 & 2h \\ -2hr'^2 & 1 - h^2 r'^2 \end{bmatrix}, \qquad r' = \frac{c}{a}\sin\frac{ka}{2}$$

Growth factors of Crank-Nicolson are eigenvalues of $\mathbf{B}^{-1}\mathbf{A}$:

$$\lambda_\pm = \frac{1 \pm 2ihr' - h^2 r'^2}{1 + h^2 r'^2}, \qquad \boxed{|\lambda_\pm| = 1}.$$

- For Forward-Euler (Explicit), the growth factors are greater than one and the solution diverges.
- For Backward-Euler (Implicit), the growth factors are less than one and the solution decays to zero.
- For CN, the growth factors are one so the solution neither grows nor decays.
- It is also 2nd-order accurate in time, while both explicit and implicit methods are 1st-order accurate (*I won't show it but it is true*).

Spectral methods

General idea (for linear PDEs):

- Find yourself a set of orthogonal functions forming a basis of your function space
- Use transforms to express trial solution and its derivative(s) in this basis, with unknown coefficients
  - Remember, any linear combination of solutions is also itself a solution
- Use transforms to project initial conditions onto that basis, and use them to determine the coefficients
- Use inverse transforms to directly obtain the solution at any specified coordinates (e.g. at any time t, without stepping through all the previous time-steps)

Examples of "set of orthogonal functions forming a basis of your function space":

- $\sin(n\pi x/L)$, $n \in \mathbb{N}$ if quantity is zero at boundaries (assuming $x = 0$, L are the boundaries) or function is odd w.r.t. midline of domain (assuming $x = 0$ at midline),
- $\cos(n\pi x/L)$, $n \in \mathbb{N}$ if quantity has zero derivatives at boundaries (assuming $x = 0$, L are the boundaries) or function is even w.r.t. midline of domain (assuming $x = 0$ at midline),
- $\exp(in\pi x/L)$, $n \in \mathbb{N}$ if quantity is periodic,
- Chebyshev polynomials for more flexible combinations of boundary conditions or non-periodic, closed domains,
- Hermite polynomials on the $(-\infty, \infty)$ real line,
- Laguerre polynomials on the $(0, \infty)$ real half-line

We focus on $\sin/\cos/\exp$ bases, sometimes called "Fourier spectral methods"

- ⊖ large down-payment cost of computing FFTs
- ⊕ large return on investment: gives you the solution at any times without stepping through previous times
  - e.g. elliptic PDEs can be solved without the need of an iterative solver like relaxation method
- ⊕ numerical stability
- ⊖ difficult or impossible to implement in complicated geometries.
- ⊖ problematic for non-linear equations

e.g. for elliptic PDEs:

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = \rho;$$
$$\begin{pmatrix}\phi\\ \rho\end{pmatrix} = \sum_i\sum_j \begin{pmatrix}\widehat{\phi}_{ij}\\ \widehat{\rho}_{ij}\end{pmatrix}\exp(i(k_i x + \ell_j y)),$$
$$\text{Use orthogonality to project } \Rightarrow \widehat{\phi}_{ij} = -\frac{\widehat{\rho}_{ij}}{k_i^2+\ell_j^2}$$

and you are just one iFFT away from getting the solution ⇒ no need to use an iterative solver!

This is particularly useful with large sets of coupled PDEs, for which just one elliptic PDE can be the main bottleneck of a non-spectral implementation.

Practical implementation of spectral methods

$$f = \sum_{n=-\infty}^{\infty}\hat{f}_n\exp(ik_nx) \Rightarrow \frac{\partial f}{\partial x} = \sum_{n=-\infty}^{\infty} ik_n\hat{f}_n\exp(ik_nx),$$

or, in shorthand,

$$\frac{\partial f}{\partial x} \to ik_n\hat{f}_n, \quad \frac{\partial^2 f}{\partial x^2} \to -k_n^2\hat{f}_n$$

Next are a couple of examples of how to express functions and their derivatives in function space.

