PHY604 Lecture 15

October 14, 2021

Review: Advection equation

- Thus, we see that there is a simpler hyperbolic equation, the advection equation:

$$\frac{\partial a}{\partial t} = -c\frac{\partial a}{\partial x}$$

- Describes the evolution of some scalar field *a* carried by a flow of velocity *c*
  - Also known as linear convection equation
  - Waves move only in one direction (to the right if $c > 0$), unlike the wave equation
- "Flux conservation" equation
  - E.g., continuity equation in electrodynamics/quantum mechanics:

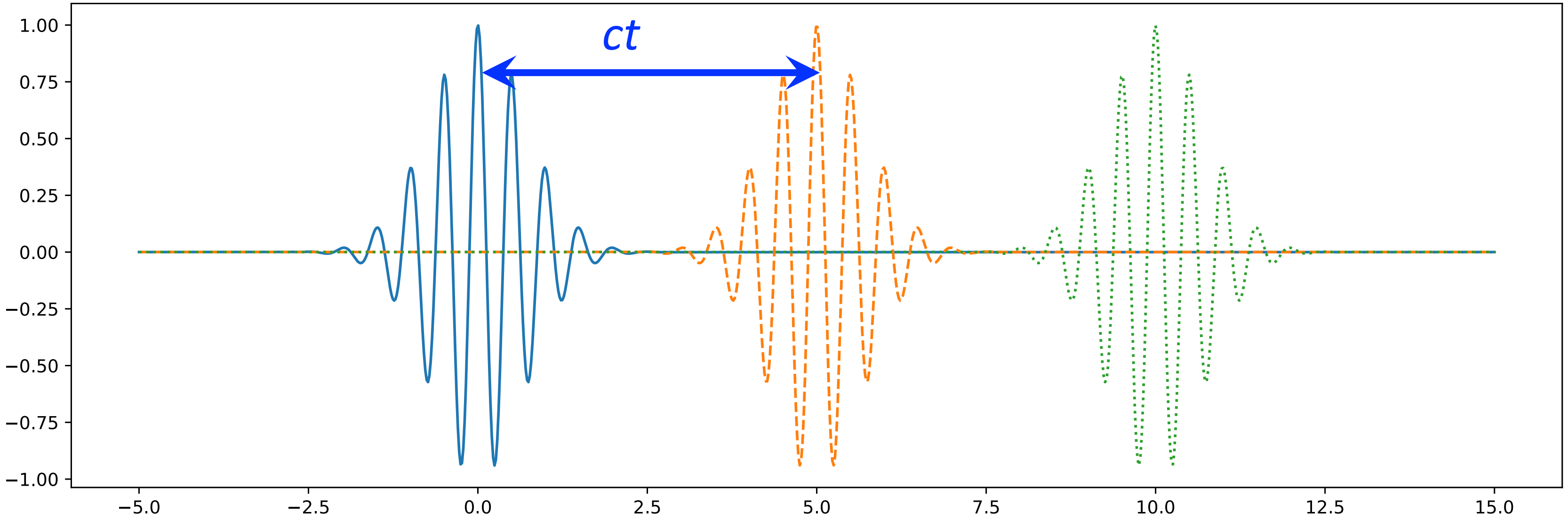
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}(p)$$

Review: Analytical solution to advection equation

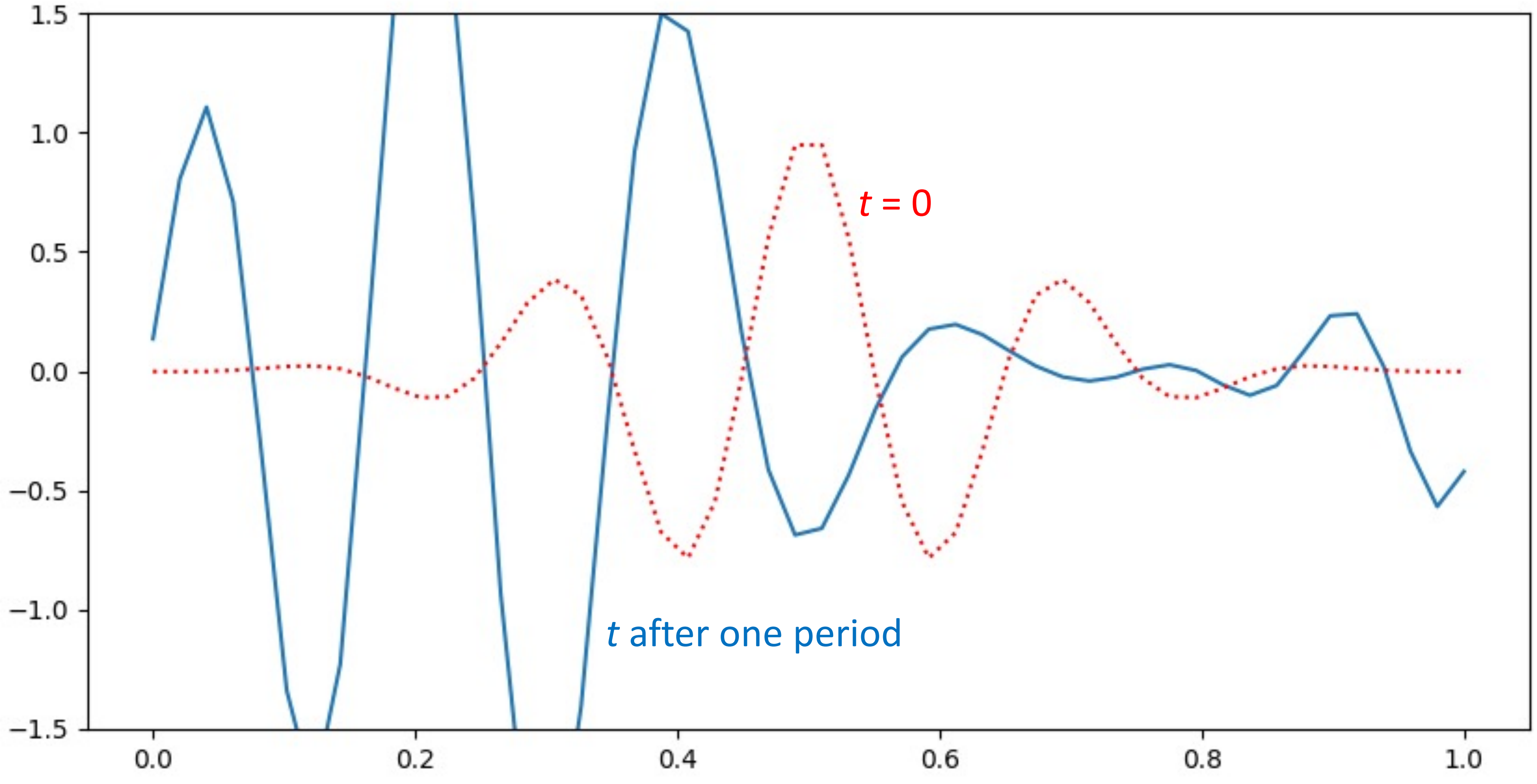
- For initial condition: $a(x, t=0) = f_0(x)$
- Solution is: $a(x,t) = f_0(x - ct)$
- Consider a wavepacket of the form:

$$a(x, t=0) = \cos[k(x - x_0)] \exp\left[-\frac{(x - x_0)^2}{2\sigma^2}\right]$$

- Solution: $a(x,t) = \cos[k((x - ct) - x_0)] \exp\left[-\frac{((x - ct) - x_0)^2}{2\sigma^2}\right]$



Review: FTCS method clearly fails for the advection equation



Review: How can we do a better job?

- We could try to adjust numerical parameters, but it will not work!
  - FTCS is unstable for any τ ! (will come back to this later)
  - Can delay the problems but not get rid of them

- Stability problem can be helped with a simple modification: The Lax method:

$$a_i^{n+1} = \frac{1}{2}(a_{i+1}^n + a_{i-1}^n) - \frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n)$$

- Simply replacing the first term with the average of the left and right neighbors

Review: Lax Wendroff

- So, we have: $a(x,t+\tau) \simeq a(x,t) - \tau \frac{\partial F(a)}{\partial x} + \frac{\tau^2}{2} \frac{\partial F'(a)}{\partial x} \frac{\partial F(a)}{\partial x}$

- Now we discretize derivatives:

$$a_i^{n+1} = a_i^n - \tau \frac{F_{i+1} - F_{i-1}}{2h} + \frac{\tau^2}{2h} \left(F'_{i+1/2} \frac{F_{i+1} - F_i}{h} - F'_{i-1/2} \frac{F_i - F_{i-1}}{h} \right)$$

- Where: $F_i \equiv F(a_i^n), \quad F'_{i\pm 1/2} \equiv F'[(a_{i\pm 1}^n + a_i^n)/2]$

- For advection equations, $F_i = c a_i^n, \quad F'_{i\pm 1/2} = c$

Discretized second derivative of a

$$a_i^{n+1} = a_i^n - \frac{c\tau}{2h}(a_{i+1}^n - a_{i-1}^n) + \frac{c^2\tau^2}{2h^2}(a_{i+1}^n + a_{i-1}^n - 2a_i^n)$$

Review: Traffic flow

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial}{\partial x}[\rho(x,t)v(x,t)]$$

- Simplest nontrivial flow: Velocity of flow is only a function of density:

$$v(x,t) = v(\rho)$$

- We will take the velocity to decrease linearly with increasing density:

$$v(\rho) = v_m(1 - \rho/\rho_m)$$

- $v_m > 0$ is the maximum velocity, $\rho_m > 0$ is the maximum density
  - Max velocity is the speed limit ;) , can be achieved if density is low
  - Max density is bumper-to-bumper, velocity is zero
- Evolution of the density may be written:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}\left[(\alpha + \frac{1}{2}\beta\rho)\rho\right], \qquad \alpha = v_m, \;\; \beta = -2v_m/\rho_m$$

Review: Setting up the traffic problem

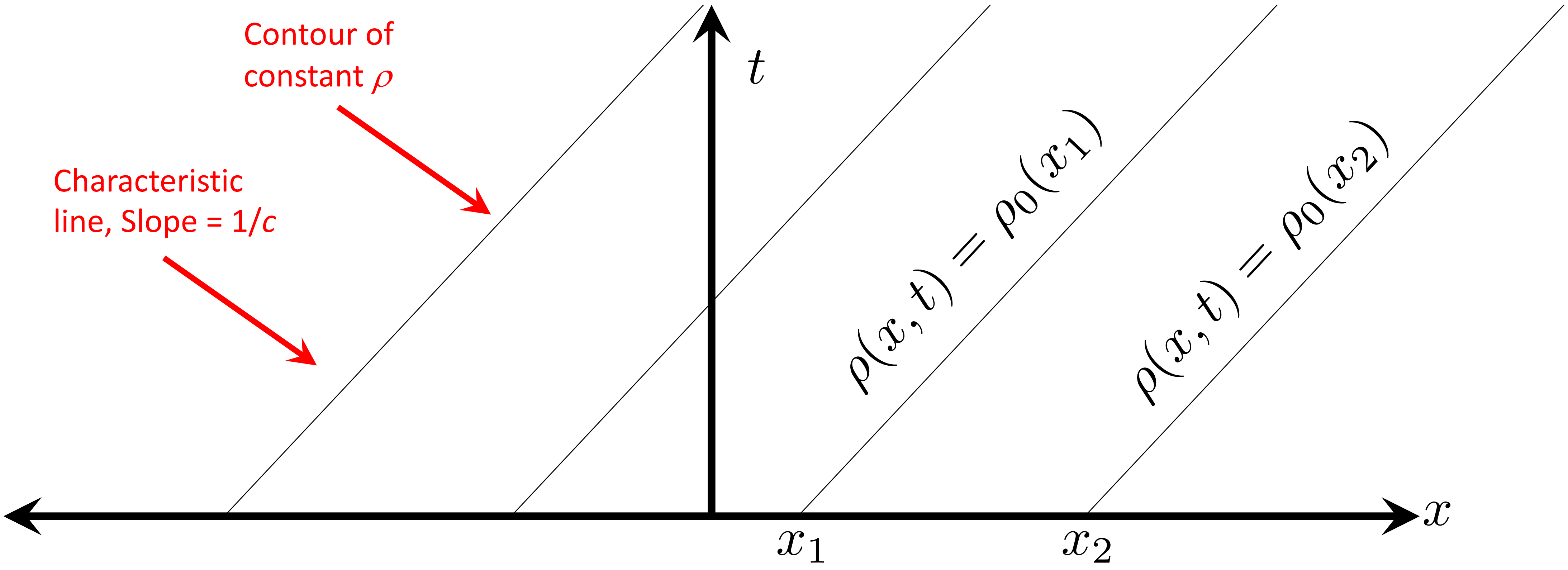
- Rewrite the nonlinear PDE: $$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}[\rho v(\rho)]$$
- As: $$\frac{\partial \rho}{\partial t} = -\left(\frac{d}{d\rho}[\rho v(\rho)]\right)\frac{\partial \rho}{\partial x} \quad \Longrightarrow \quad \frac{\partial \rho}{\partial t} = -c(\rho)\frac{\partial \rho}{\partial x}$$
- Where: $c(\rho) = v_m(1 - 2\rho/\rho_m)$
- $c(0) = v_m$ and $c(\rho_m) = -v_m$
- $c(\rho)$ is not the speed of traffic; speed disturbances (waves) travel
- Since $c(\rho) \leq v(\rho)$, waves can never travel faster than cars

