Computational Physics (PHYS6350)

Lecture 16: Partial Differential Equations Part II

- Initial value problems
  - Heat equation
  - Wave equation

Reference: Chapter 9 of *Computational Physics* by Mark Newman

March 23, 2023

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Course materials: https://github.com/vlvovch/PHYS6350-ComputationalPhysics

Initial value problem in PDEs

Many PDEs describe time evolution of fields u(t,x)

For example *heat equation* describing the temperature profile

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2}$$

This equation describes the time evolution of u(t,x) given initial profile

$$u(t = 0, x) = u_0(x),$$

and boundary conditions

$$u(t, x = 0) = u_{\text{left}}(t),$$
$$u(t, x = L) = u_{\text{right}}(t).$$

If boundary conditions are static, the solution will approach a stationary profile at large times

Finite difference approach to heat equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

First, one discretizes the spatial coordinate into a grid with N+1 points, i.e.

$$x_k = ak, \qquad k = 0 \ldots N, \qquad a = L/N,$$

The spatial 2nd derivative is approximate with central difference

$$\frac{\partial^2 u(t,x)}{\partial x^2} \approx \frac{u(t,x+a) - 2u(t,x) + u(t,x-a)}{a^2}.$$

How to discretize time derivative?

Three common options:

- FTCS scheme
- Implicit scheme
- Crank-Nicolson method

Finite difference approach to heat equation: FTCS scheme

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2},$$

FTCS (Forward Time Centered Space) scheme

Time derivative approximated by forward difference

$$\frac{\partial u(t,x)}{\partial t} \approx \frac{u(t+h,x) - u(t,x)}{h}$$

This gives the following discretized PDE

$$\frac{u(t+h,x) - u(t,x)}{h} = D \frac{u(t,x+a) - 2u(t,x) + u(t,x-a)}{a^2}.$$

The method is explicit: to evaluate *u(t+h,x)* one only needs *u(t,x)* at the present time

Discretized form

$$u_k^{n+1} = u_k^n + r\,(u_{k+1}^n - 2u_k^n + u_{k-1}^n), \qquad k = 1 \ldots N-1.$$

$$r \equiv \frac{Dh}{a^2}$$

FTCS scheme for heat equation

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2},$$

```python
# Single iteration of the FTCS scheme in the time direction
# r = Dh/a^2 is the dimensionless parameter
def heat_FTCS_iteration(u, r):
    N = len(u) - 1

    unew = np.empty_like(u)

    # Boundary conditions
    unew[0] = u[0]
    unew[N] = u[N]


    # FTCS scheme
    for i in range(1,N):
        unew[i] = u[i] + r * (u[i+1] - 2 * u[i] + u[i-1])

    return unew
```

```python
# Perform nsteps FTCS time iterations for the heat equation
# u0: the initial profile
# h: the size of the time step
# nsteps: number of time steps
# a: the spatial cell size
# D: the diffusion constant
def heat_FTCS_solve(u0, h, nsteps, a, D = 1.):
    u = u0.copy()
    r = h * D / a**2
    for i in range(nsteps):
        u = heat_FTCS_iteration(u, r)

    return u
```

Example

Let us consider Example 9.3 from M. Newman, *Computational Physics*:

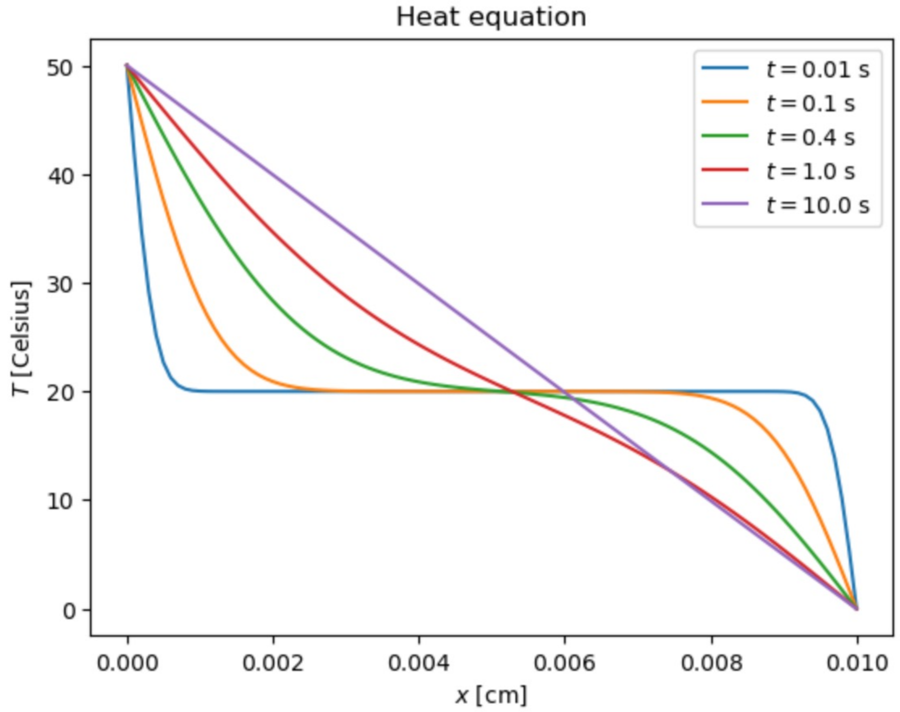
We have a 1 cm long steel container, initially at a temperature 20° C. It is placed in bath of cold water at 0° C and filled on top with hot water at 50° C. Our goal is to calculate the temperature profile as function of time. The thermal diffusivity constant for stainless steel is $D = 4.25 \cdot 10^{-6}$ m^2 s^{-1}.