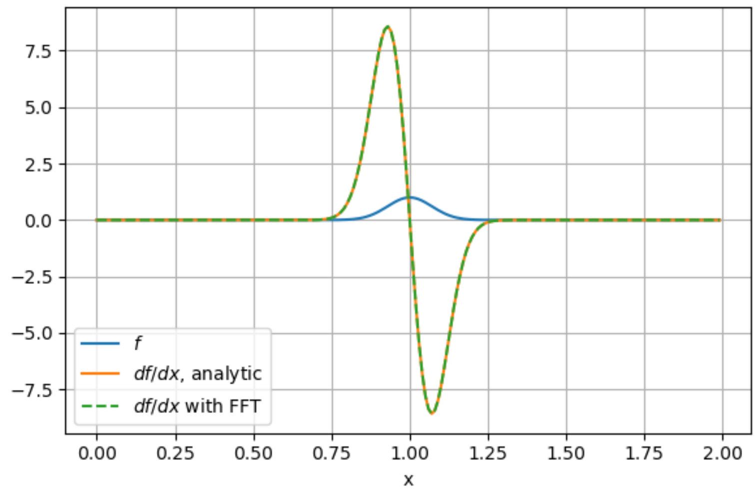
First derivative

$$f(x) = \exp\left(\frac{-(x-L/2)^2}{\Delta^2}\right)$$

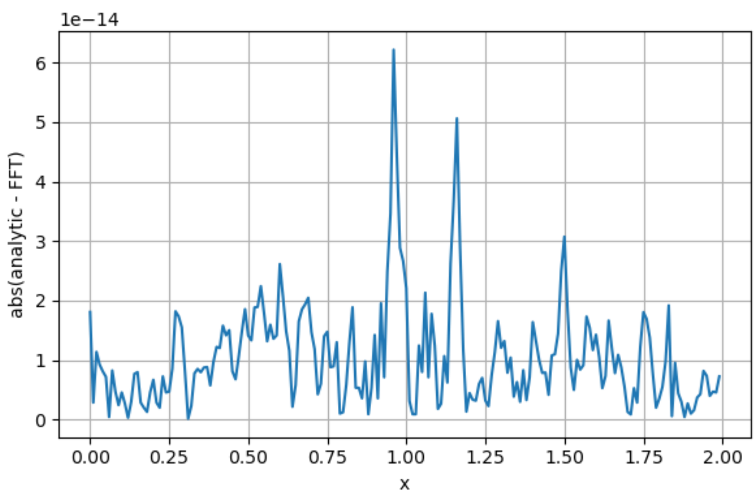
In [1]:
```
# Based on derivative_fft.py
import numpy as np
import matplotlib.pyplot as plt
from numpy.fft import rfft, irfft

#define function and its derivative
def f(x):
    return np.exp(-(x-L/2)**2/Delta**2)
def dfdx(x):
    return -2*(x-L/2)/Delta**2*np.exp(-(x-L/2)**2/Delta**2)

# define problem parameters
L = 2.0
Delta = 0.1
nx = 200

# define x, f(x), f'(x)
x = np.arange(0, L, L/nx)
farr = f(x)
farr_derivative = dfdx(x)
```

In [3]:
```
# now do the same thing spectrally:
fhat = rfft(farr)  # fourier transform
karray = np.arange(nx/2+1)*2*np.pi/L  # define k
fhat_derivative = complex(0, 1)*karray*fhat  # define ik*fhat
f_derivative_fft = irfft(fhat_derivative)  # and transform back
```

In [5]:
```python
plt.figure(dpi=100)
plt.plot(x, farr, label='$f$')
plt.plot(x, farr_derivative, label='$df/dx$, analytic')
plt.plot(x, f_derivative_fft, '--', label='$df/dx$ with FFT')
plt.legend(loc=3)
plt.xlabel('x')
plt.grid()
plt.tight_layout()
plt.show()
```



In [6]:
```python
plt.figure(dpi=100)
plt.plot(x, abs(farr_derivative-f_derivative_fft))
plt.xlabel('x')
plt.ylabel('abs(analytic - FFT)')
plt.grid()
plt.tight_layout()
plt.show()
```



Second derivative

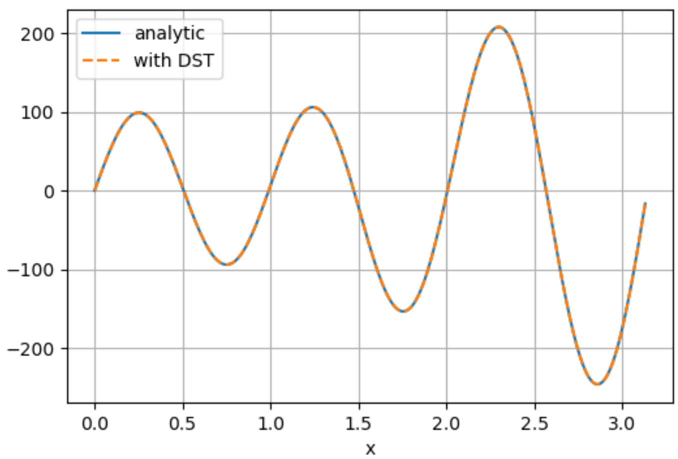
$$f = \sin(x) - 2\sin(4x) + 3\sin(5x) - 4\sin(6x)$$