Today’s lecture:
PDEs

- Hyperbolic PDEs: Traffic problem
- Elliptical PDEs: Relaxation methods

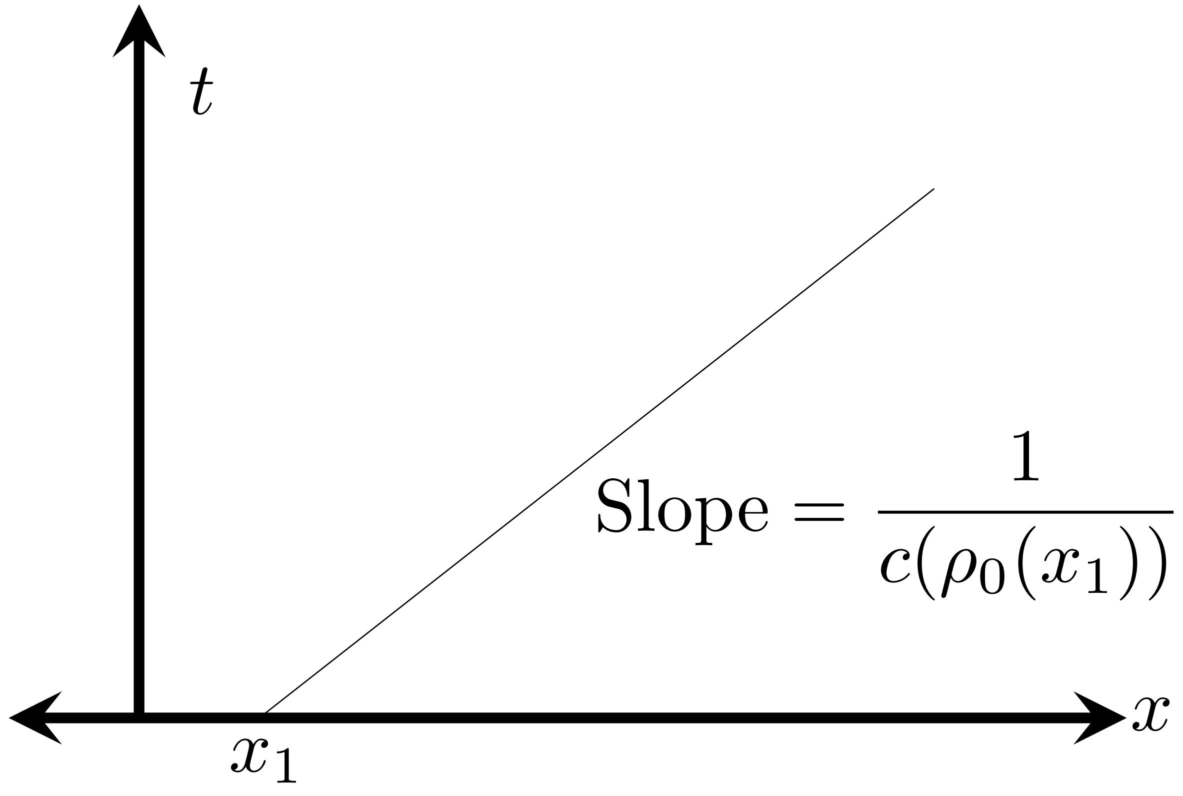
Solving the traffic problem: Method of characteristics

- We can learn about the behavior of this PDE by comparing to the advection equation we have already solved
  - Recall that the initial condition $\rho(x,t=0) = \rho_0(x)$ is rigidly translated with speed c
- We can represent this with "characteristic lines" of constant ρ



Characteristic lines for nonlinear problem

- Even in the nonlinear problem, ρ is constant on the characteristic line!



Constant density along characteristic line

- Using the chain rule:

$$\frac{d}{dt}\rho[x(t),t] = \frac{\partial}{\partial t}\rho[x(t),t] + \frac{dx}{dt}\frac{\partial}{\partial x}\rho[x(t),t]$$

- Along the characteristic line:

$$\frac{d}{dt}\rho[x(t),t] = \frac{\partial}{\partial t}\rho[x(t),t] + c[\rho_0(x)]\frac{\partial}{\partial x}\rho[x(t),t]$$

- But from the original PDE:

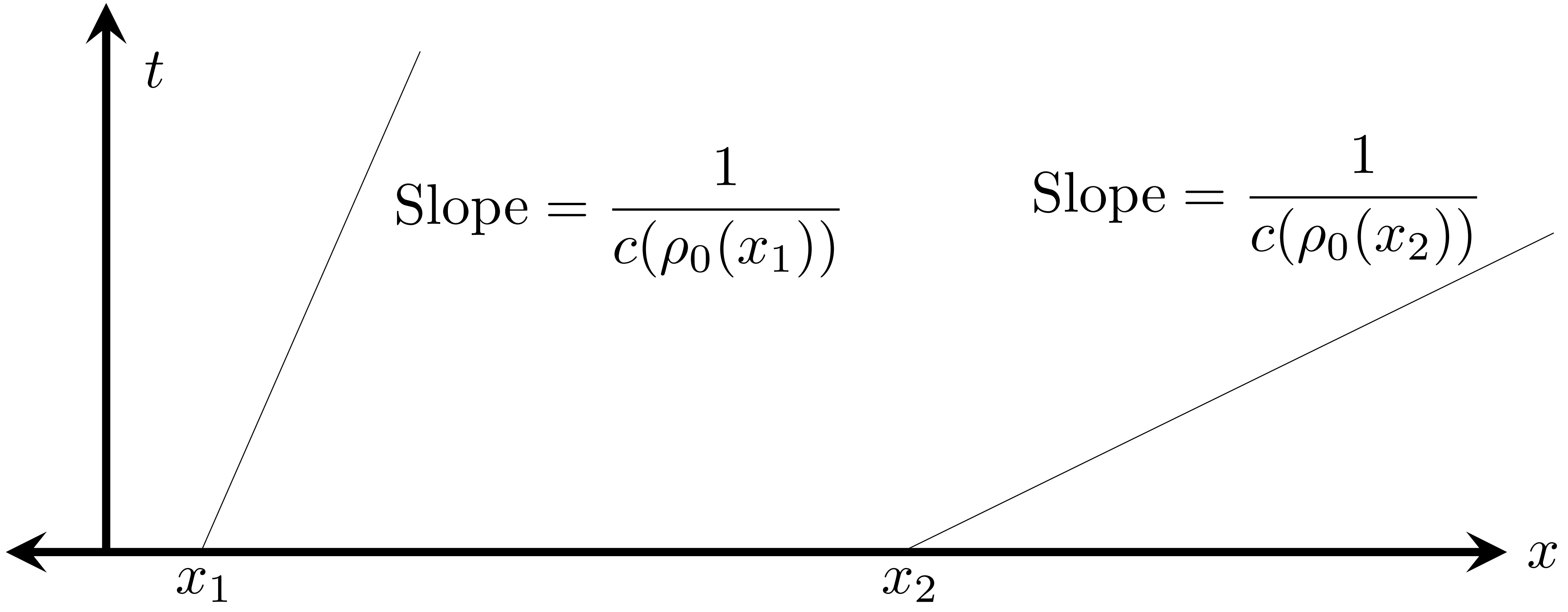
$$\frac{\partial \rho}{\partial t} = -c(\rho)\frac{\partial \rho}{\partial x}$$

- So, on the characteristic line:

$$\frac{d}{dt}\rho[x(t),t] = 0$$

Constructing a solution with the method of characteristics

- Draw a characteristic line from each point on the x axis
- This will form a contour map of $\rho(x,t)$

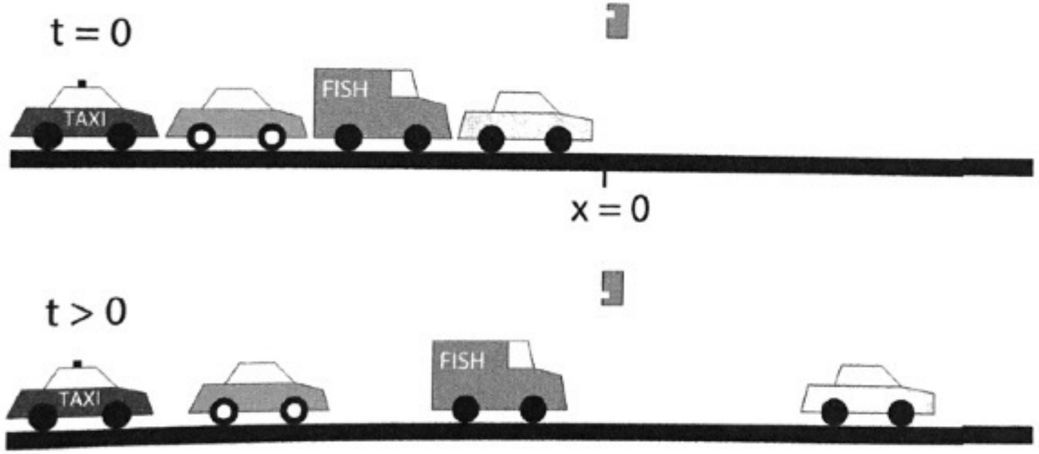


Method of characteristics to solve traffic at a stoplight

- Consider the initial distribution:

$$\rho_0(t) = \begin{cases} \rho_m, & x < 0 \\ 0, & x > 0 \end{cases}$$

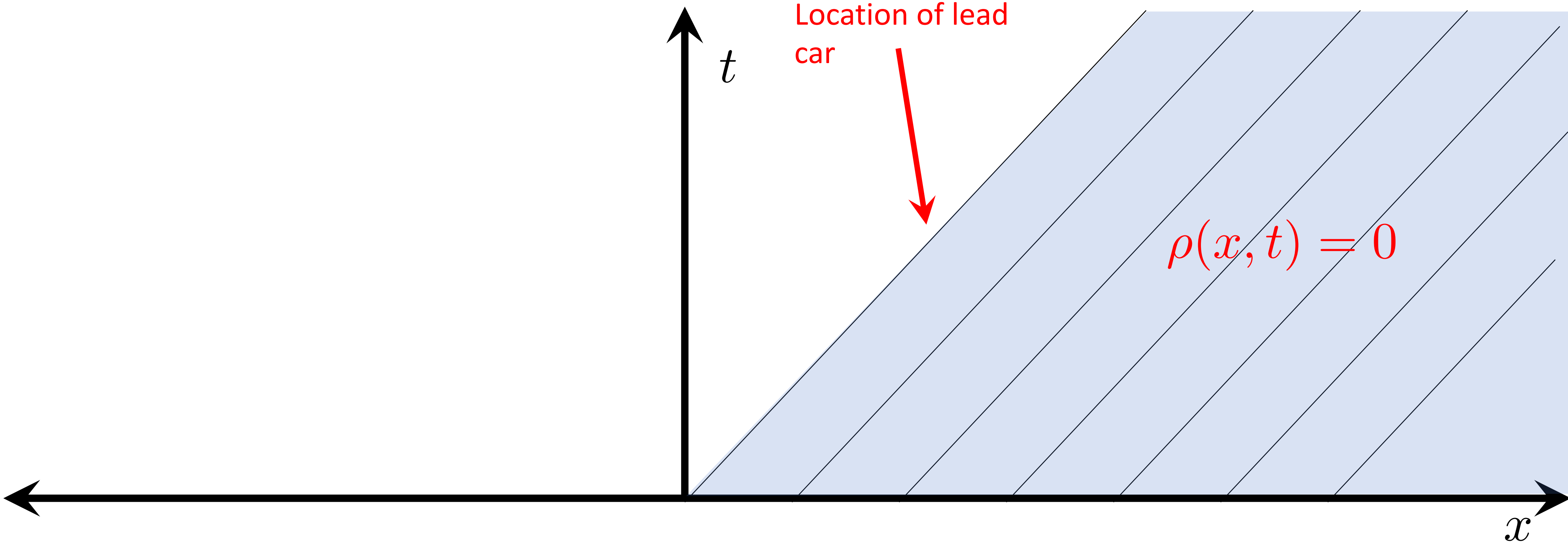
- i.e., cars stopped at a stoplight positioned at *x* = 0



- At time *t* = 0, the light turns green
  - Not all cars can move at once, density decrease as cars separate
  - Effect propagates back
  - “Rarefaction” wave problem

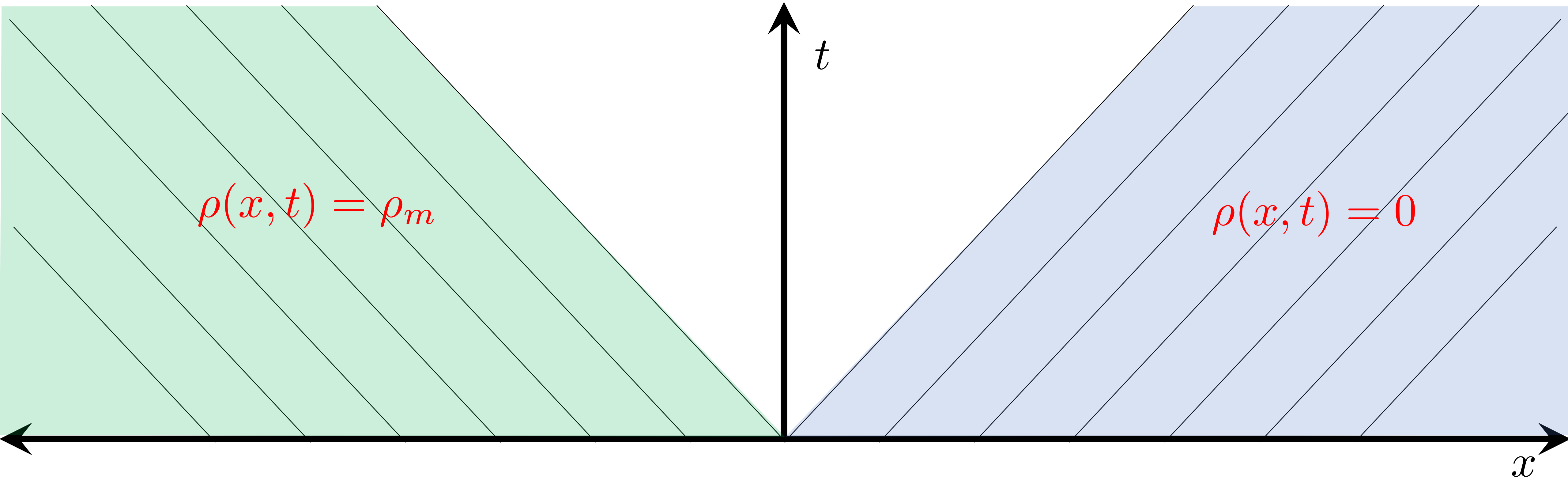
Start by drawing characteristic lines for $x > 0$

- All lines will have slope $c(0)=v_m$ since $\rho(x,t)=0$ for all x > 0



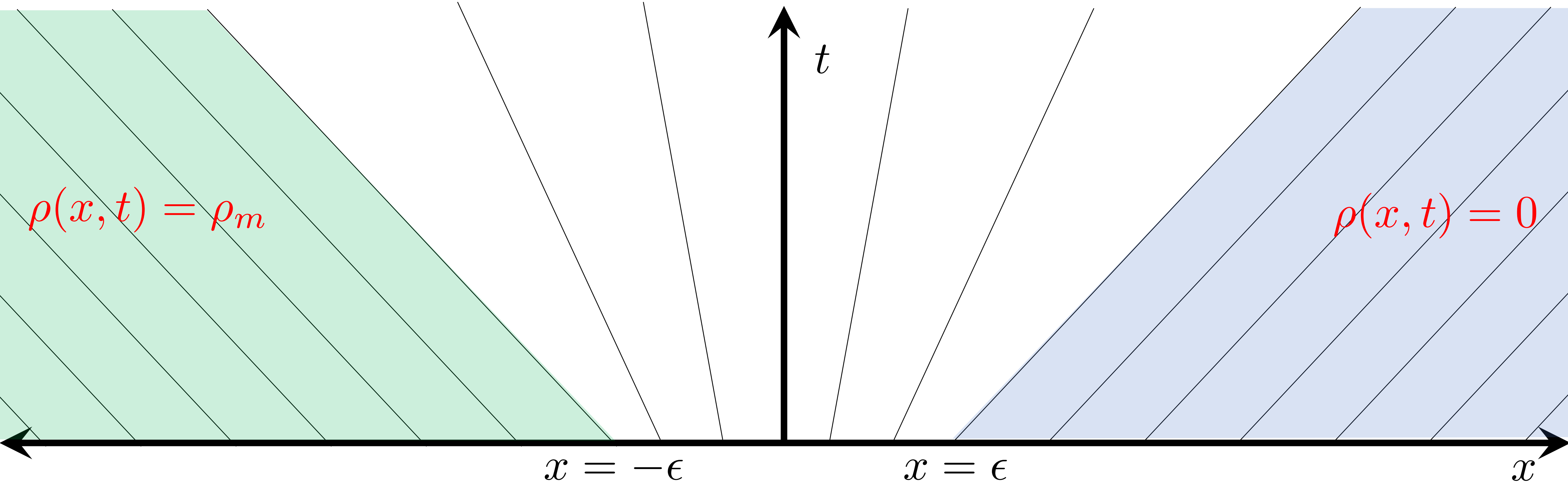
Now draw characteristic lines for $x < 0$

- At $t = 0$ we have density ρ_m, and $c(\rho_m) = -v_m$



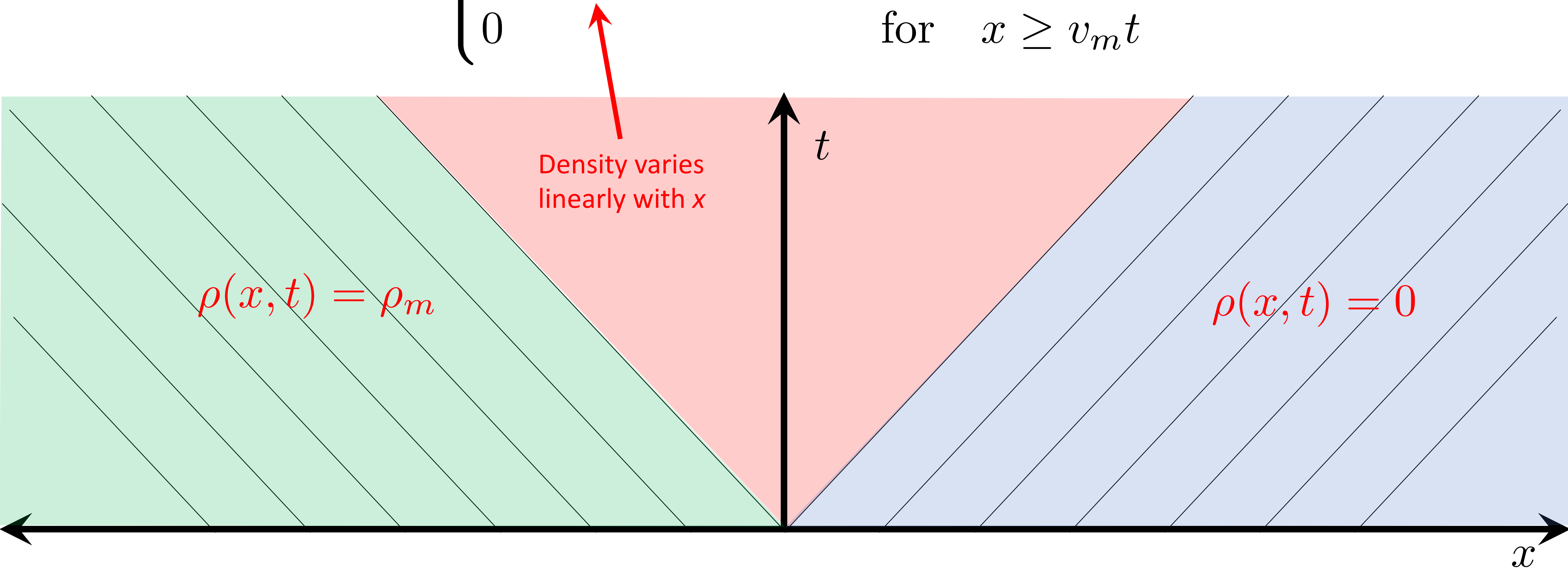
What about in between?

- Consider instead of ρ_0 as a step function, varying continuously in region 2ε
- Characteristic lines interpolate between $-v_m$ and v_m
  - Take ε to zero



Final solution for $\rho(x,t)$

$$\rho(x,t,) = \begin{cases} \rho_m & \text{for} \quad x \le -v_m t \\ \frac{1}{2}\left(1 - \frac{x}{v_m t}\right)\rho_m & \text{for} \quad -v_m t < x < v_m t \\ 0 & \text{for} \quad x \ge v_m t \end{cases}$$



Numerical solution to the traffic problem

- Starting with a general continuity equation:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial F(\rho)}{\partial x}$$

- In our case: $F(\rho) = \rho(x,t)v[\rho(x,t)] = \rho(x,t)v_m(1-\rho/\rho_m)$
- FTCS scheme:

$$\rho_i^{n+1} = \rho_i^n - \frac{\tau}{2h}(F_{i+1}^n - F_{i-1}^n)$$

- Lax scheme:

$$\rho_i^{n+1} = \frac{1}{2}(\rho_{i+1}^n + \rho_{i-1}^n) - \frac{\tau}{2h}(F_{i+1}^n - F_{i-1}^n)$$

- Lax-Wendroff scheme:

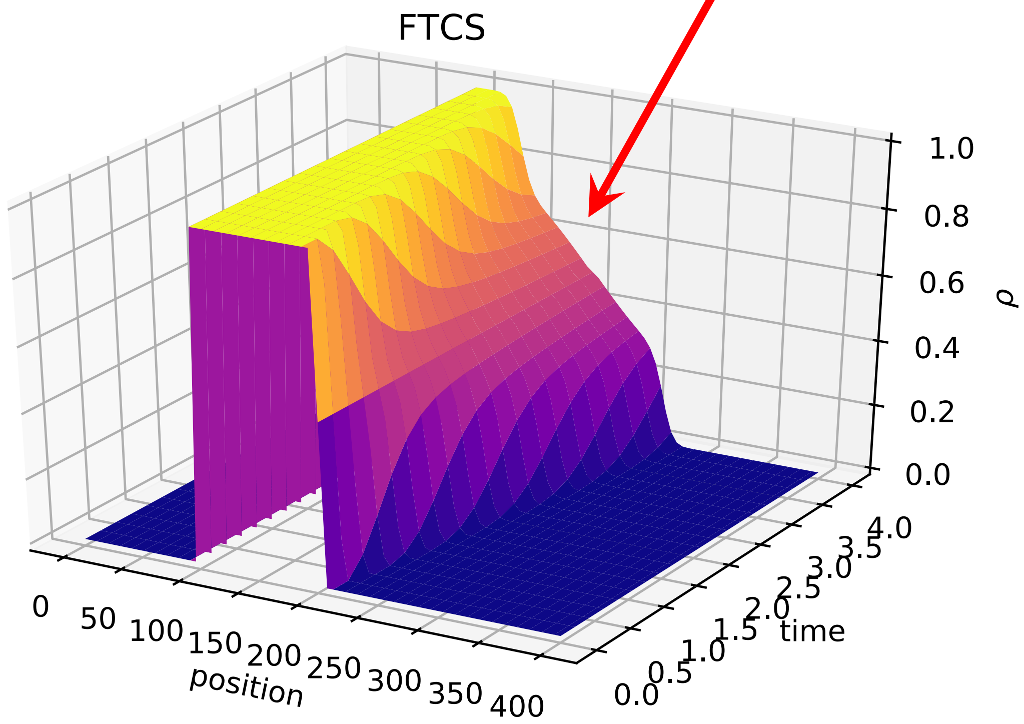
$$\rho_i^{n+1} = \rho_i^n - \frac{\tau}{2h}(F_{i+1}^n - F_{i-1}^n) + \frac{\tau^2}{2h^2}\left[c_{i+\frac{1}{2}}(F_{i+1}^n - F_i^n) - c_{i-\frac{1}{2}}(F_i^n - F_{i-1}^n\right]$$

  - Where:

$$c_{i\pm\frac{1}{2}} \equiv c(\rho_{i\pm\frac{1}{2}}^n), \quad \rho_{i\pm\frac{1}{2}}^n \equiv \frac{\rho_{i\pm 1}^n + \rho_i^n}{2}$$

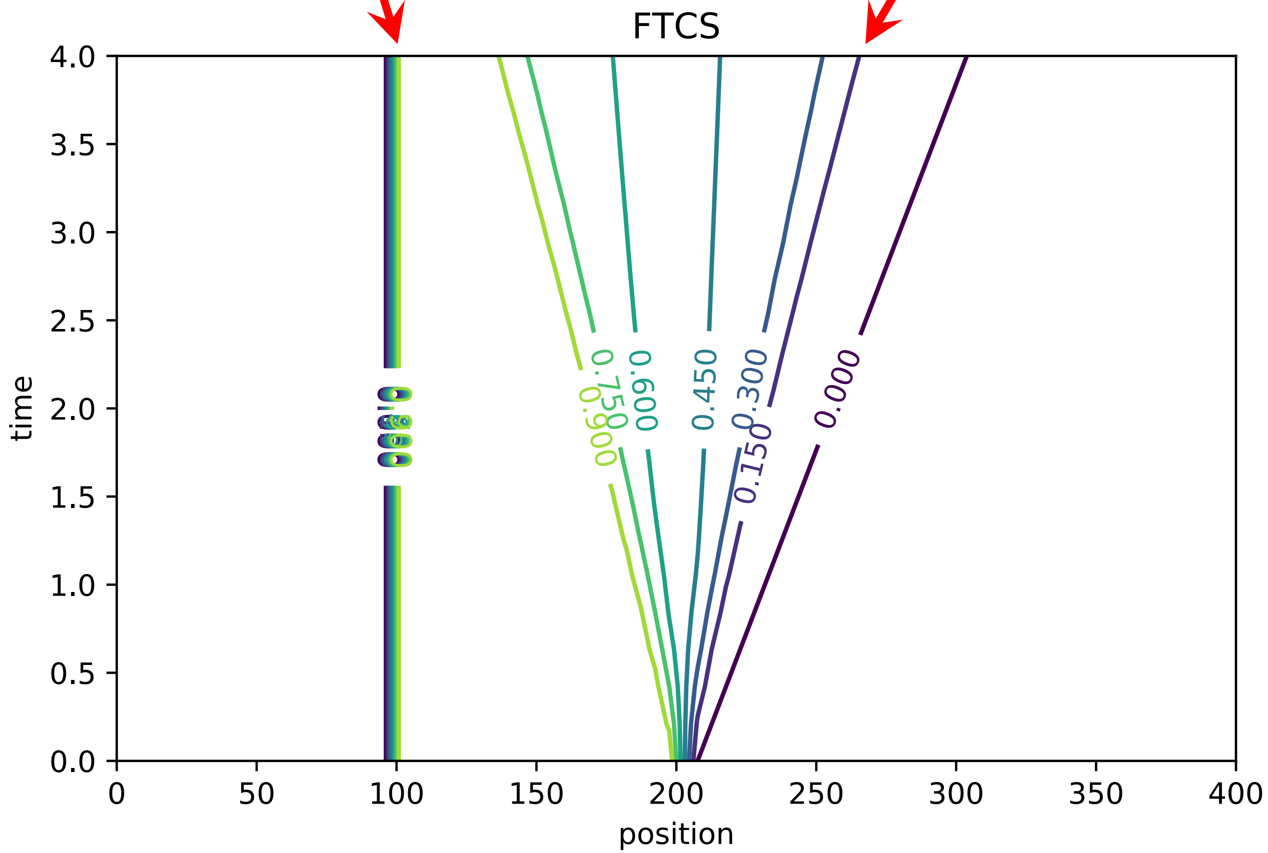
Numerical solution with FTCS method:

Curved, should expand as a straight line (lead car moving at constant velocity)



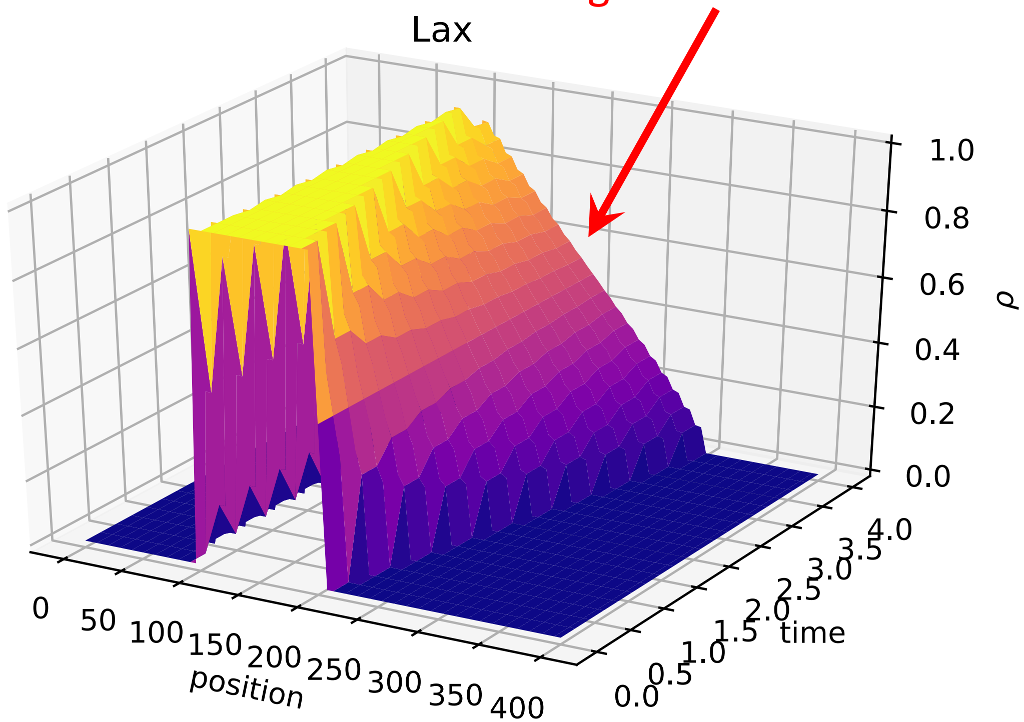
Shock front on left edge

Slope of contours should vary continuously



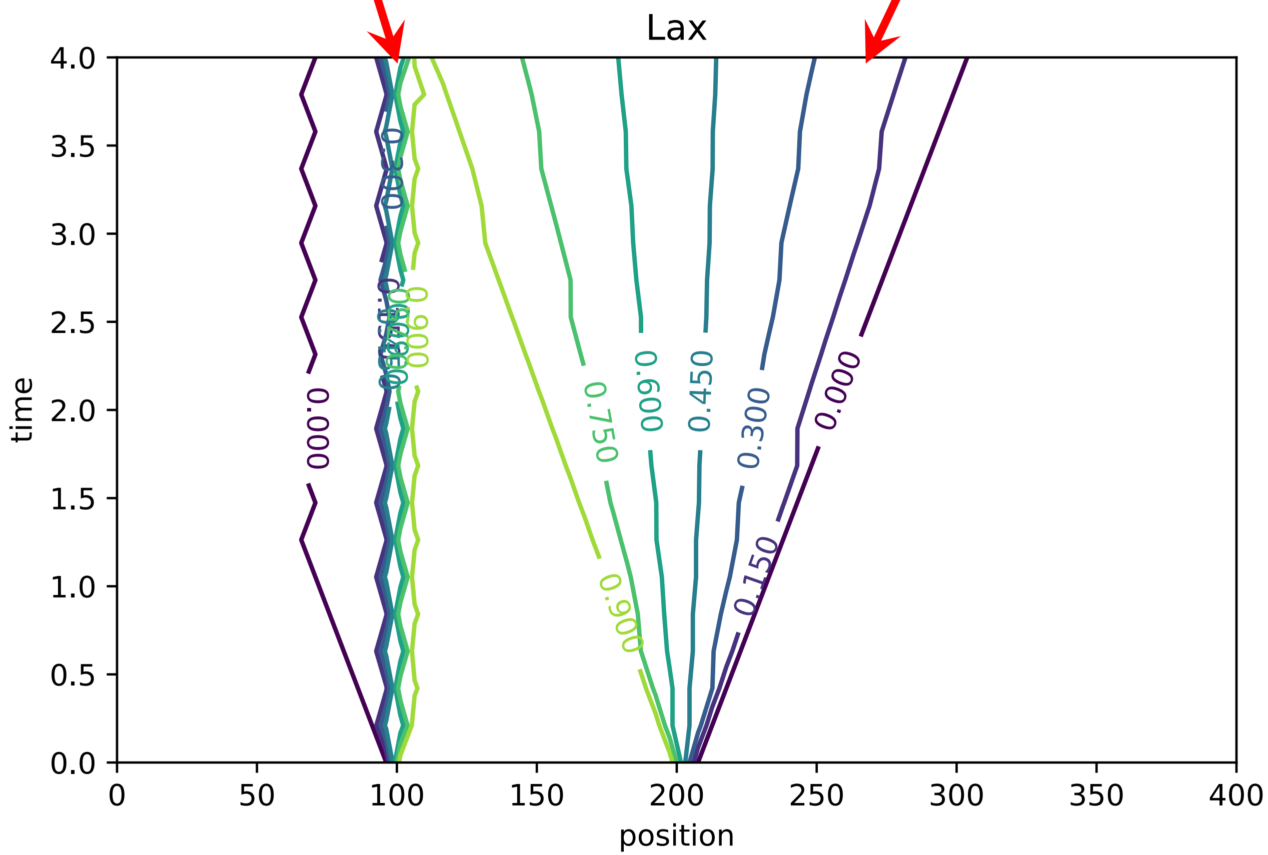
Numerical solution with Lax method:

Straighter, but some significant noise

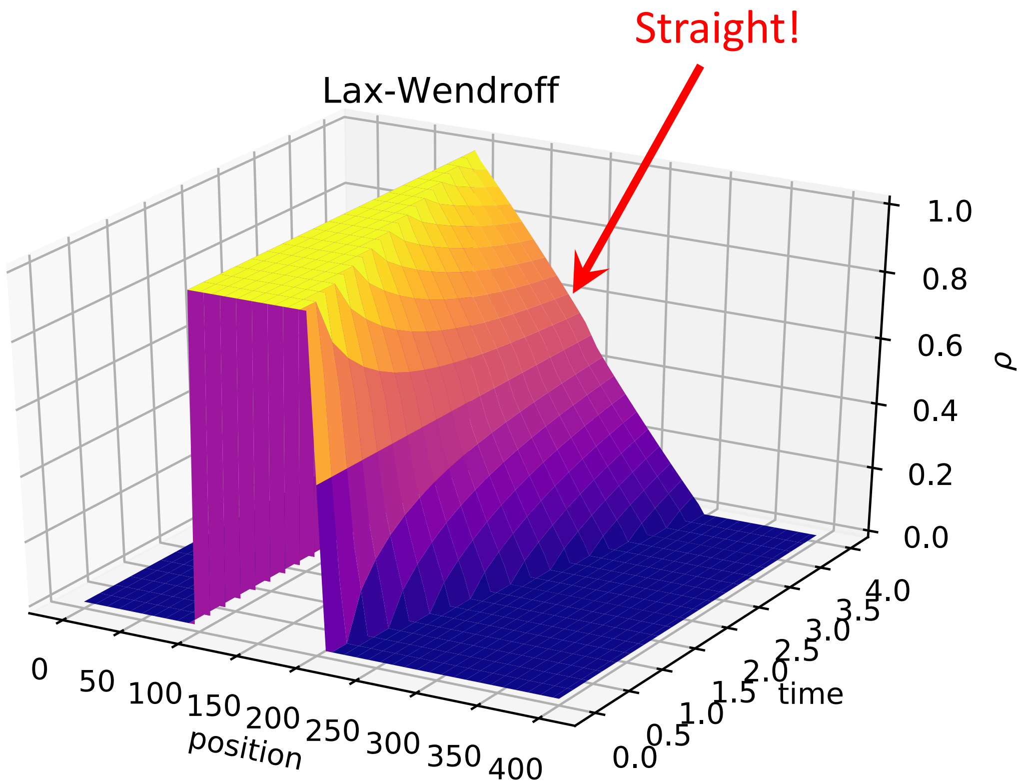


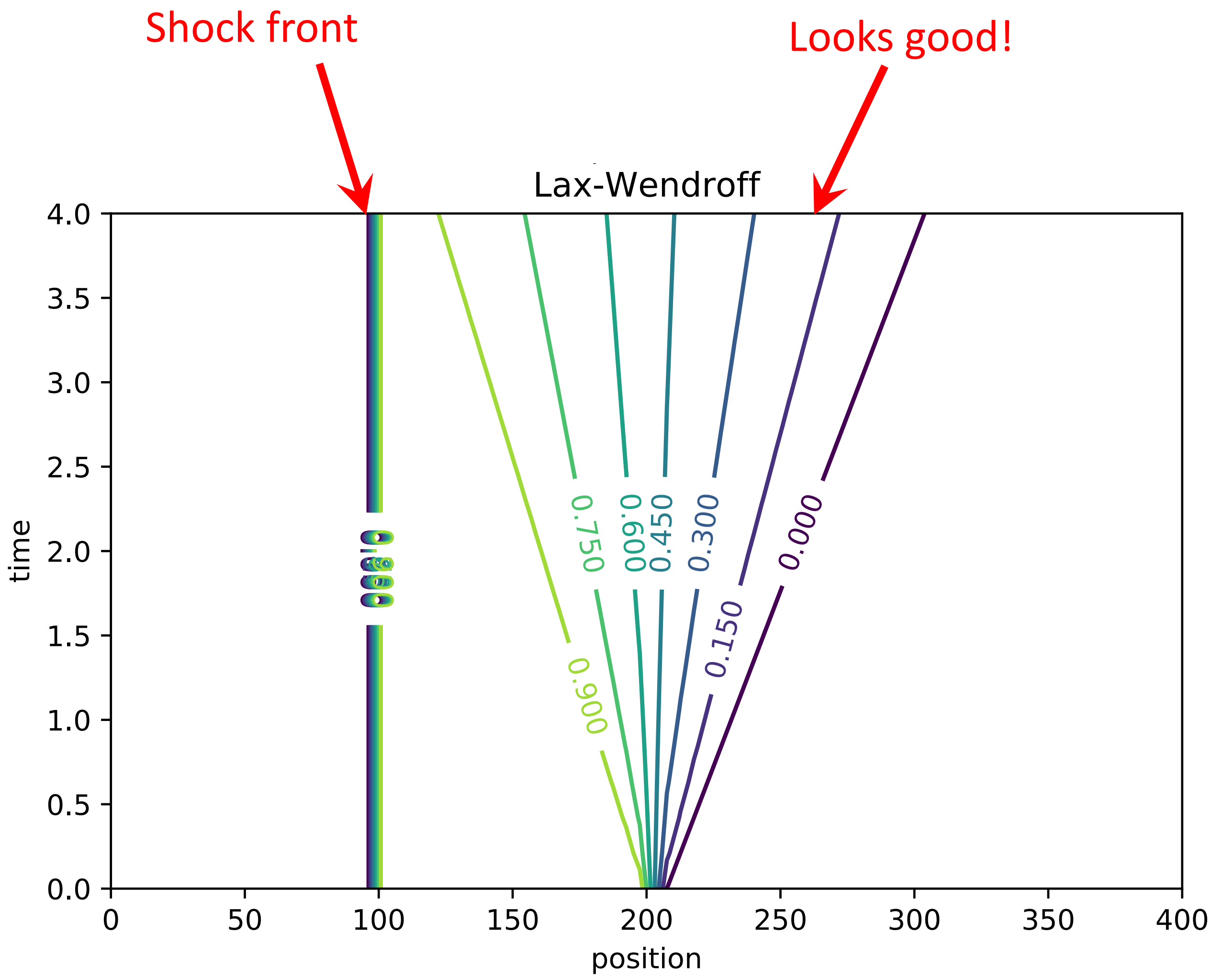
Shock front

Better, but some significant noise and wandering of LHS.



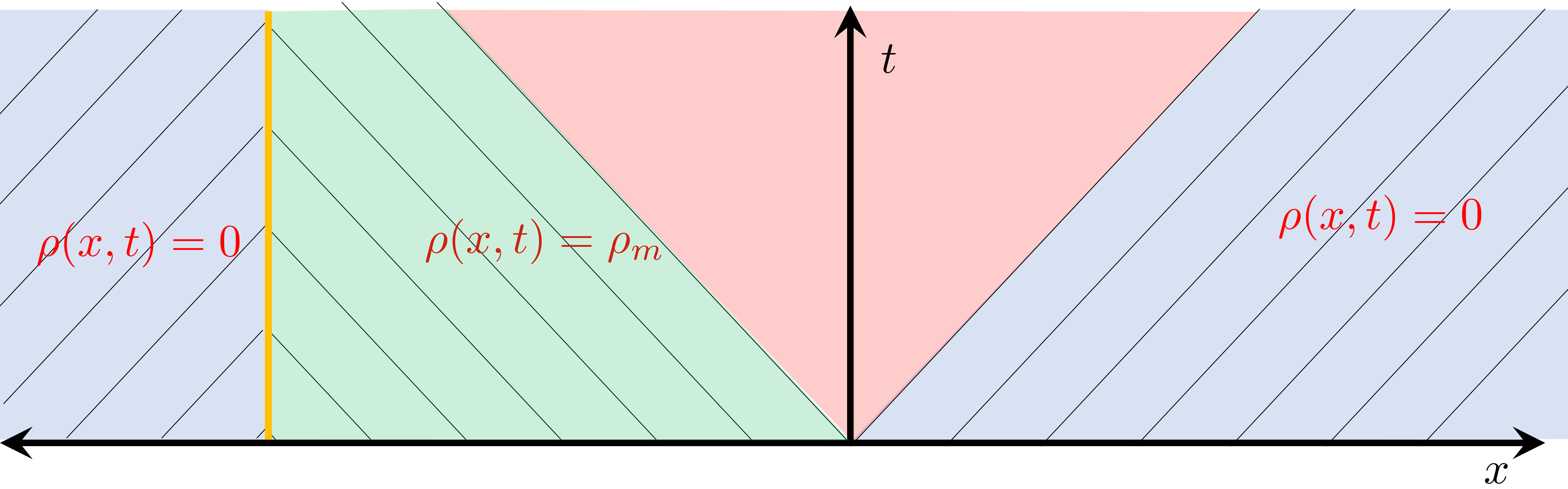
Numerical solution with Lax-Wendroff method:



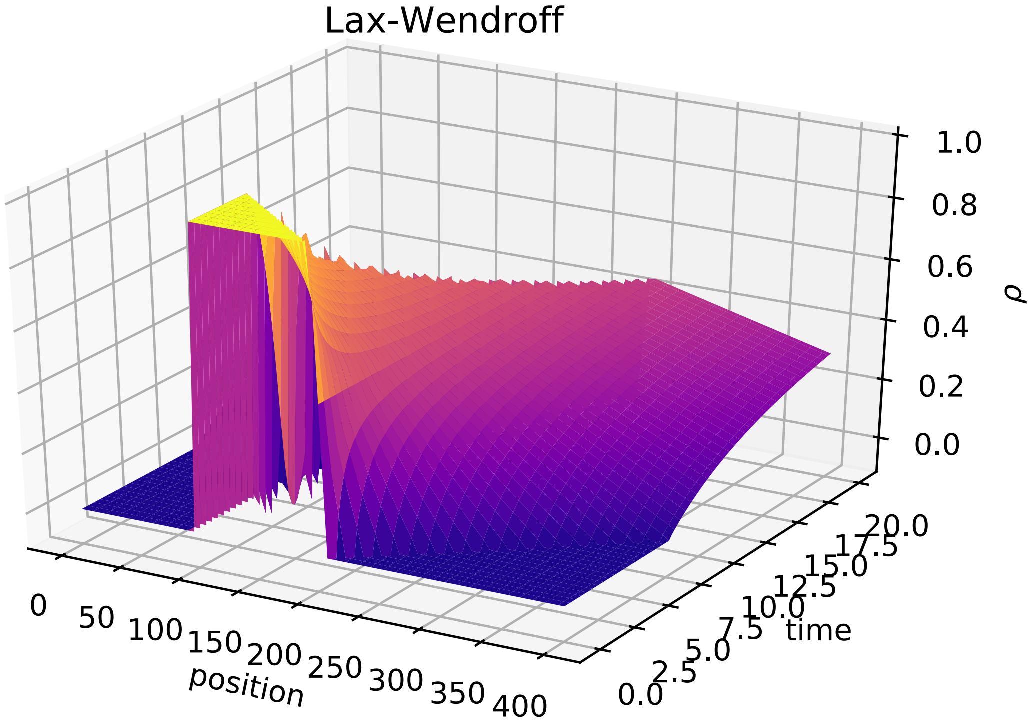


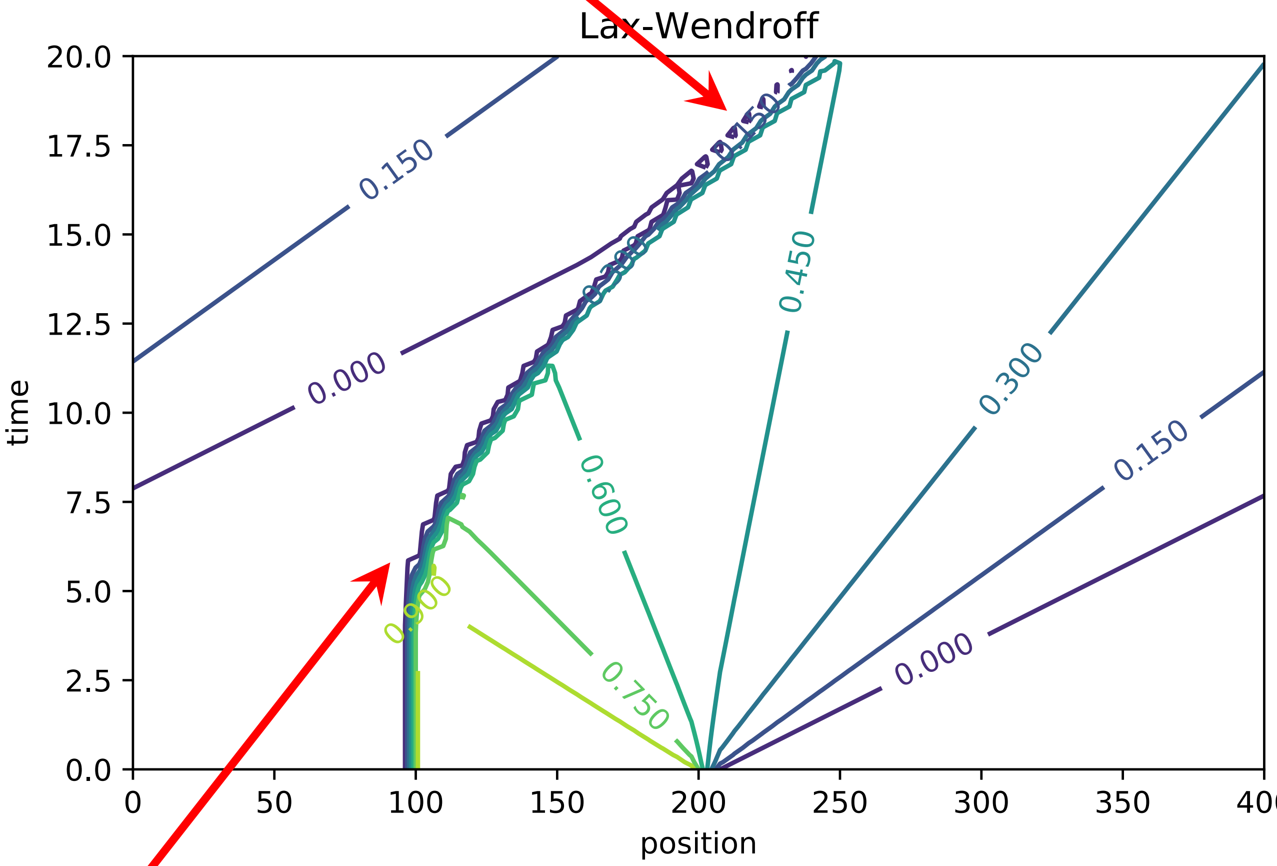
Shock front in the traffic problem

- Shock front is arising from discontinuity at the left edge, since lines of high and low density intersect
- Once red region intersects with shock, last cars start to move
- But what about the cars coming in from the left (because of PBCs)?



Shock front in the traffic problem





Last car starts to move

Final note on the hyperbolic equations

- We used the method of characteristics to find an analytical solution
  - We can also use it as a numerical method: Along the line, we have ODEs instead of PDEs
- For the wave equation, we have two sets of characteristic equations, left and right moving waves
- Shocks are the principal difficulty for solving hyperbolic PDEs
  - Solution is discontinuous
  - Can be mitigated by using uneven grids to concentrate grid points near the shock

Today’s lecture:
PDEs

- Hyperbolic PDEs: Traffic problem

- Elliptical PDEs: Relaxation methods

Elliptical equations: e.g., Laplace equation

- The PDEs we will discuss here represent boundary-value problems
  - Solution is a static field
- Consider Laplace's equation: $$\frac{\partial^2 \Phi(x,y)}{\partial x^2} + \frac{\partial^2 \Phi(x,y)}{\partial y^2} = 0$$
- Φ is the electrostatic potential
- As usual it is useful to solve a simple problem analytically so that we can benchmark numerical methods

Separation of variables for Laplace's equation

- Write Φ as the product: $\Phi(x,y) = X(x)Y(y)$
- Insert into Laplace's equation and divide by Φ:

$$\frac{1}{X(x)}\frac{d^2X}{dx^2} + \frac{1}{Y(y)}\frac{d^2Y}{dy^2} = 0$$

- This equation should hold for all *x* and *y*, so each term must be a constant:

$$\frac{1}{X(x)}\frac{d^2X}{dx^2} = -k^2, \qquad \frac{1}{Y(y)}\frac{d^2Y}{dy^2} = k^2$$

  - *k* is a complex constant
  - Writing constant as k^2 to simplify notation later
  - Signs can be switched
- Now we have two ODEs

Solution of Laplace's eq. ODEs

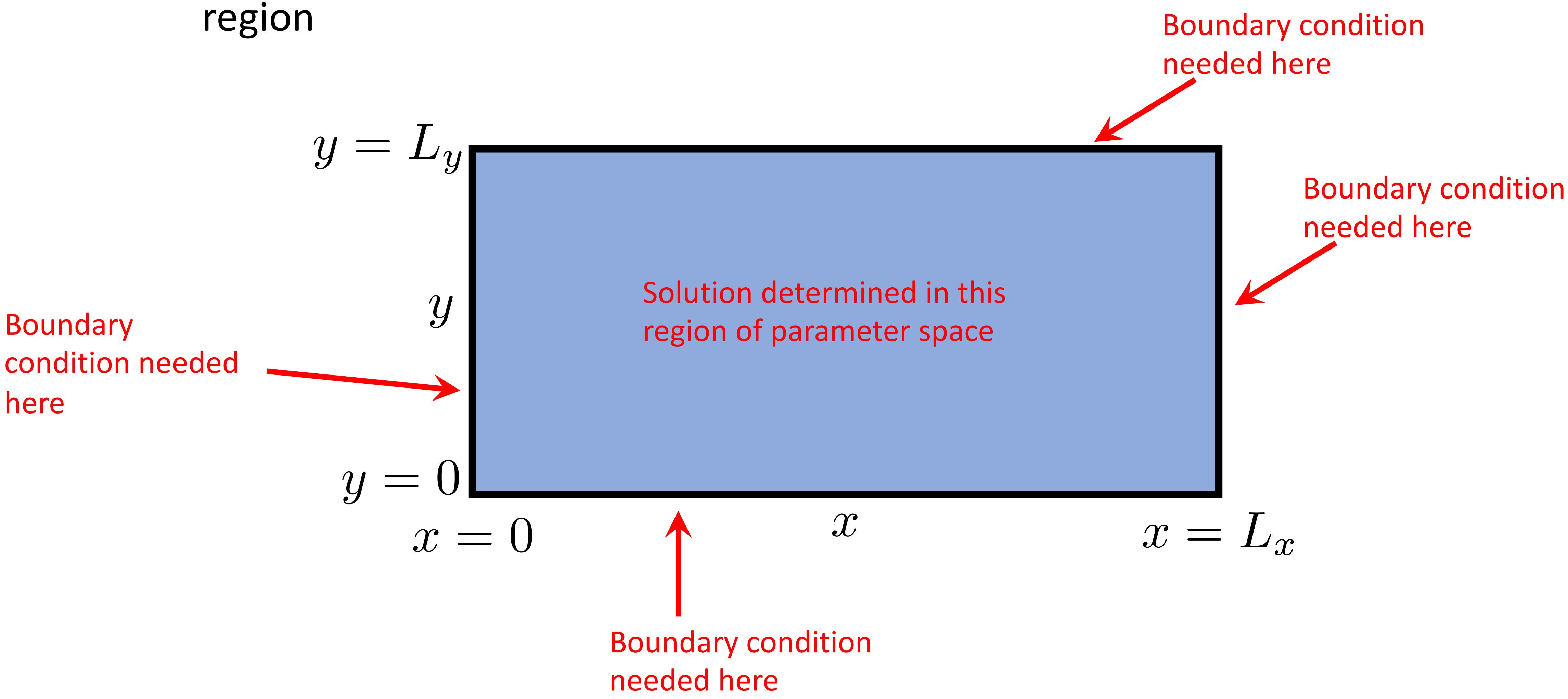
- Solution of these equations are well known:

$$X(x) = C_s \sin(kx) + C_c \cos(kx), \qquad Y(y) = C'_s \sinh(ky) + C'_c \cosh(ky)$$

  - Recall that k is complex, so solutions are "symmetric"
- To get the coefficients, we need to specify the boundary conditions

Boundary value problems

- All boundary values are specified at the outset
  - E.g., Laplace's equation in electrostatics, potential fixed on for sides of spatial region



Solution of Laplace’s eq. ODEs

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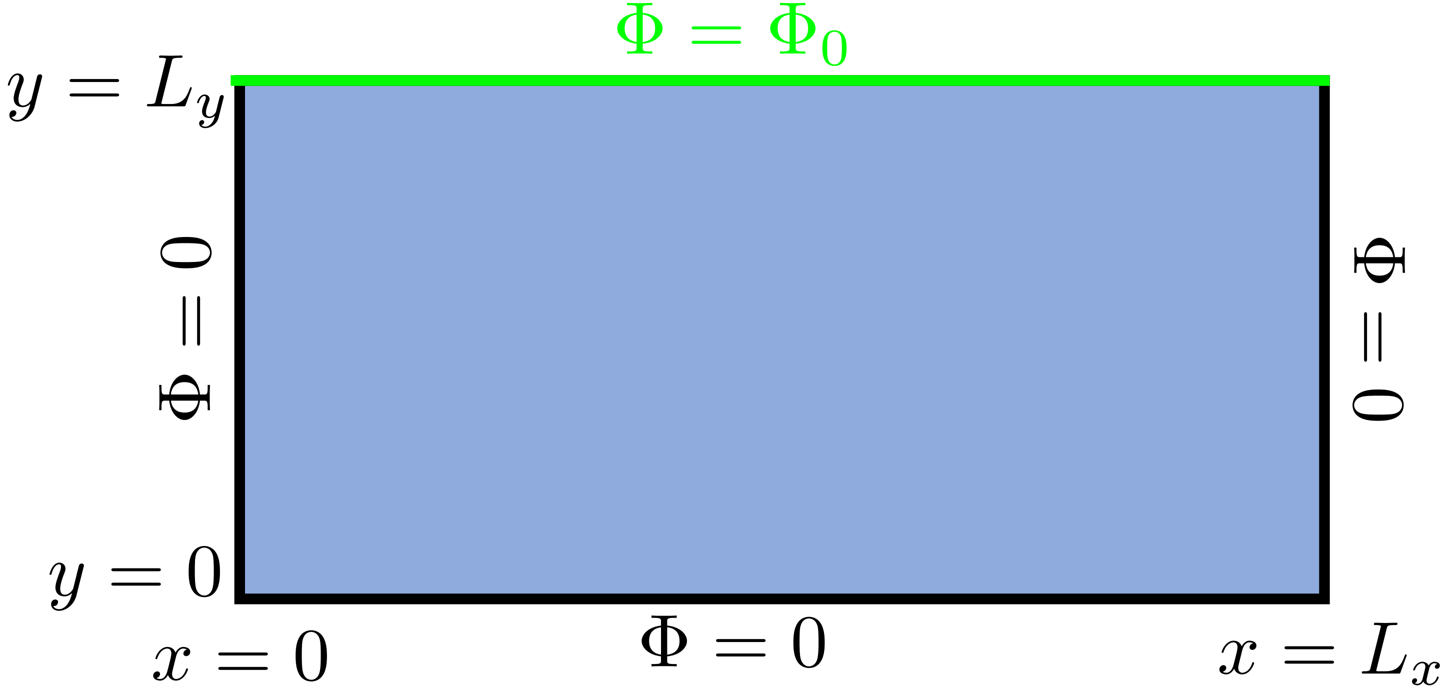
  - Recall that k is complex, so solutions are “symmetric”

- To get the coefficients, we need to specify the boundary conditions

$$\Phi(x=0,y) = \Phi(x=L_x,y) = \Phi(x,y=0) = 0, \quad \Phi(x,y=L_y) = \Phi_0$$



Solution of Laplace’s eq. ODEs

$$X(x) = C_s \sin(kx) + C_c \cos(kx), \qquad Y(y) = C'_s \sinh(ky) + C'_c \cosh(ky)$$

- Use our boundary conditions:

$$\Phi(x=0,y)=0 \implies C_c = 0$$
$$\Phi(x,y=0)=0 \implies C'_c = 0$$
$$\Phi(x=L_x,y)=0 \implies k = \frac{n\pi}{L_x},\ n = 1,2,\ldots$$

- So, we have solutions of the form:

$$c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi y}{L_x}\right)$$

- Any linear combination is also a solution, so:

$$\Phi(x,y) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi y}{L_x}\right)$$

Solution of Laplace's equation

- Now we use our last boundary condition:

$$\Phi_0 = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L_x}\right) \sinh\left(\frac{n\pi L_y}{L_x}\right)$$

- To solve the equation, multiply both sides by sin($m\pi x/L_x$) and integrate from 0 to L_x:

$$\int_0^{L_x} dx \Phi_0 \sin\left(\frac{m\pi x}{L_x}\right) = \sum_{n=1}^{\infty} c_n \sinh\left(\frac{n\pi L_y}{L_x}\right) \int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) \sin\left(\frac{n\pi x}{L_x}\right)$$

- Left-hand side integral:

$$\int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right) = \begin{cases} 2L_x/\pi, & m \text{ odd} \\ 0, & m \text{ even} \end{cases}$$

Solution of Laplace's equation

- Sum on the right-hand side simplifies because:

$$\int_0^{L_x} dx \sin\left(\frac{m\pi x}{L_x}\right)\sin\left(\frac{n\pi x}{L_x}\right) = \frac{L_x}{2}\delta_{n,m}$$

- So, we have:

$$\Phi_0 \frac{2L_x}{\pi m} = c_m \sinh\left(\frac{m\pi L_y}{L_x}\right)\frac{L_x}{2}, \quad m = 1, 3, 5, \ldots$$

- So:

$$c_m = \frac{4\Phi_0}{\pi m \sinh\left(\frac{m\pi L_y}{L_x}\right)}, \quad m = 1, 3, 5, \ldots$$

Solution of Laplace’s equation

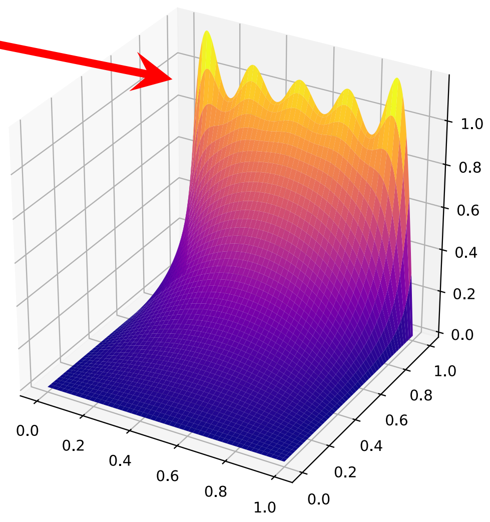
- Our final solution of Laplace’s equation with our chosen boundary conditions:

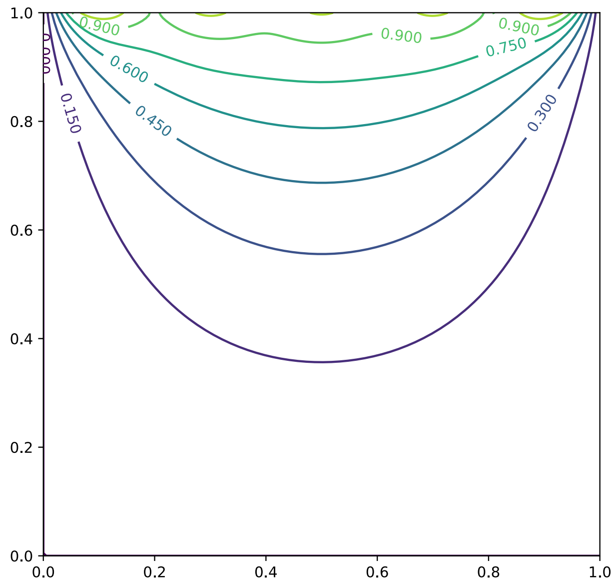
$$\Phi(x,y) = \Phi_0 \sum_{n=1,3,5,\ldots}^{\infty} \frac{4}{\pi n} \sin\left(\frac{n\pi x}{L_x}\right) \frac{\sinh\left(\frac{n\pi y}{L_x}\right)}{\sinh\left(\frac{n\pi L_y}{L_x}\right)}$$

Analytical solution to Laplace equation

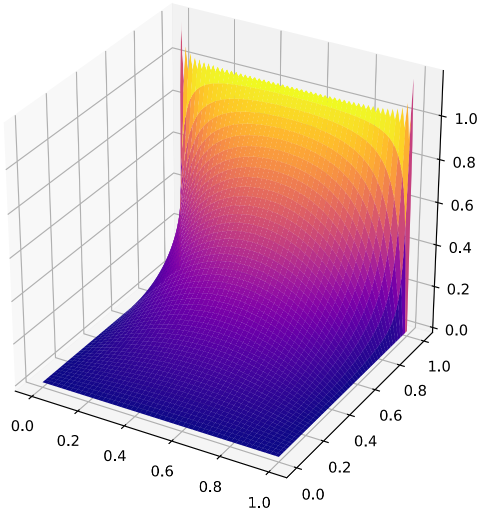
“Gibbs phenomenon,” oscillations of Fourier series for discontinuous function

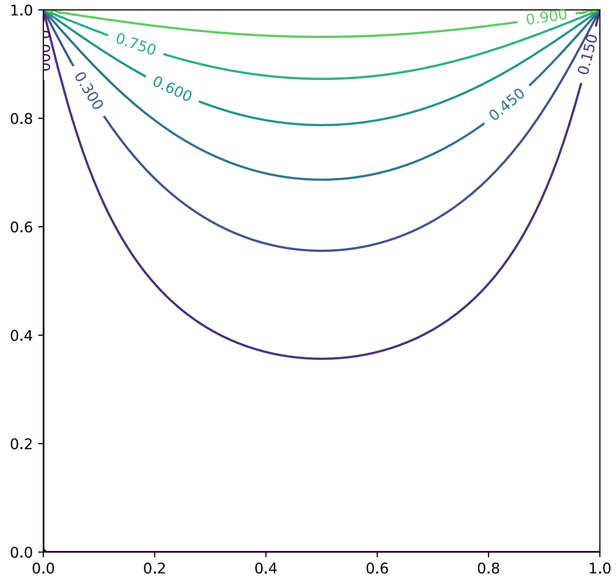
5 terms in the sum:





50 terms in the sum:





Numerical solution of the Laplace equation

- To do this, we'll go back to the *diffusion* equation we have solved previously, this time in two spatial dimensions:

$$\frac{\partial T(x,y,t)}{\partial t} = \kappa \left(\frac{\partial^2 T(x,y,t)}{\partial x^2} + \frac{\partial^2 T(x,y,t)}{\partial y^2} \right)$$

- Given an initial temperature profile and stationary boundary conditions, the solution will eventually relax to some steady state:

$$\lim_{t \to \infty} T(x,y,t) = T_s(x,y)$$

- In this state $\partial T / \partial t = 0$, so:

$$\frac{\partial^2 T_s}{\partial x^2} + \frac{\partial^2 T_s}{\partial y^2} = 0$$

- We can think of the Laplace equation as the steady-state of the diffusion equation

Relaxation methods

- Methods based on this physical intuition are called relaxation methods
- We can use the FTCS method that we have used previously for the diffusion equation
- Start with the 2D "diffusion" equation:

$$\frac{\partial \Phi}{\partial t} = \mu \left(\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right)$$

Remember, solving an electrostatic problem, so Φ does not actually have time dependence

Will drop out later

Relaxation methods

- Methods based on this physical intuition are called relaxation methods
- We can use the FTCS method that we have used previously for the diffusion equation
- Start with the 2D "diffusion" equation:

$$\frac{\partial \Phi}{\partial t} = \mu \left(\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right)$$

- Discretize:

$$\Phi_{i,j}^{n+1} = \Phi_{i,j}^{n} + \frac{\mu\tau}{h_x^2}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n} - 2\Phi_{i,j}^{n}) + \frac{\mu\tau}{h_y^2}(\Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n} - 2\Phi_{i,j}^{n})$$

- *n* here is not really time, more an improved guess for the solution

Jacobi relaxation method

- Recall that FTCS is stable for $\mu\tau/h^2 \leq 1/2$
- In 2D the stability criteria is :

$$\frac{\mu\tau}{h_x^2} + \frac{\mu\tau}{h_y^2} \leq \frac{1}{2}$$

- If $h_x = h_y = h$, then the criterion is

$$\frac{\mu\tau}{h^2} \leq \frac{1}{4}$$

- Since we want to take *n* to infinity, we choose the largest timestep:

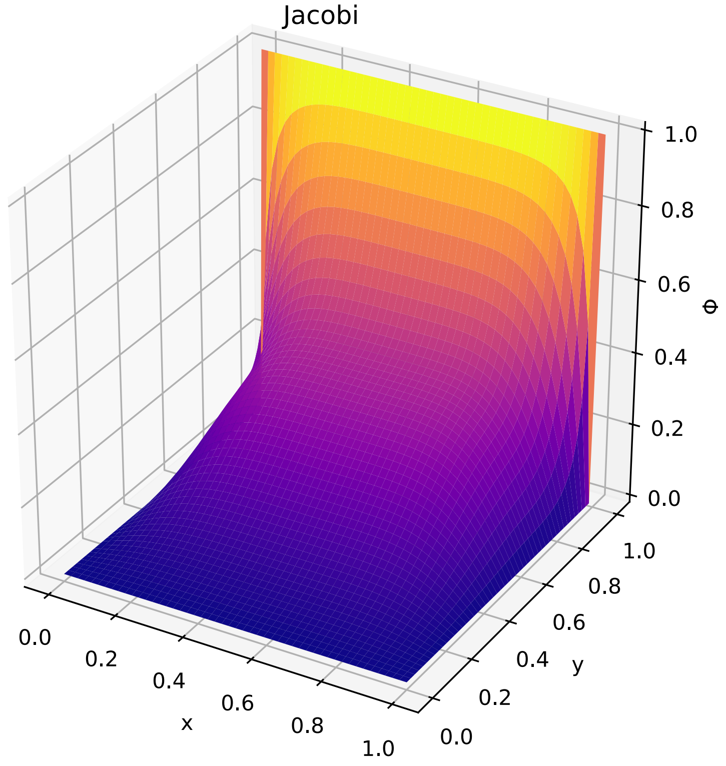
$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^n + \Phi_{i-1,j}^n + \Phi_{i,j+1}^n + \Phi_{i,j-1}^n)$$

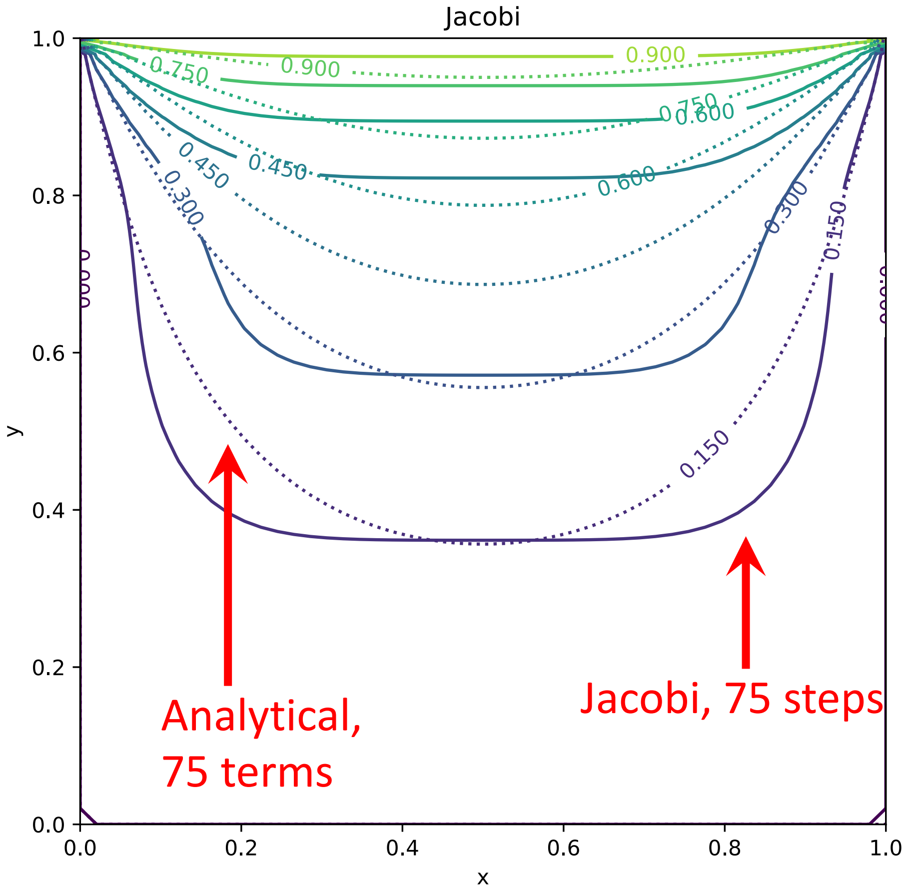
Jacobi method for Laplace equation

$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n})$$

- Note that the μ has dropped out
- Involves replacing the value of the potential at a point with the average value of the four nearest neighbors
  - Discrete version of mean-value theorem for the electrostatic potential
- This equation is for the interior points (exterior are set by boundary conditions)
- Simple to generalize for Poisson equation (i.e.,

Jacobi method for Laplace equation





Gauss-Seidel and simultaneous overrelaxation

- Gauss-Seidel: We can improve the convergence over the Jacobi method by using updated values of the potential as they are calculated:

$$\Phi_{i,j}^{n+1} = \frac{1}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n+1})$$

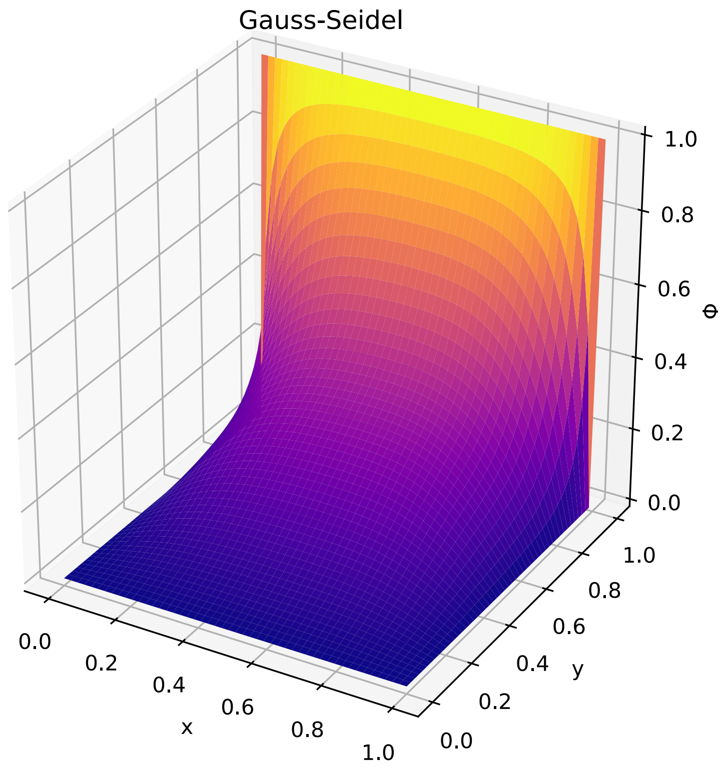
- Simultaneous overrelaxation: Choose a mixing parameter ω:

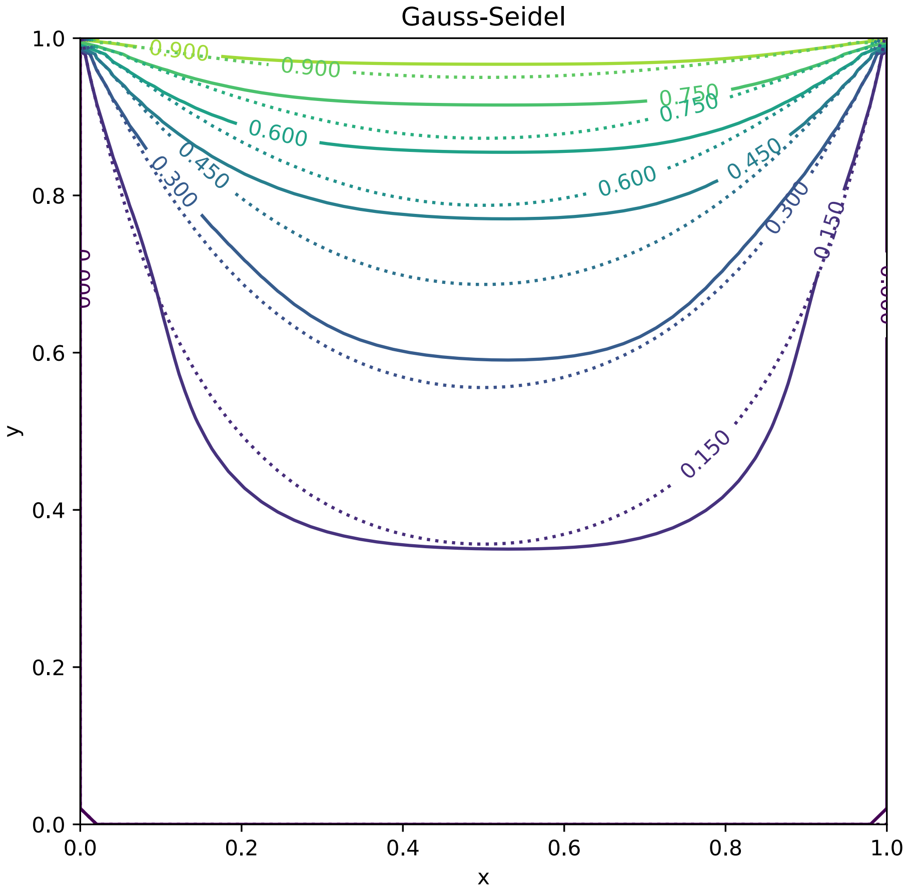
$$\Phi_{i,j}^{n+1} = (1-\omega)\Phi_{i,j}^{n} + \frac{\omega}{4}(\Phi_{i+1,j}^{n} + \Phi_{i-1,j}^{n+1} + \Phi_{i,j+1}^{n} + \Phi_{i,j-1}^{n+1})$$

  - $\omega < 1$ slows convergence, $\omega > 2$ is unstable
  - Often chosen by trial and error
  - E.g., for a square geometry with equal discretization, often a good choice:

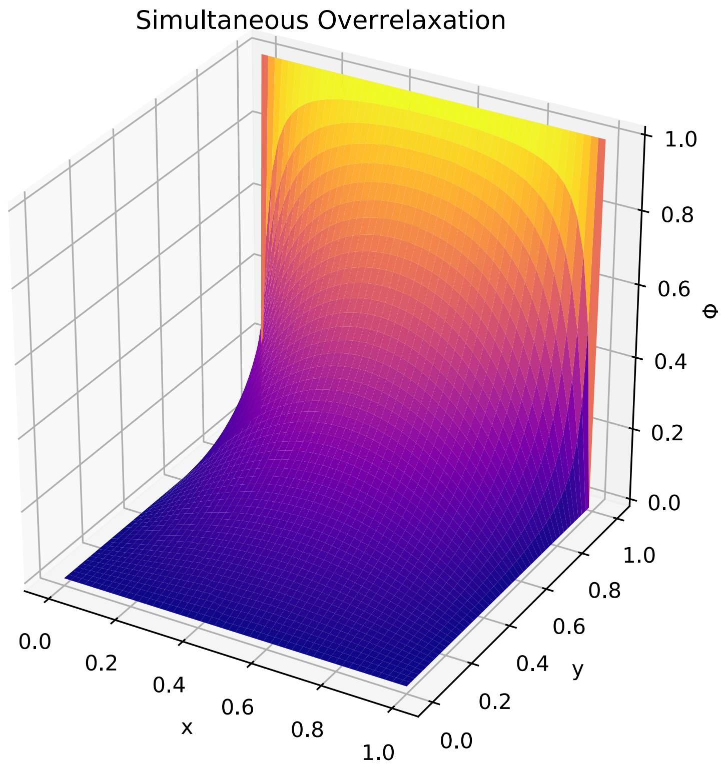
$$\omega_{\mathrm{opt}} = \frac{2}{1+\sin(\pi/N)}$$

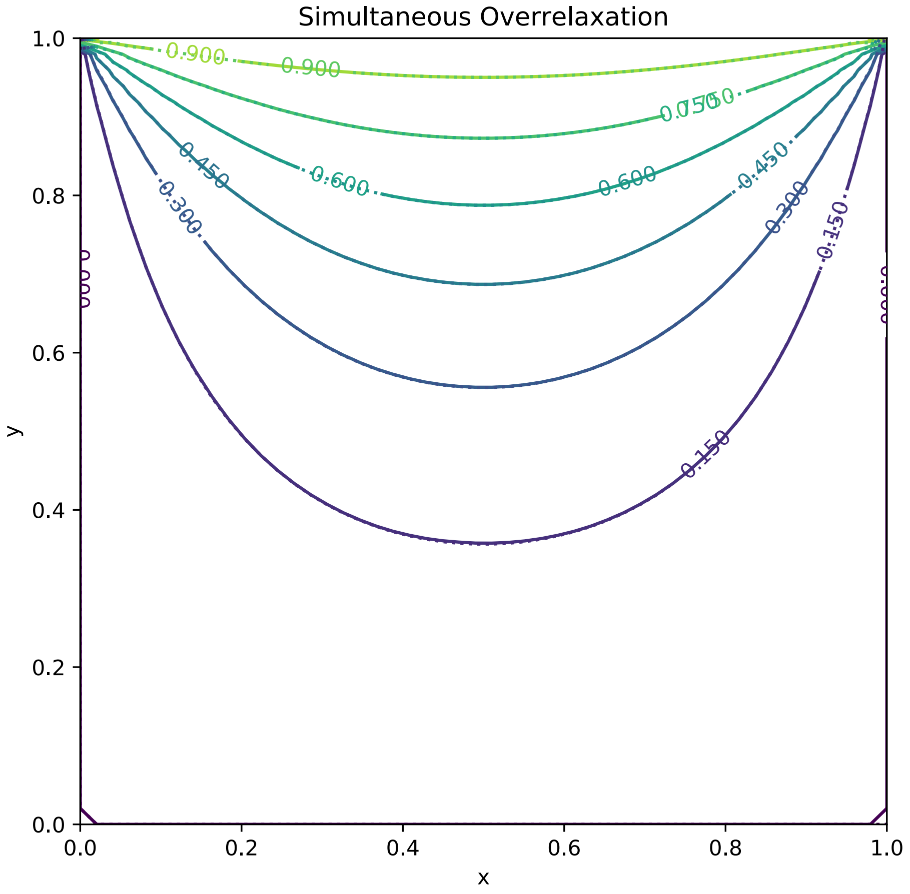
Gauss-Seidel for Laplace equation





Simultaneous overrelaxation for Laplace eq.





After class tasks

- Homework 3 due today Thursday Oct. 14
  - Let me know if you need more time!
- Homework 2 graded, see GRADES.md in your repositories
- Homework 4 will be posted soon

- Readings
  - Garcia Chapters 7
  - [MIke Zingale's notes on computational hydrodynamics]