We will calculate the profile at times $t = 0.01$ s, 0.1 s, 0.4 s, 1 s, and 10 s.

```
# Constants
L = 0.01       # Thickness of steel in meters
D = 4.25e-6    # Thermal diffusivity
N = 100        # Number of divisions in grid
a = L/N        # Grid spacing
h = 1e-4       # Time-step (in s)

print("Solving the heat equation with FTCS scheme")
print("r = h*D/a^2 =",h*D/a**2)

Tlo  = 0.0     # Low temperature in Celsius
Tmid = 20.0    # Intermediate temperature in Celsius
Thi  = 50.0    # High temperature in Celsius

# Initialize
u = np.zeros([N+1],float)
# Initial temperature
u[1:N] = Tmid
# Boundary conditions
u[0] = Thi
u[N] = Tlo
```

```
current_time = 0.
for time in times:
    nsteps = round((time - current_time)/h)
    u = heat_FTCS_solve(u, h, nsteps, a, D)
    profiles.append(u.copy())
    current_time = time
```

```
Solving the heat equation with FTCS scheme
r = h*D/a^2 = 0.0425
```



Animation

Let us consider Example 9.3 from M. Newman, *Computational Physics*:

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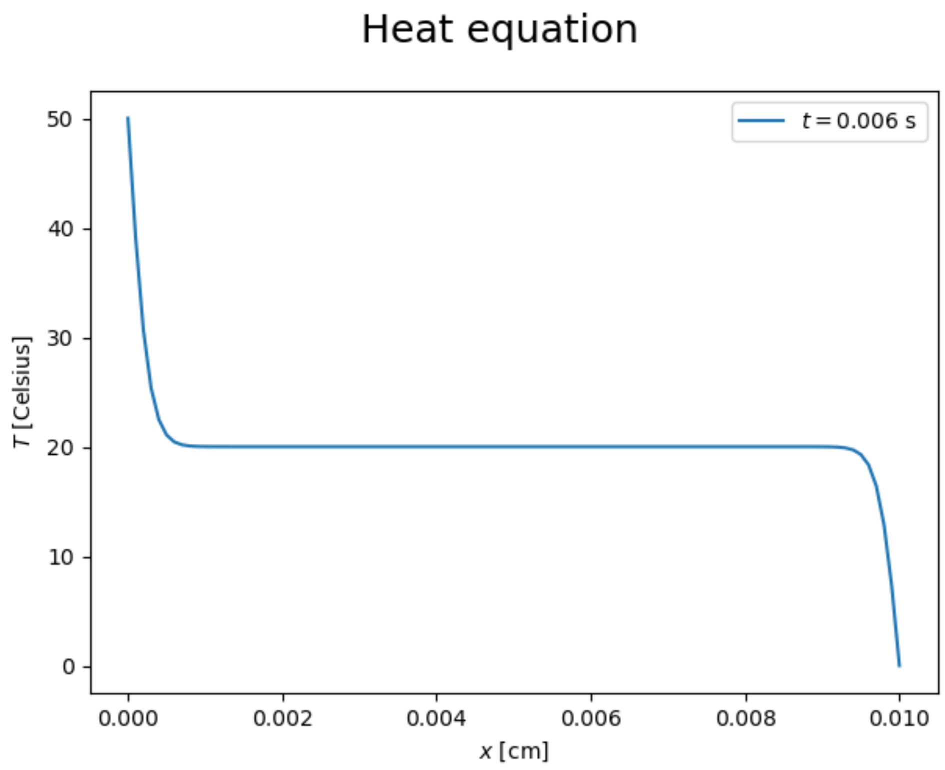
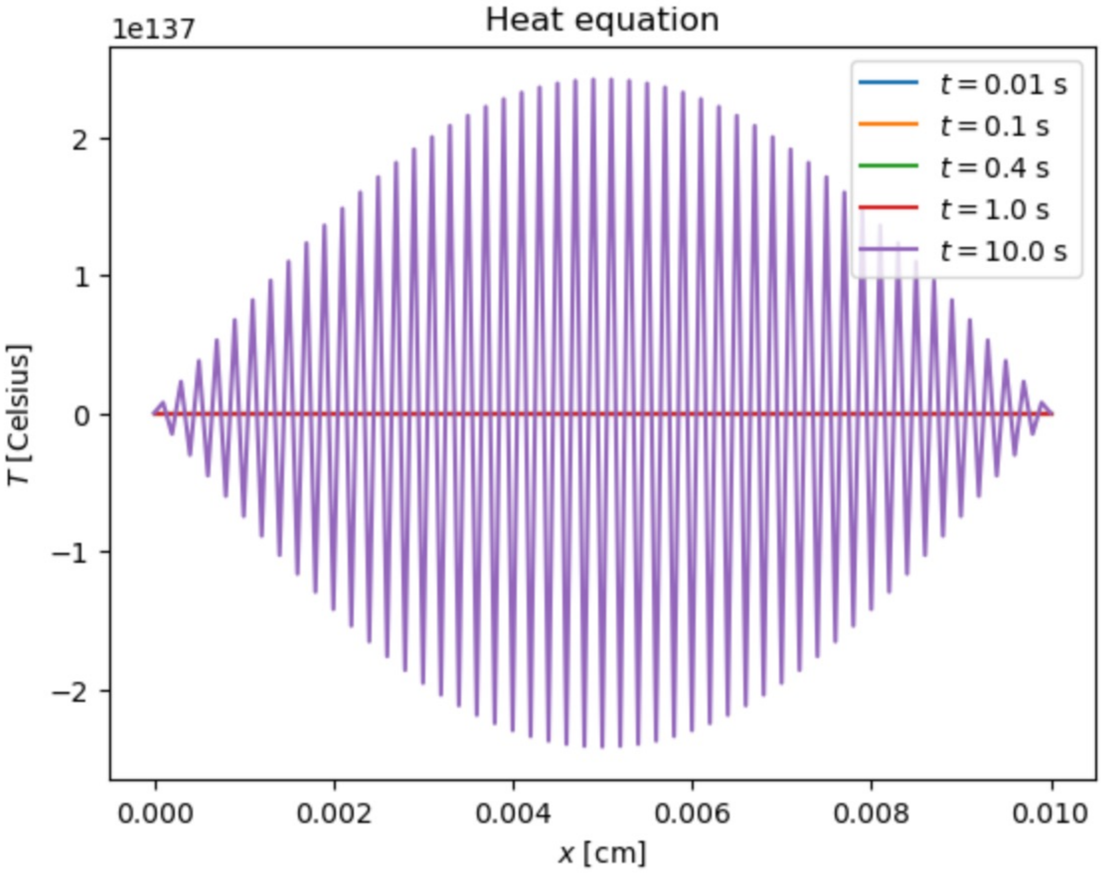
We will calculate the profile at times $t = 0.01$ s, 0.1 s, 0.4 s, 1 s, and 10 s.



Try a larger time step

```
Solving the heat equation with FTCS scheme
r = h*D/a^2 = 0.5099999999999999
```



The method is unstable if r $>$ 0.5

Stability analysis: Neumann method

Recall Fourier transform $u(t,x) = \sum_k c_k(t)\, e^{ikx}$

Analyze the following solutions: $u(t,x) = c_k(t) e^{ikx}$

Plugging into

$$\frac{u(t+h,x) - u(t,x)}{h} = D\frac{u(t,x+a) - 2u(t,x) + u(t,x-a)}{a^2}$$

one gets

$$u(t+h,x) = [1 - 4r\sin^2(ka/2)]c_k(t)e^{ikx}$$

i.e.

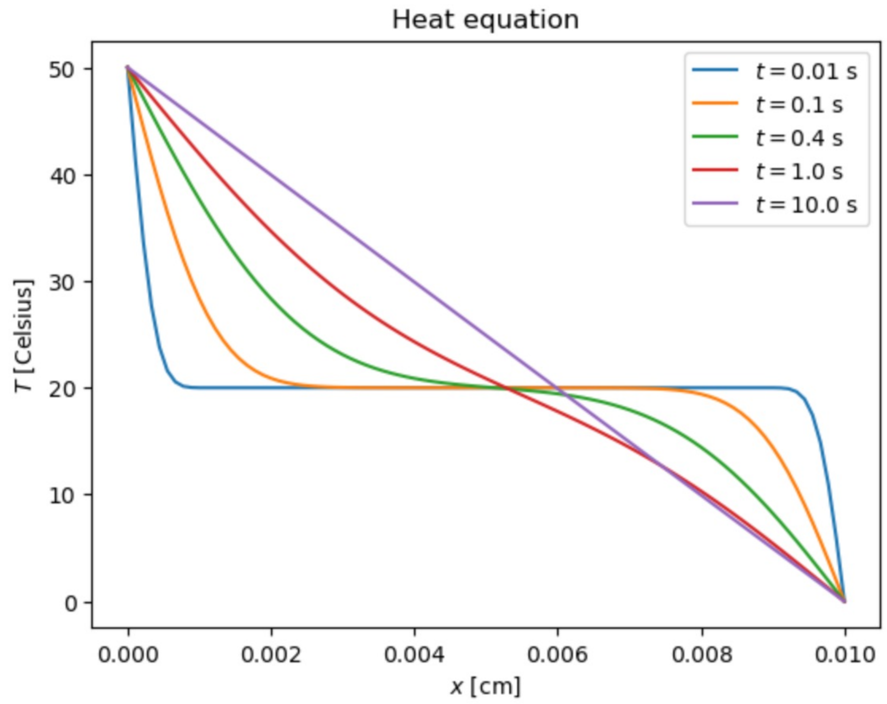
$$c_k(t+h) = [1 - 4r\sin^2(ka/2)]c_k(t), \qquad c_k^{n+1} = [1 - 4r\sin^2(ka/2)]^n c_k^0$$

The method is stable if $r<1/2$

Try a larger space step to compensate for large time step

```
# Constants
L = 0.01        # Thickness of steel in meters
D = 4.25e-6     # Thermal diffusivity
N = 90          # Number of divisions in grid
a = L/N         # Grid spacing
h = 1.2e-3      # Time-step (in s)
```

```
Solving the heat equation with FTCS scheme
r = h*D/a^2 = 0.41309999999999986
```



Implicit scheme

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2},$$

Time derivative approximated by backward difference

$$\frac{\partial u(t+h,x)}{\partial t} \approx \frac{u(t+h,x)-u(t,x)}{h}$$

This gives the following discretized PDE

$$\frac{u(t+h,x)-u(t,x)}{h} = D\frac{u(t+h,x+a)-2u(t+h,x)+u(t+h,x-a)}{a^2}$$

Discretized form

$$u_k^{n+1} = u_k^n + r\,(u_{k+1}^{n+1} - 2u_k^{n+1} + u_{k-1}^{n+1}), \qquad k = 1\ldots N-1$$

Tridiagonal system of linear equations at each step

$$-ru_{k-1}^{n+1} + (1+2r)u_k^{n+1} - ru_{k+1}^{n+1} = u_k^n, \qquad k = 1\ldots N-1$$

Neumann stability analysis: method is stable for any r

Implicit scheme for heat equation

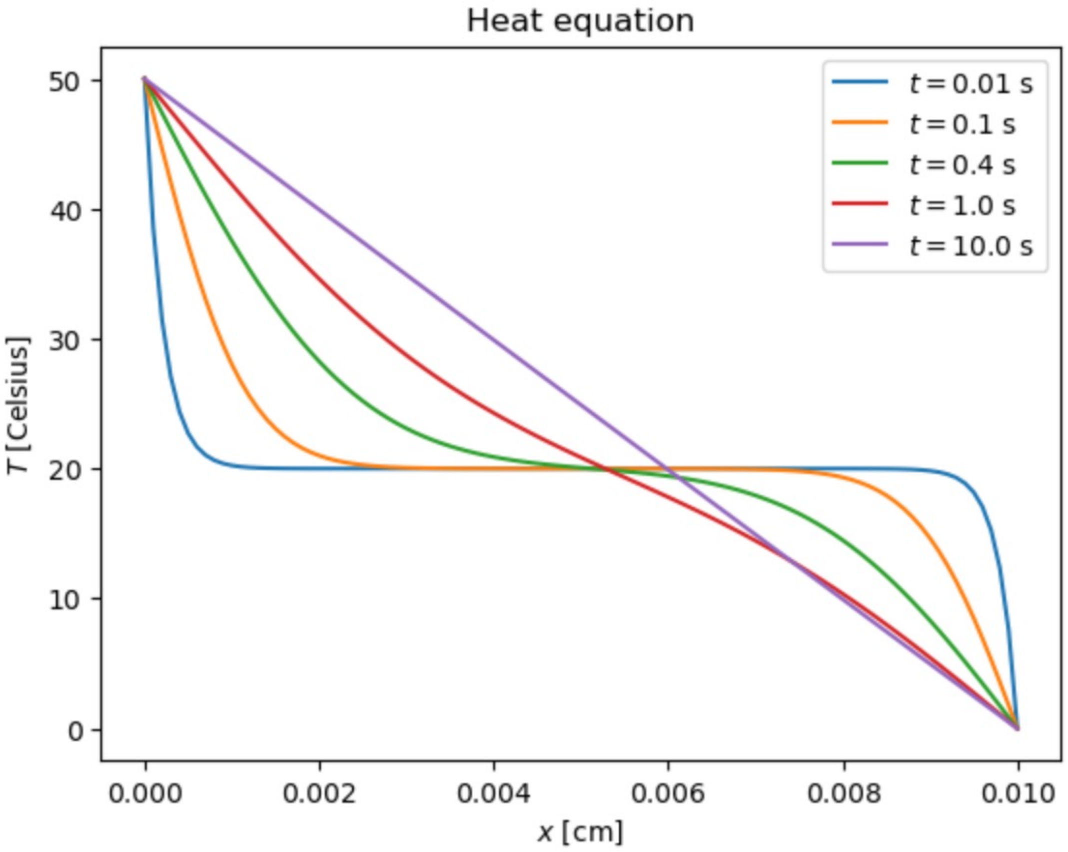
$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2},$$

```python
# Single iteration of the FTCS scheme in the time direction
# The new field is written into unew
# r = Dh/a^2 is the dimensionless parameter
def heat_implicit_iteration(u, r):
    N = len(u) - 1

    unew = np.empty_like(u)

    # Boundary conditions
    unew[0] = u[0]
    unew[N] = u[N]

    d  = np.full(N-1, 1+2.*r)
    ud = np.full(N-1, -r)
    ld = np.full(N-1, -r)
    v  = np.array(u[1:N])
    v[0]   += r * u[0]
    v[N-2] += r * u[N]

    unew[1:N] = linsolve_tridiagonal(d,ld,ud,v)

    return unew
```

```python
# Perform nsteps FTCS time iterations for the heat equation
# u0: the initial profile
# h: the size of the time step
# nsteps: number of time steps
# a: the spatial cell size
# D: the diffusion constant
def heat_implicit_solve(u0, h, nsteps, a, D = 1.):
    u = u0.copy()
    r = h * D / a**2
    # print("Heat equation with r =", r)
    for i in range(nsteps):
        u = heat_implicit_iteration(u, r)

    return u
```

Implicit scheme: large time step

```
Solving the heat equation with implicit scheme
r = h*D/a^2 = 4.25
```



Crank-Nicolson scheme

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2};$$

"Average" between forward and backward difference

$$\frac{\partial u(t,x)}{\partial t} \approx \frac{1}{2}\left[D\frac{\partial^2 u(t+h,x)}{\partial x^2} + D\frac{\partial^2 u(t,x)}{\partial x^2}\right]$$

Essentially a trapezoidal rule for the time integration (more accurate than forward/backward differences)

$$\frac{u(t+h,x)-u(t,x)}{h} = D\frac{u(t+h,x+a)-2u(t+h,x)+u(t+h,x-a)}{a^2}$$

Discretized form

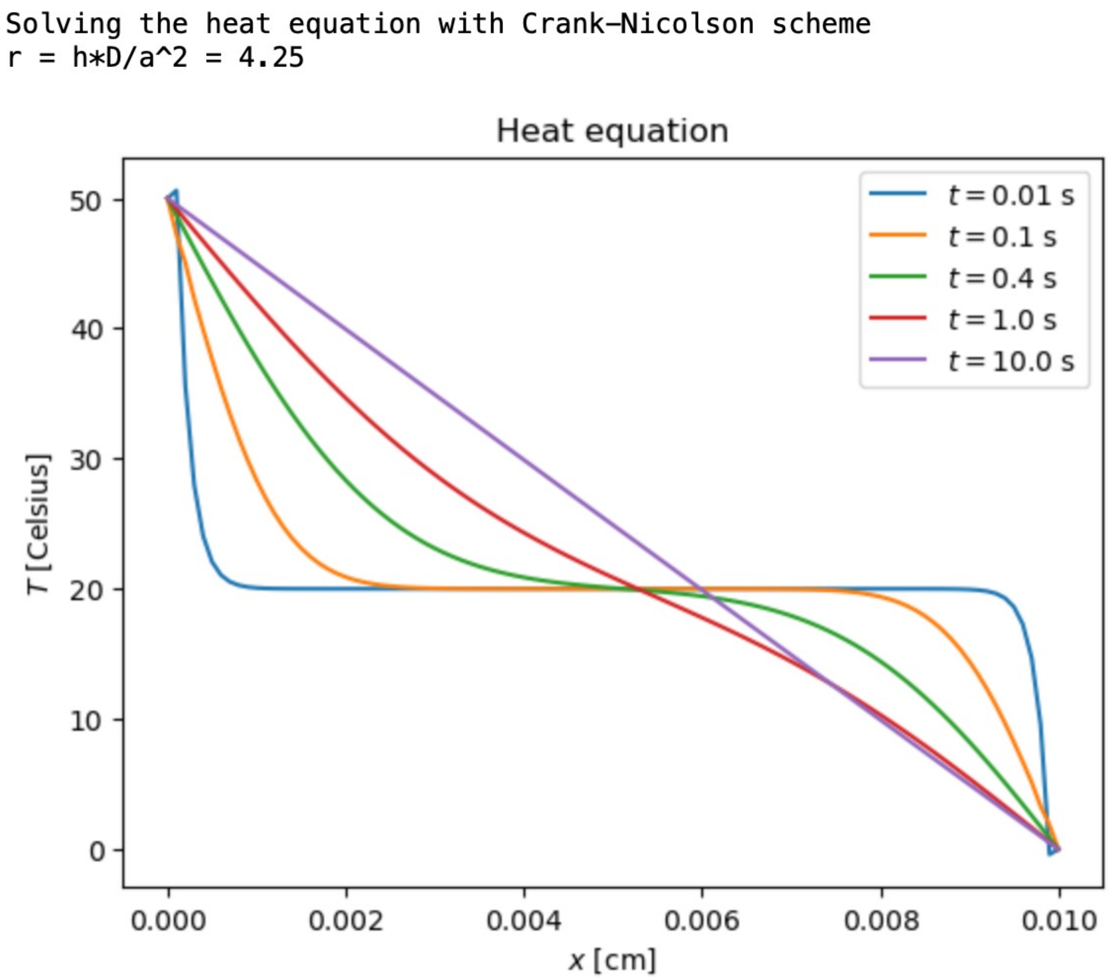
$$\frac{u(t+h,x)-u(t,x)}{h} = \frac{D}{2}\frac{u(t+h,x+a)-2u(t+h,x)+u(t+h,x-a)}{a^2} + \frac{D}{2}\frac{u(t,x+a)-2u(t,x)+u(t,x-a)}{a^2}.$$

Tridiagonal system of linear equations at each step

$$-ru_{k-1}^{n+1} + 2(1+r)u_k^{n+1} - ru_{k+1}^{n+1} = ru_{k-1}^n + 2(1-r)u_k^n + ru_{k+1}^n, \qquad k = 1\ldots N-1.$$

Neumann stability analysis: method is stable for any r

Crank-Nicolson scheme: large time step



Heat equation in two dimensions

In two dimensions the heat equation reads

$$\frac{\partial u}{\partial t} = D\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right].$$

This equation describes the time evolution of $u(t, x, y)$ given initial profile

$$u(t = 0, x, y) = u_0(x, y),$$

and boundary conditions

$$\begin{aligned} u(t, x = 0, y) &= u_{\text{left}}(t; y), \\ u(t, x = L, y) &= u_{\text{right}}(t; y), \\ u(t, x = 0, y) &= u_{\text{bottom}}(t; x), \\ u(t, x = L, y) &= u_{\text{top}}(t; x). \end{aligned}$$

Now we have two perform discretization in both x and y directions. Taking the same step size a in both directions, we obtain the following discretized FTCS scheme:

$$u_{i,j}^{n+1} = u_{i,j}^n + r\,(u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n) + r\,(u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n), \qquad i = 1 \ldots N-1, \quad j = 1 \ldots M-1.$$

Here, as before,

$$r \equiv \frac{Dh}{a^2},$$

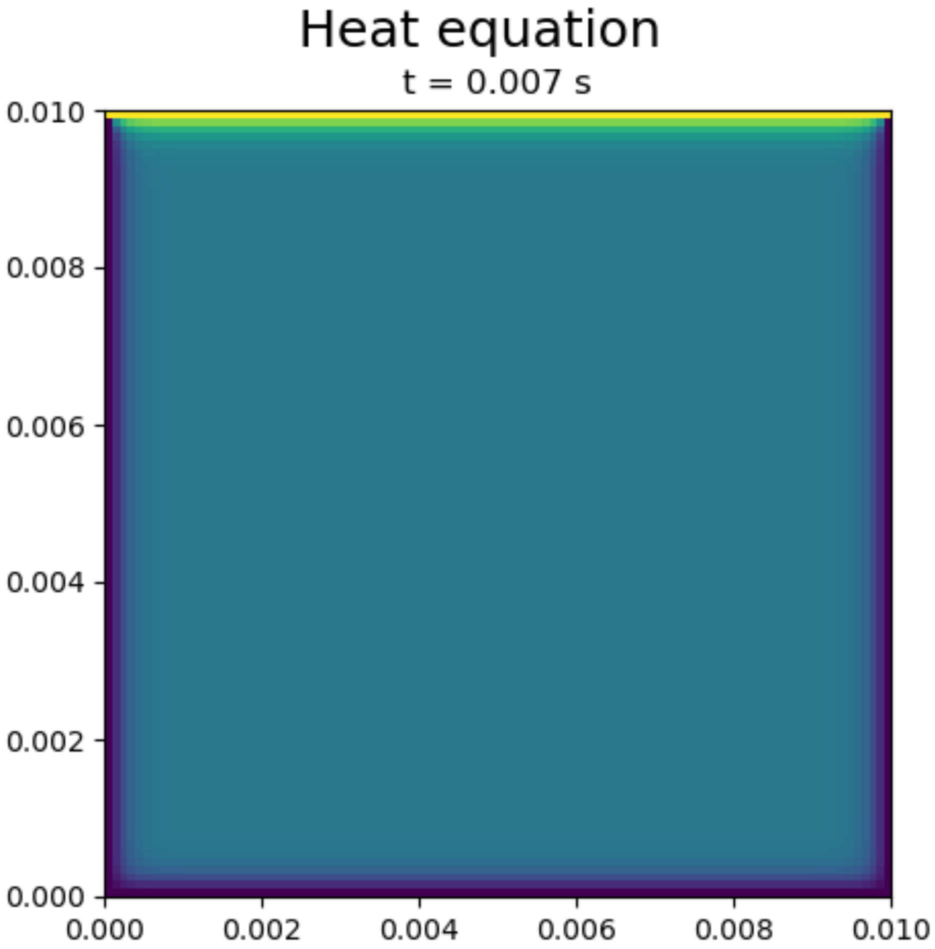
$N = L_x/a$, $M = L_y/a$, and

$$u_{i,j}^n = u(t + hn, ai, aj).$$

Heat equation in two dimensions: FTCS scheme

```
# Single iteration of the 2D FTCS scheme in the time direction
# r = Dh/a^2 is the dimensionless parameter
def heat_FTCS_iteration_2D(u, r):
    N, M = u.shape

    unew = np.empty_like(u)

    # Boundary conditions
    unew[  0, :]   = u[ 0, :]
    unew[N-1, :]   = u[N-1, :]
    unew[ :, 0]    = u[ :, 0]
    unew[ :, M-1]  = u[ :, M-1]

    # FTCS scheme
    for i in range(1, M-1):
        for j in range(1, N-1):
            unew[i, j] = u[i, j] + r * (u[i+1, j] - 2 * u[i, j] + u[i-1, j]) + r * (u[i, j+1] - 2 * u[i, j] + u[i,

    return unew

# Perform nsteps 2D FTCS time iterations for the heat equation
# u0: the initial profile
# h: the size of the time step
# nsteps: number of time steps
# a: the spatial cell size
# D: the diffusion constant
def heat_FTCS_solve_2D(u0, h, nsteps, a, D = 1.):
    u = u0.copy()
    r = h * D / a**2
    for i in range(nsteps):
        u = heat_FTCS_iteration_2D(u, r)

    return u
```

Heat equation in two dimensions: FTCS scheme



Wave equation

Wave equation is an example of a second-order linear PDE describing the waves and standing wave fields. In one dimensions it reads

$$\frac{\partial^2 \phi}{\partial t^2} = v^2 \frac{\partial^2 \phi}{\partial x^2}.$$

Since it is a 2nd order PDE, it is supplemented by initial conditions for both $\phi(t = 0, x)$ and $\phi_t'(t = 0, x)$:

$$\phi(t = 0, x) = \phi_0(x),$$
$$\phi_t'(t = 0, x) = \phi_0'(x).$$

The boundary conditions can be of either Dirichlet

$$\phi(t, x = 0) = \phi_{\text{left}}(t),$$
$$\phi(t, x = L) = \phi_{\text{right}}(t),$$

or Neumann

$$\phi_x'(t, x = 0) = \phi_{\text{left}}'(t),$$
$$\phi_x'(t, x = L) = \phi_{\text{right}}'(t),$$

forms.

We shall focus on the Dirichlet form.

Finite difference approach

Finite difference approach

To deal with the second-order time derivative we denote

$$\psi(t,x) \equiv \frac{\partial \phi}{\partial t}.$$

This way we are dealing with a system of first-order (in t) PDEs

$$\frac{\partial \phi}{\partial t} = \psi(t,x),$$
$$\frac{\partial \psi}{\partial t} = v^2 \frac{\partial^2 \phi}{\partial x^2}.$$

To apply the finite difference method we first approximate the derivative $\partial^2\phi/\partial x^2$ by the lowest order central difference, just like for the heat equation,

$$\frac{\partial^2 \phi(t,x)}{\partial x^2} \approx \frac{\phi(t,x+a) - 2\phi(t,x) + \phi(t,x-a)}{a^2}.$$

To solve the PDEs numerically we apply the same procedure as for the heat equation, but for $\phi(t,x)$ and $\psi(t,x)$ simultaneously. Denoting $\phi(t=nh, x=ka) = \phi_k^n$ and $\psi(t=nh, x=ka) = \psi_k^n$ we get

FTCS scheme

$$\begin{aligned}
\phi_k^{n+1} &= \phi_k^n + h\psi_k^n, \\
\psi_k^{n+1} &= \psi_k^n + r\,(\phi_{k+1}^n - 2\phi_k^n + \phi_{k-1}^n), \qquad k = 1 \ldots N-1.
\end{aligned}$$

Wave equation

```python
# Single iteration of the FTCS scheme in the time direction
# h is the time step
# r = Dh/a^2 is the dimensionless parameter
def wave_FTCS_iteration(phi, psi, h, r):
    N = len(phi) - 1

    phinew = np.empty_like(phi)
    psinew = np.empty_like(psi)

    # Boundary conditions (here static Dirichlet)
    phinew[0] = phi[0]
    phinew[N] = phi[N]
    psinew[0] = 0.
    psinew[N] = 0.


    # FTCS scheme
    for i in range(1,N):
        phinew[i] = phi[i] + h * psi[i]
        psinew[i] = psi[i] + r * (phi[i+1] - 2 * phi[i] + phi[i-1])

    return phinew, psinew
```

```python
# Perform nsteps FTCS time iterations for the heat equation
# u0: the initial profile
# h: the size of the time step
# nsteps: number of time steps
# a: the spatial cell size
# D: the diffusion constant
def wave_FTCS_solve(phi0, psi0, h, nsteps, a, v = 1.):
    phi = phi0.copy()
    psi = psi0.copy()
    r = h * v**2 / a**2
    for i in range(nsteps):
        phi, psi = wave_FTCS_iteration(phi, psi, h, r)

    return phi, psi
```

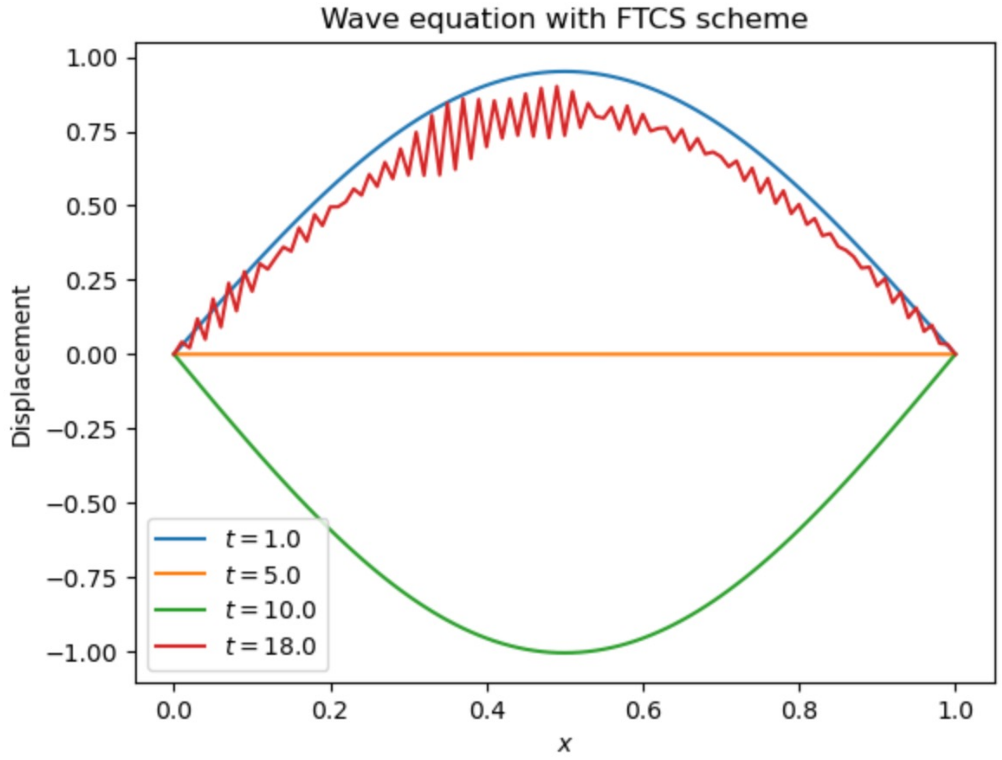
Wave equation

```
# Constants
L = 1          # Length
v = 0.1        # Wave propagation speed
N = 100        # Number of divisions in grid
a = L/N        # Grid spacing
h = 1e-2       # Time-step

print("Solving the wave equation with FTCS scheme")
print("r = h*v^2/a^2 =",h*v**2/a**2)



# Initialize
phi = np.array([np.sin(k*np.pi/N) for k in range(N+1)])
psi = np.zeros([N+1],float)
```



FTCS scheme is unstable

Wave equation

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# Constants
L = 1          # Length
v = 0.1        # Wave propagation speed
N = 100        # Number of divisions in grid
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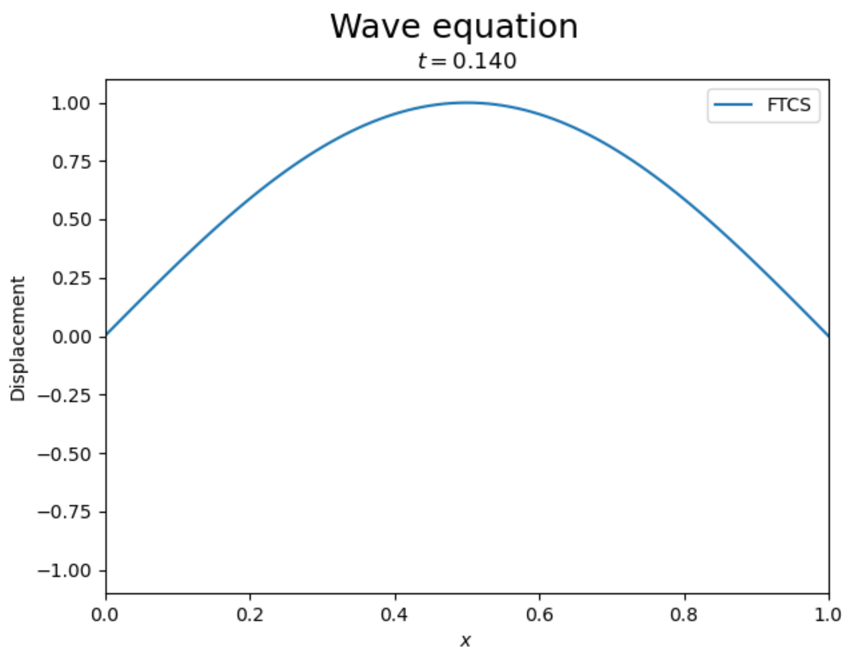
```



FTCS scheme is unstable

Wave equation: other schemes

Implicit scheme

$$\phi_k^{n+1} = \phi_k^n + h\psi_k^{n+1},$$
$$\psi_k^{n+1} = \psi_k^n + r\,(\phi_{k+1}^{n+1} - 2\phi_k^{n+1} + \phi_{k-1}^{n+1}), \qquad k = 1 \ldots N-1.$$

Substituting the first equation into the second one gets the tridiagonal system of linear equations for ψ_k^{n+1}:

$$-rh\psi_{k+1}^{n+1} + (1+2rh)\psi_k^{n+1} - rh\psi_{k-1}^{n+1} = \psi_k^n + r\,(\phi_{k+1}^n - 2\phi_k^n + \phi_{k-1}^n), \qquad k = 1 \ldots N-1$$

Stable, but has exponential decay (waves don't propagate forever)

Crank-Nicolson scheme

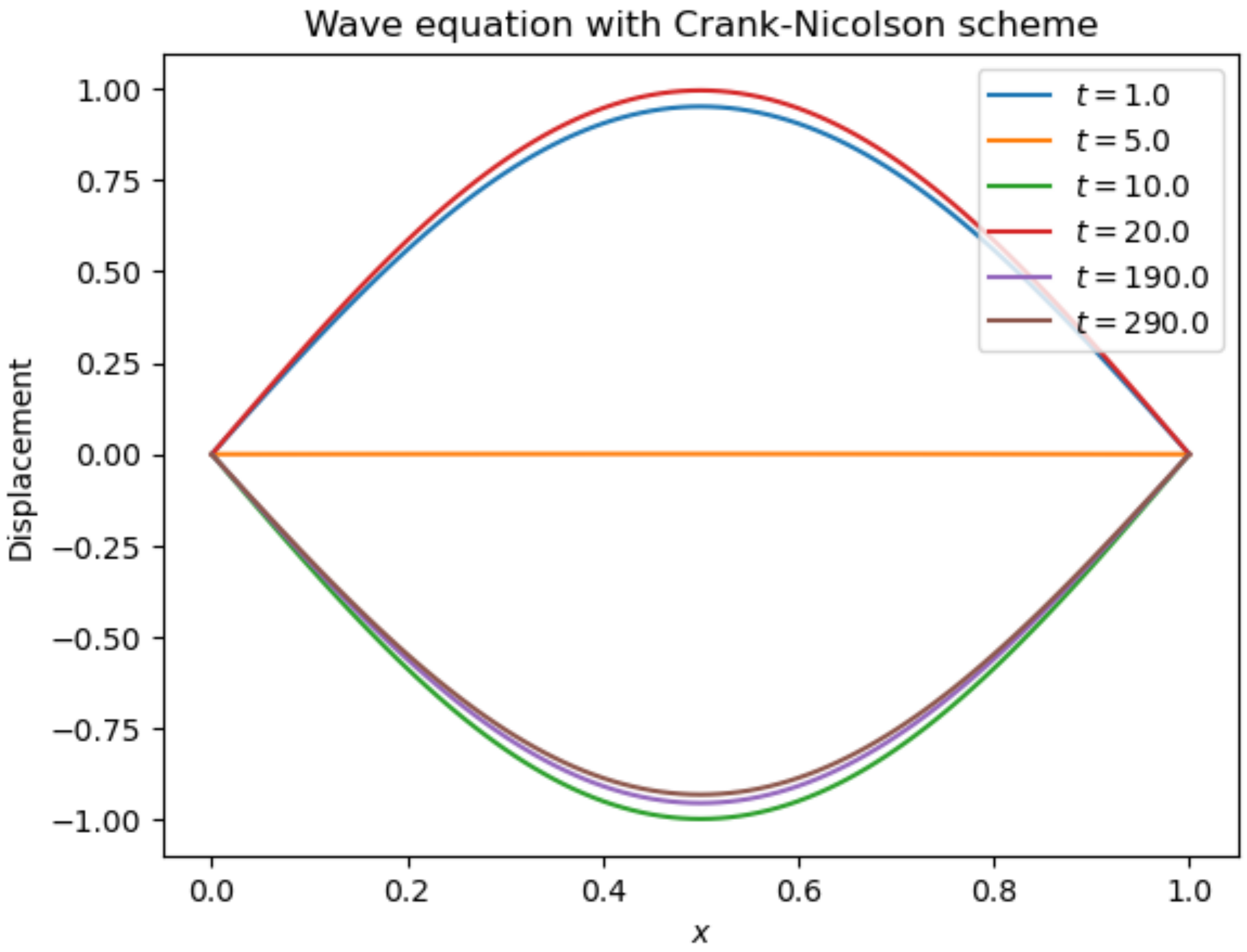
$$\phi_k^{n+1} = \phi_k^n + \frac{h}{2}\left[\psi_k^{n+1} + \psi_k^n\right],$$
$$\psi_k^{n+1} = \psi_k^n + \frac{r}{2}\,(\phi_{k+1}^{n+1} - 2\phi_k^{n+1} + \phi_{k-1}^{n+1}) + \frac{r}{2}\,(\phi_{k+1}^n - 2\phi_k^n + \phi_{k-1}^n), \qquad k = 1 \ldots N-1.$$

Substituting the first equation into the second one gets the tridiagonal system of linear equations for ψ_k^{n+1}:

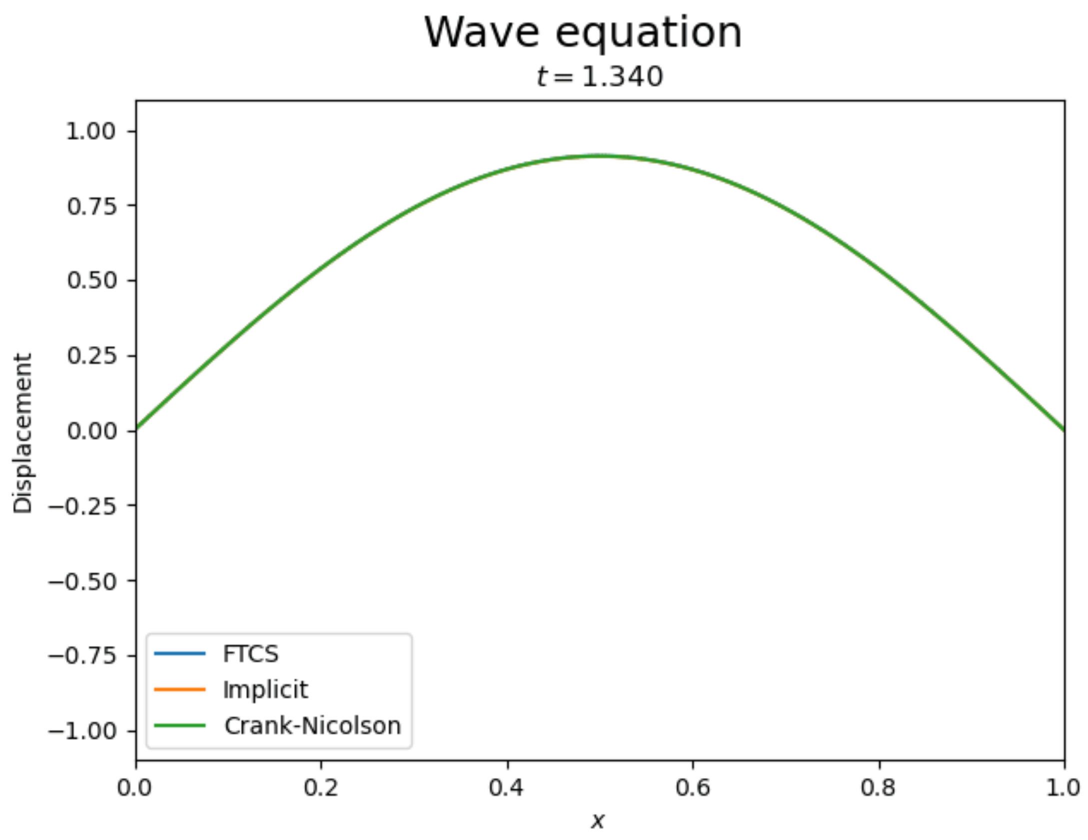
$$-rh\psi_{k+1}^{n+1} + 2(1+rh)\psi_k^{n+1} - rh\psi_{k-1}^{n+1} = 2\psi_k^n + 2r\,(\phi_{k+1}^n - 2\phi_k^n + \phi_{k-1}^n) + rh\,(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n), \qquad k = 1 \ldots N-1.$$

Stable, no growth or decay

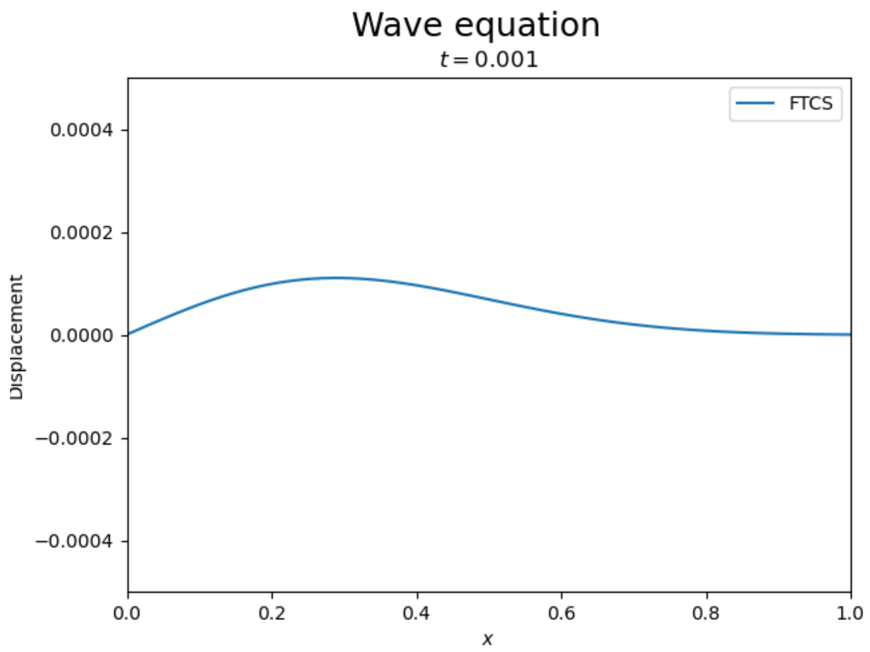
Wave equation with Crank-Nicolson scheme



Wave equation: Comparison



Wave equation: Pulses



Wave equation: Pulses