In [7]:
```python
from dcst import dst, idst, dct, idct  # From Newman's dcst.py

N = 256
x = np.arange(N)*np.pi/N  # x = pi*n/N
farr = np.sin(x) - 2*np.sin(4*x) + 3*np.sin(5*x) - 4*np.sin(6*x)  # function is a sine series
fCoeffs = dst(farr)  # do fourier sine series
print('Original series: f = sin(x) - 2sin(4x) + 3sin(5x) - 4sin(6x)')
for j in range(7):
    print('Coefficient of sin({0}x): {1:.2e}'.format(j, fCoeffs[j]/N))
```

```
Original series: f = sin(x) - 2sin(4x) + 3sin(5x) - 4sin(6x)
Coefficient of sin(0x): 0.00e+00
Coefficient of sin(1x): 1.00e+00
Coefficient of sin(2x): -4.58e-17
Coefficient of sin(3x): -5.64e-16
Coefficient of sin(4x): -2.00e+00
Coefficient of sin(5x): 3.00e+00
Coefficient of sin(6x): -4.00e+00
```

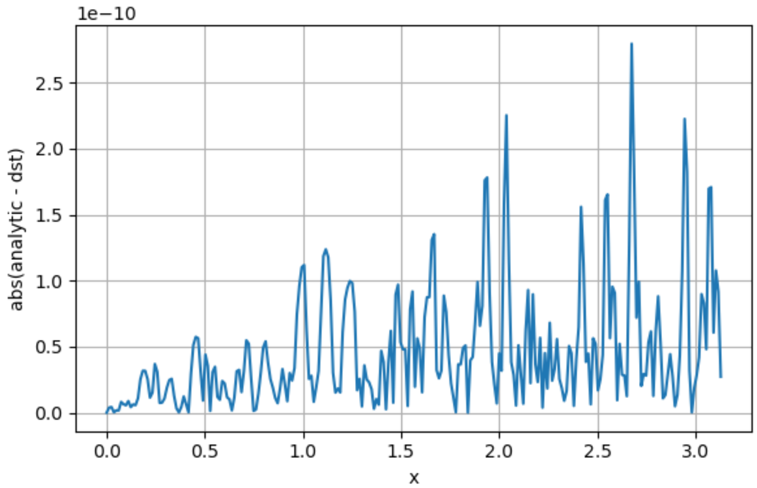
In [9]:
```python
# Below: 2nd derivative also a sine series
d2f_dx2_a = -np.sin(x) + 32*np.sin(4*x) - 75*np.sin(5*x) + 144*np.sin(6*x)

# 2nd derivative using Fourier transform
DerivativeCoeffs = -np.arange(N)**2*fCoeffs
d2f_dx2_b = idst(DerivativeCoeffs)
```

In [12]:
```python
plt.figure(dpi=100)
plt.plot(x, d2f_dx2_a, label='analytic')
plt.plot(x, d2f_dx2_b, '--', label='with DST')
plt.xlabel('x')
plt.legend()
plt.grid()
plt.show()
```



In [13]:

```
plt.figure(dpi=100)
plt.plot(x, abs(d2f_dx2_a - d2f_dx2_b))
plt.xlabel('x')
plt.ylabel('abs(analytic - dst)')
plt.tight_layout()
plt.grid()
plt.show()
```



Summary

- Last week: FTCS was
  - an explicit scheme,
  - unstable for hyperbolic PDEs (wave eqn.)
- This week, FTCS with implicit time stepping:
  - infers what RHS of next step is based on present step, and inverts.
  - stable for hyperbolic PDEs, but decays (bad accuracy)

- Crank-Nicolson:
  - average of implicit and explicit, also requires matrix inversion,
  - neither grows nor decays
- Spectral methods:
  - leverage $\partial_x f \to ik\hat{f}$ and powerful FFT methods,
  - can be much faster than grid-based schemes (though it depends),
  - Very accurate
  - Not too flexible when it comes to domain shape.

In [ ]: