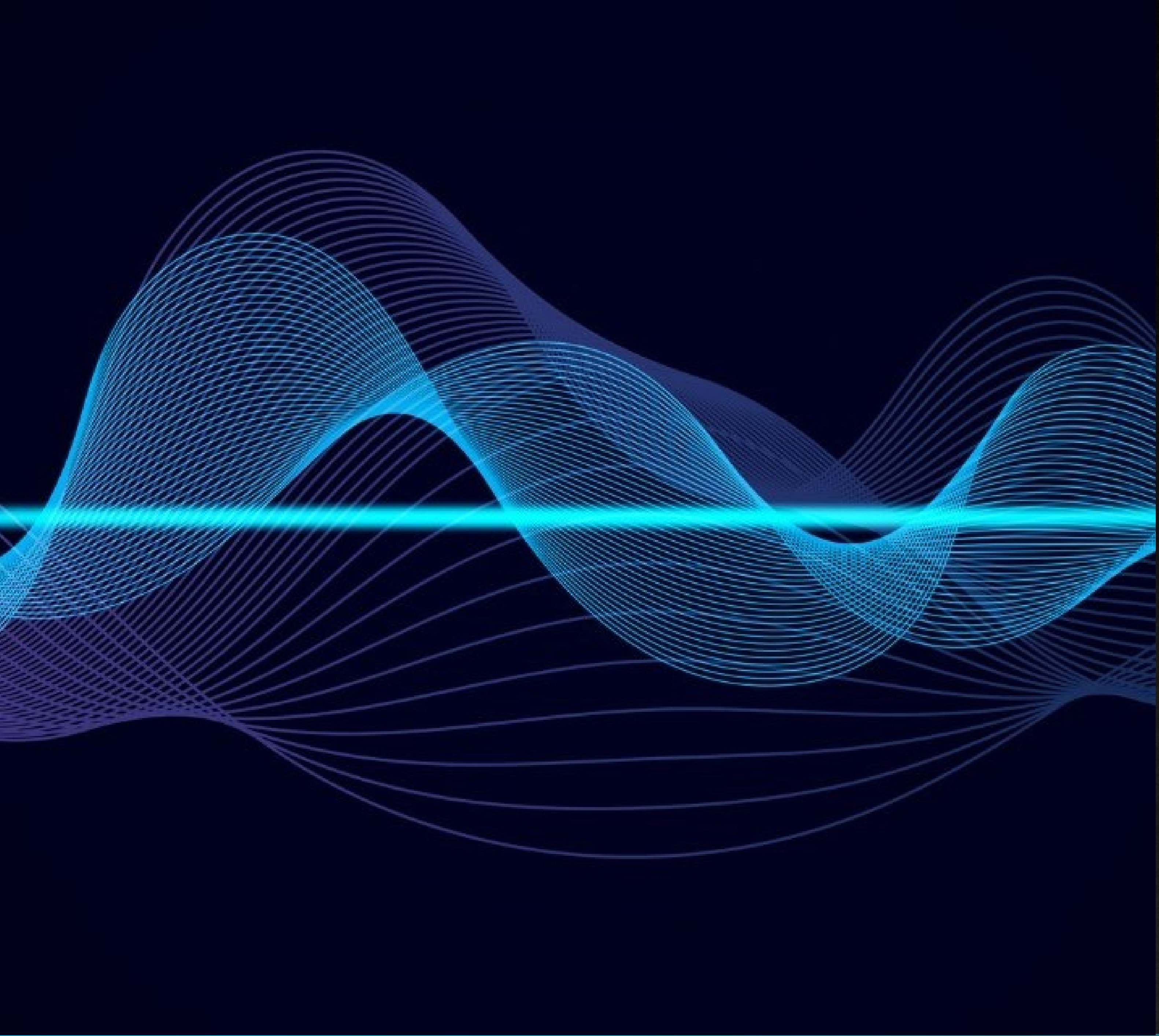


Computational Physics

PHYS 6260

PDEs: Initial value problems (II)

Announcements:

- HW3: Due Friday 1/31

Lecture Outline

We will cover these topics

- Implicit method
- Crank-Nicolson method
- Spectral methods

Implicit methods

- Recall that the FTCS method is inherently unstable for the wave equation
- Luckily we can workaround this shortcoming
- Method: Go backwards in time to the previous timestep and predict current timestep from it
- First, let's substitute h → -h into the wave equation

$$\phi(x, t-h) = \phi(x,t) - h\psi(x,t)$$

$$\psi(x, t-h) = \phi(x,t) - h\frac{v^2}{a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right]$$

- Make a 2nd substitution t → t + h

$$\phi(x,t) = \phi(x,t+h) - h\psi(x,t+h)$$

$$\psi(x,t) = \psi(x,t+h) - h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]$$

Implicit methods

$$\phi(x,t) = \phi(x,t+h) - h\psi(x,t+h)$$
$$\psi(x,t) = \psi(x,t+h) - h\frac{v^2}{a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]$$

- This set gives the solution at t+h indirectly
- These equations is a set of simulataneous equations at each grid point
- We can solve these with Linear Algebra methods, like Gaussian elimination

- Let's perform a von Neumann analysis on it.

$$\mathbf{B}\mathbf{c}(t+h) = \mathbf{c}(t), \qquad \text{with} \qquad \mathbf{B} = \begin{pmatrix} 1 & -h \\ hr^2 & 1 \end{pmatrix}$$

- Here $r = \left(\frac{2v}{a}\right)\sin\left(\frac{ka}{2}\right)$

Implicit methods

- Let's perform a von Neumann analysis on it. One would find

$$\mathbf{B}\mathbf{c}(t+h) = \mathbf{c}(t), \qquad \text{with} \qquad \mathbf{B} = \begin{pmatrix} 1 & -h \\ hr^2 & 1 \end{pmatrix}$$

- Here $r = \left(\frac{2v}{a}\right)\sin\left(\frac{ka}{2}\right)$
- We can solve for **c**(t+h) by multiplying by $\mathbf{B}^{-1}$
- The determinant of the inverse of **B** gives the eigenvalues

$$\lambda = \frac{1 \pm ihr}{1 + h^2r^2}$$
$$|\lambda| = (1 + h^2r^2)^{-1/2}.$$

- This value is always less than one and is **unconditionally stable** but not necessarily correct

Crank-Nicolson method

- The optimal method would be a hybrid of FTCS and implicit methods
- The Crank-Nicolson method takes the average of these two methods

$$\phi(x,t+h) - \tfrac{1}{2}h\psi(x,t+h) = \phi(x,t) + \tfrac{1}{2}\psi(x,t),$$

$$\begin{aligned}\psi(x,t+h) - h\frac{v^2}{2a^2}\left[\phi(x+a,t+h) + \phi(x-a,t+h) - 2\phi(x,t+h)\right]& \\ = \psi(x,t) + h\frac{v^2}{2a^2}\left[\phi(x+a,t) + \phi(x-a,t) - 2\phi(x,t)\right].&\end{aligned}$$

- These equations are indirect (just like the implicit method) and need to solve the system of equations

Crank-Nicolson method

- Is it stable? If so, when is it stable?
- The Crank-Nicolson method has a solution: **B**c(t+h) = **A**c(t), where A and B are as defined before (matrix A in previous lecture)
- Rearrange to have the time-update on the LHS

$$c(t+h) = B^{-1}Ac(t)$$

$$\mathbf{B}^{-1}\mathbf{A} = \frac{1}{1+h^2r^2}\begin{pmatrix} 1 & h \\ -hr^2 & 1 \end{pmatrix}\begin{pmatrix} 1 & h \\ -hr^2 & 1 \end{pmatrix} = \frac{1}{1+h^2r^2}\begin{pmatrix} 1-h^2r^2 & 2h \\ -2hr^2 & 1-h^2r^2 \end{pmatrix}$$

- That has eigenvalues of

$$\lambda = \frac{1-h^2r^2 \pm 2ihr}{1+h^2r^2}$$

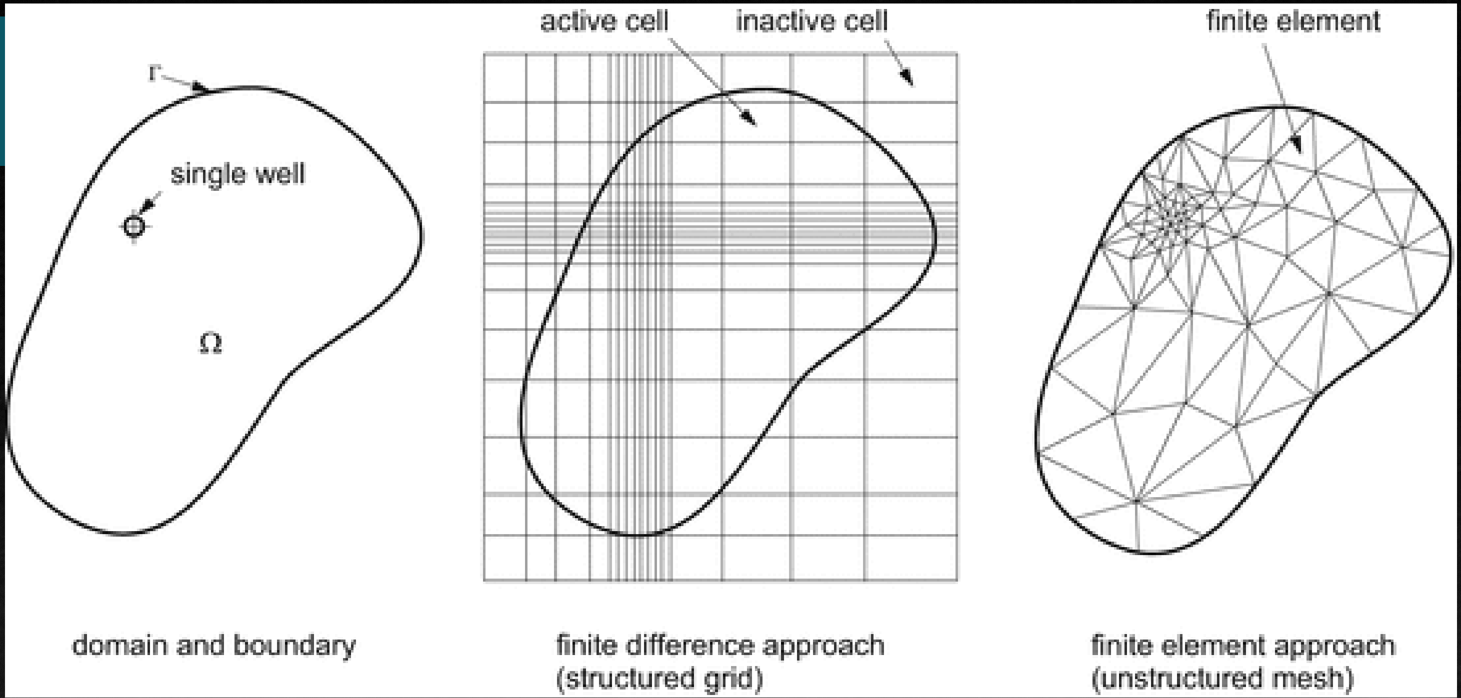
Crank-Nicolson method

$$\lambda = \frac{1 - h^2 r^2 \pm 2ihr}{1 + h^2 r^2}$$

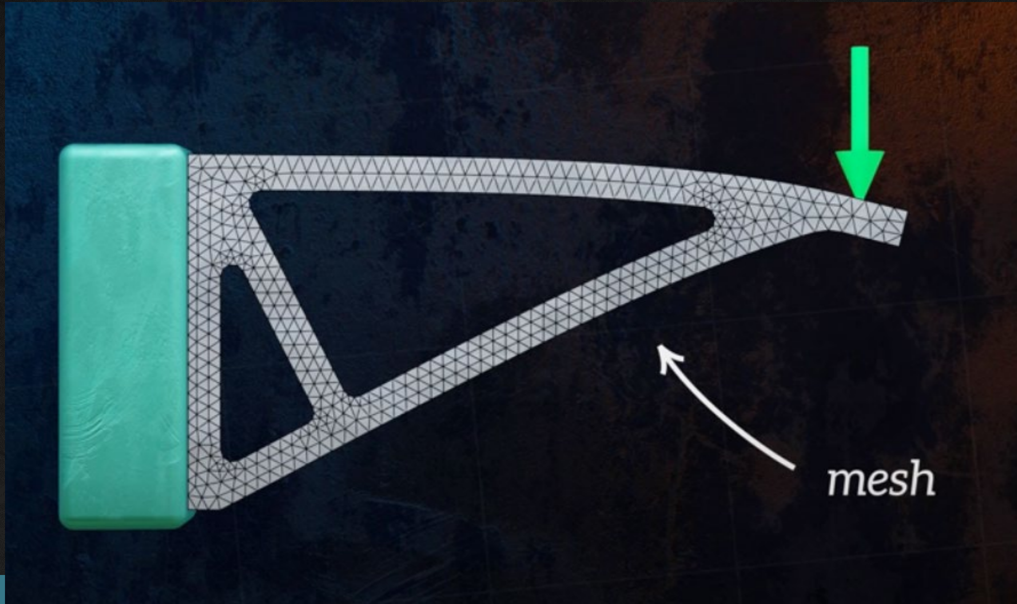
- These eigenvalues have the same value and are exactly one
- Suits the wave equation very well, where the solution is neither amplified or suppressed

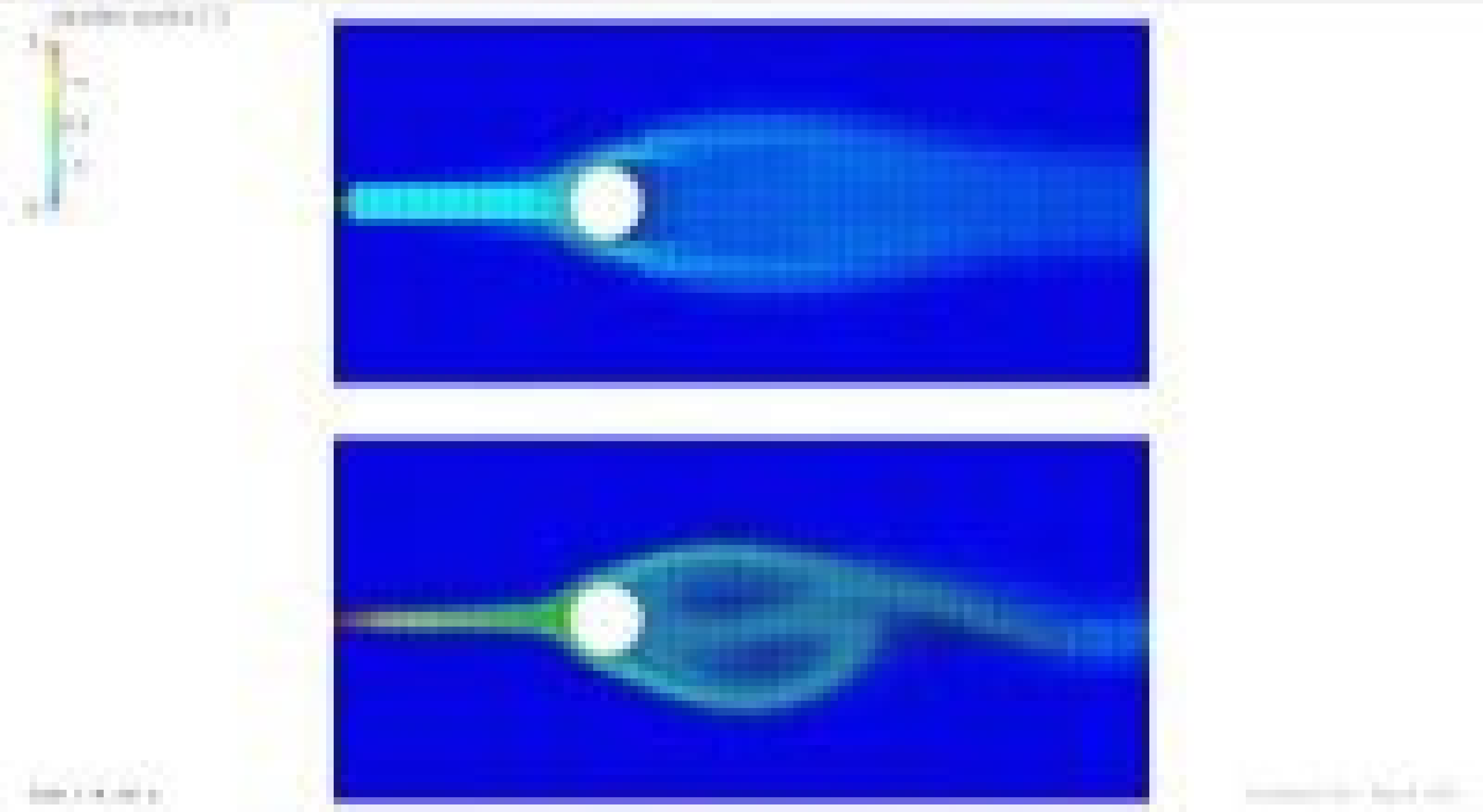
- Although the Crank-Nicolson method is more complicated than FTCS, it is still relatively fast and only depends on neighboring grid points
- Therefore, one would have a tridiagonal matrix to solve

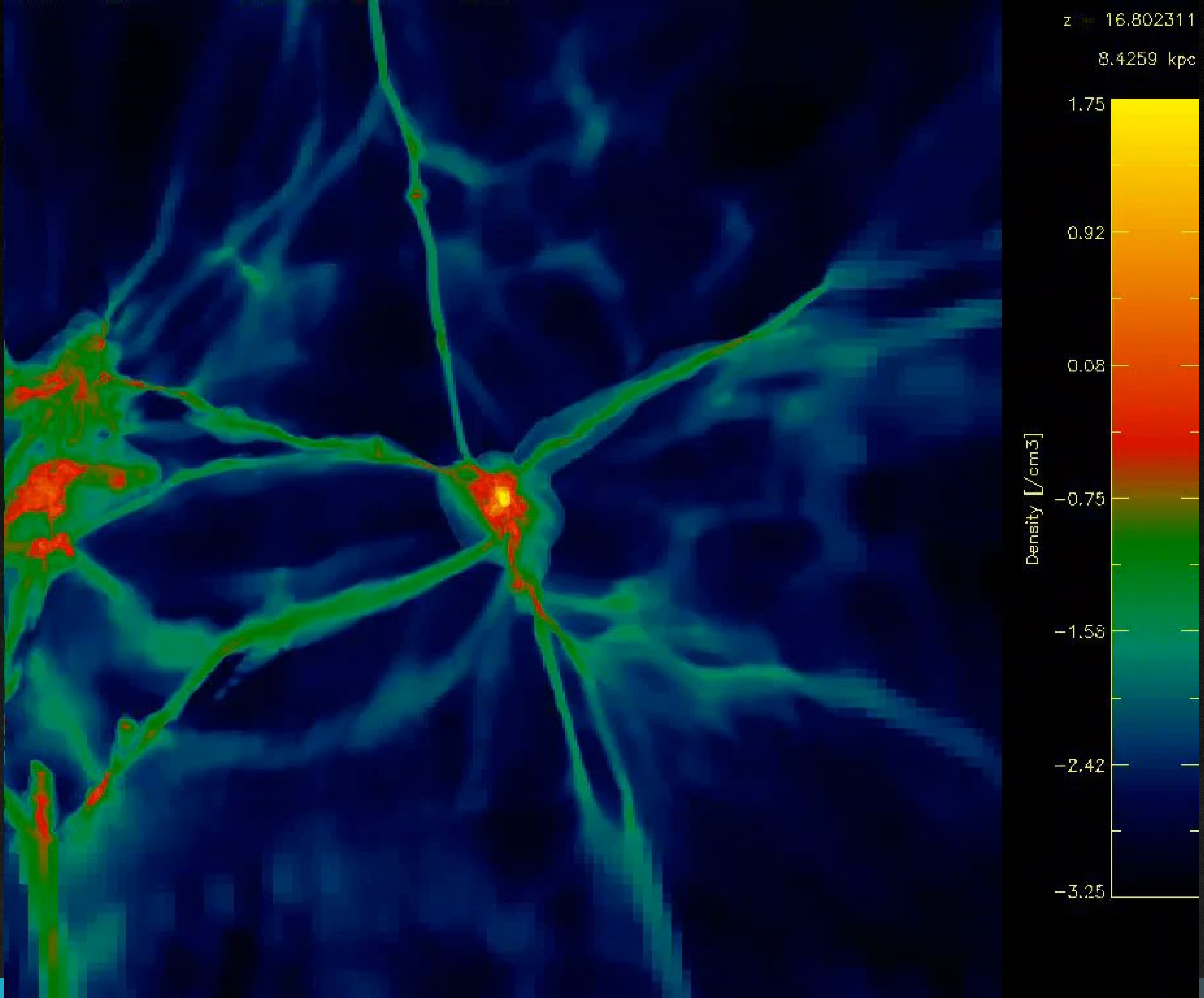
Finite element methods



- There are alternatives to finite differencing methods
- Fewer stability problems and more accurate solutions in particular problems
- One method is the finite element method
- These solve the PDEs in small elements of space and time
- Stitching together at the volume boundaries to form a solution
- This method is highly complex but popular in academia and industry
- We won’t cover it because of its complexity



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8.4259 kpc
1.75
0.92
0.08
-0.75
-1.58
-2.42
-3.25
Density [/cm3]

Spectral methods

- Spectral methods are less complex than finite element
- Still has better accuracy than finite differencing
- Let's consider the wave equation again

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

- Consider a trial solution to this PDE

$$\phi_k(x,t) \sin\left(\frac{\pi k x}{L}\right) e^{ikx}$$

- For now, let's assume that it is real. (In the long run, it is more convenient to carry around the full solution)

Spectral methods

- Trial solution: $\phi_k(x,t)\ \sin\left(\frac{\pi k x}{L}\right) e^{ikx}$
- As long as k is an integer, the solution satisfies the boundary conditions (fixed at zero)

- Divide domain into N intervals with positions: x_n = (n/N) L
- The solution at these points is

$$\phi_k(x_n, t) = \ \sin\left(\frac{\pi k n}{N}\right) \exp\left(i \frac{\pi v k t}{L}\right)$$

- The wave equation is linear, so any linear combination of the k-solutions is also a solution

$$\phi_k(x_n, t) = \frac{1}{N} \sum_{k=1}^{N-1} b_k \sin\left(\frac{\pi k n}{N}\right) \exp\left(i \frac{\pi v k t}{L}\right)$$

Spectral methods

- We can use the initial solution (t=0) to understand the coefficient evolution
- First, let's express them as $b_k = \alpha_k + i\eta_k$
- The real part of the solution is

$$\phi(x_n, 0) = \frac{1}{N} \sum_{k=1}^{N-1} \alpha_k \sin\left(\frac{\pi k n}{N}\right),$$

- This Fourier sine series can represent any solution
- We can inspect the time derivatives, which is just another sine series with different cofficients

$$\frac{\partial \phi}{\partial t} = -\left(\frac{\pi v}{L}\right) \frac{1}{N} \sum_{k=1}^{N-1} k\eta_k \sin\left(\frac{\pi k n}{N}\right),$$

Spectral methods

- We can match the initial values and derivatives for a given set of coefficients (b_k, α_k, η_k)
- Knowing these coefficients, we know the solution for any time t!

- Because the solution is a Fourier series, we can solve the problem with FFTs, i.e. the coefficients
- Once they are known, we can calculate the solution

$$\phi(x_n, t) = \frac{1}{N} \sum_{k=1}^{N-1} \left[\alpha \cos\left(\frac{\pi v k t}{L}\right) - \eta_k \sin\left(\frac{\pi v k t}{L}\right)\right] \sin\left(\frac{\pi k n}{N}\right).$$

- At some time t with an inverse FFT
- Limitations: only works well when (1) BCs are simple, and (2) with linear differential eqns