Numerical Solutions to PDEs

Lecture Notes #15
— Second Order Equations —
Boundary Conditions; 2D and 3D

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Outline

1. Recap
   - Second Order Equations
2. Boundary Conditions
   - Fundamentals
   - Higher Order Accurate Schemes
3. 2D and 3D
   - Example: An Order (2,4) Scheme

Previously: Second Order Equations,

We started looking at problems with more than one time-derivative, *e.g.* the wave equation, and the Euler-Bernoulli beam equation.

Many of our previous definitions and theorems go through without change: consistency, convergence, and order of accuracy; however, the **definition and machinery for checking stability** had to be modified a little.

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Previously: Second Order Equations, 2 of 2

The stability definition was modified to allow for **linear growth** in the ℓ_2-norm over time (to match the growth of the PDE), and in the **von Neumann** analysis we allowed for double roots of the amplification polynomial on the unit circle.

Further, we augmented our definitions of Schur and von Neumann polynomials (with the von-Neumann-Order), so that a finite difference scheme for a second order (time) problem is stable if and only if its amplification polynomial is a von Neumann polynomial of second order.

Boundary Conditions for Second-Order Equations

Since the solutions to the second order wave equation

$$u_{tt} - a^2 u_{xx} = 0$$

consist of two parts moving at characteristic speeds $\pm\mathbf{a}$, it is clear that in a finite domain, *e.g.* $0 \leq x \leq 1$, we must specify **one** boundary condition at each boundary.

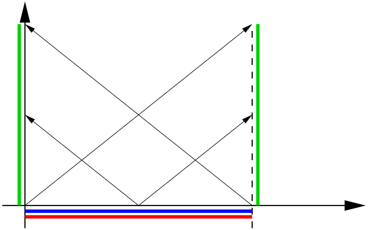

Figure: We must specify two initial conditions *e.g.* $u(0, x) = u_0(x)$, $u_t(0, x) = u_1(x)$, and two boundary conditions *e.g.* $u(t, 0) = f_0(t)$, and $u(t, 1) = f_1(t)$.

Boundary Conditions for Second-Order Equations

The specified boundary conditions can be of Dirichlet type (u specified), or Neumann type (u_x specified), or a combination thereof:

$$\alpha_0 u(0,t) + \beta_0 u_x(0,t) = \tilde{f}_0(x), \quad \min\{|\alpha_0|, |\beta_0|\} > 0$$
$$\alpha_1 u(1,t) + \beta_1 u_x(1,t) = \tilde{f}_1(x), \quad \min\{|\alpha_1|, |\beta_1|\} > 0$$

When $\beta_i = 0$, the numerical implementation of the boundary condition is trivial

$$\alpha_i v_I^n = \tilde{f}_I^n, \quad I = \begin{cases} 0 & \text{when } i = 0 \\ M & \text{when } i = 1 \end{cases}$$

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Neumann (or Mixed-Type) Boundary Conditions

When $\beta_i \neq 0$, then several possibilities present themselves. For a pure Neumann boundary condition at $x = 0$

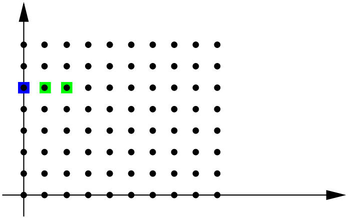
$$u_x(t, 0) = 0, \quad \text{no-flux}$$

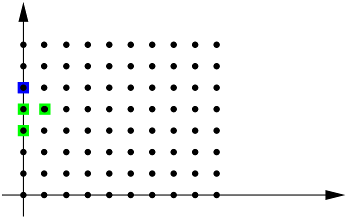
We can use

$$v_0^{n+1} = \frac{4v_1^{n+1} - v_2^{n+1}}{3}$$

or

$$v_0^{n+1} = 2v_0^n - v_0^{n-1} - 2a^2\lambda^2(v_0^n - v_1^n)$$





The first formula originates from the second-order accurate one-sided approximation

$$u_x(0) = \frac{4u(h) - 3u(0) - u(2h)}{2h} + \mathcal{O}\left(h^2\right),$$

and the second from applying the scheme

$$\frac{v_m^{n+1} - 2v_m^n + v_m^{n-1}}{k^2} = a^2 \frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2},$$

at $m = 0$, and eliminating the **ghost point** v_{-1}^n using the central second-order difference

$$\frac{v_1^n - v_{-1}^n}{2h} = 0.$$

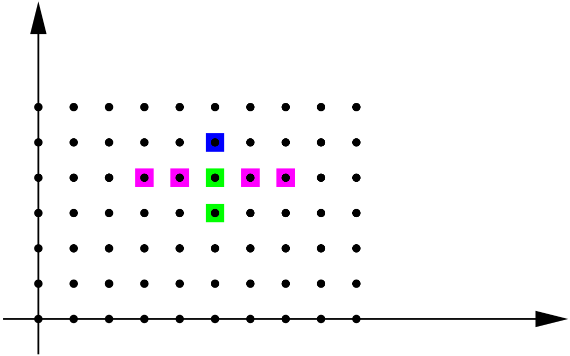
First-order one-sided differences should be avoided, since they will degrade the overall accuracy of the scheme.

BC's for Higher Order Accurate Schemes

The scheme

$$\frac{v_m^{n+1} - 2v_m^n + v_m^{n-1}}{k^2} = a^2 \left(1 - \frac{h^2}{12}\delta^2\right) \delta^2 v_m^n$$

is accurate of order (2,4) for the wave equation $u_{tt} = a^2 u_{xx}$.



BC's for Higher Order Accurate Schemes

If the value on the boundary is specified, then the value next to the boundary can be determined by interpolation, *e.g.*

$$v_1^{n+1} = \frac{1}{4}\left(v_0^{n+1} + 6v_2^{n+1} - 4v_3^{n+1} + v_4^{n+1}\right)$$

which comes from (the numerical BC — $\frac{\partial^4}{\partial x}u = 0$):

$$h^4 \delta_+^4 v_0^{n+1} = 0.$$

Applying this scheme with Neumann/mixed boundary conditions becomes quite challenging; — we can use (1) two layers of "ghost points," v_{-1}^n, and v_{-2}^n, which must be eliminated; or (2) non-symmetric finite differencing in the x-direction. In both settings we (α) have to match the order of the scheme, and (β) analyze the stability [lecture notes #19].

BC's for the Euler-Bernoulli Equation

Next, we consider the Euler-Bernoulli equation

$$u_{tt} = -b^2 u_{xxxx}$$

and the second order accurate scheme

$$\frac{v_m^{n+1} - 2v_m^n + v_m^{n-1}}{k^2} = -b^2 \frac{v_{m+2}^n - 4v_{m+1}^n + 6v_m^n - 4v_{m-1}^n + v_{m-2}^n}{h^4}$$

Here, we are going to need 2 boundary conditions at each end-point:

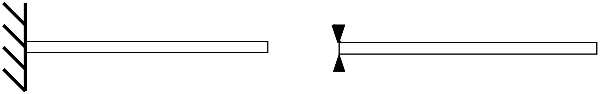


Figure: Illustration of physical boundary conditions, in the left figure the beam is clamped in at $x = 0$, and we have $u(t, 0) = u_x(t, 0) = 0$; in the right figure the beam is fixed in place at $x = 0$ but is allowed to pivot, and we have $u(t, 0) = u_{xx}(t, 0) = 0$. In both cases the right end of the beam is free to move, and the boundary conditions are $u_{xx}(t, L) = u_{xxx}(t, L) = 0$.

BC's for the Euler-Bernoulli Equation

Boundary Type	**u**	**u′**	**u″**	**u‴**
Free End			$u'' = 0$	$u''' = 0$
Clamp at End	fixed	fixed		
Simply Supported End	fixed		$u'' = 0$	
Point Force at End			$u'' = 0$	specified
Point Torque at End			specified	$u''' = 0$
	$\boldsymbol{\Delta}$**u**	$\boldsymbol{\Delta}$**u′**	$\boldsymbol{\Delta}$**u″**	$\boldsymbol{\Delta}$**u‴**
Interior Clamp	$\Delta u = 0$	$\Delta u' = 0$		
Interior Simple Support	$\Delta u = 0$	$\Delta u' = 0$	$\Delta u'' = 0$	
Interior Point Force	$\Delta u = 0$	$\Delta u' = 0$	$\Delta u'' = 0$	$\Delta u'''$ specified
Interior Point Torque	$\Delta u = 0$	$\Delta u' = 0$	$\Delta u''$ specified	$\Delta u''' = 0$

Note: Here $\Delta u'' \equiv u''(x_{\text{right}}) - u''(x_{\text{left}})$.

http://en.wikipedia.org/wiki/Euler-Bernoulli_beam_equation

BC's for the Euler-Bernoulli Equation

The finite difference implementations of these boundary conditions are quite straight-forward, but require some thought...

Second order accurate approximations for u_x, u_{xx} and u_{xxx} can be used at the boundary points

$$\frac{v_1^n - v_{\mathbf{-1}}^n}{2h}, \quad \frac{v_1^n - 2v_0^n + v_{\mathbf{-1}}^n}{h^2}, \quad \frac{v_2^n - 2v_1^n + 2v_{\mathbf{-1}}^n - v_{\mathbf{-2}}^n}{2h^3},$$

$$\frac{v_{\mathbf{M+1}}^n - v_{M-1}^n}{2h}, \quad \frac{v_{\mathbf{M+1}}^n - 2v_M^n + v_{M-1}^n}{h^2}, \quad \frac{v_{\mathbf{M+2}}^n - 2v_{\mathbf{M+1}}^n + 2v_{M-1}^n - v_{M-2}^n}{2h^3},$$

after which we must eliminate the values at the "ghost points" $\mathbf{v_{-1}^n}$, $\mathbf{v_{-2}^n}$, $\mathbf{v_{M+1}^n}$, and $\mathbf{v_{M+2}^n}$. It's "just" a "book-keeping" problem!

Second-Order Equations in 2D and 3D

In terms of definitions and theory, nothing much changes as we move our finite difference schemes into 2D and 3D.

The wave equation in 2D / 3D is given by

$$u_{tt} = a^2\left(u_{xx} + u_{yy}\right), \quad u_{tt} = a^2\left(u_{xx} + u_{yy} + u_{zz}\right),$$

and the most straight-forward second order schemes are given by

$$\begin{aligned} \delta_t^2 v_{\ell,m}^n &= a^2\left(\delta_x^2 v_{\ell,m}^n + \delta_y^2 v_{\ell,m}^n\right) \\ \delta_t^2 v_{k,\ell,m}^n &= a^2\left(\delta_x^2 v_{k,\ell,m}^n + \delta_y^2 v_{k,\ell,m}^n + \delta_z^2 v_{k,\ell,m}^n\right), \end{aligned}$$

When $\Delta x = \Delta y = \Delta z = h$ the stability conditions for 2D and 3D are

$$a\lambda \leq \frac{1}{\sqrt{2}}, \quad a\lambda \leq \frac{1}{\sqrt{3}}$$

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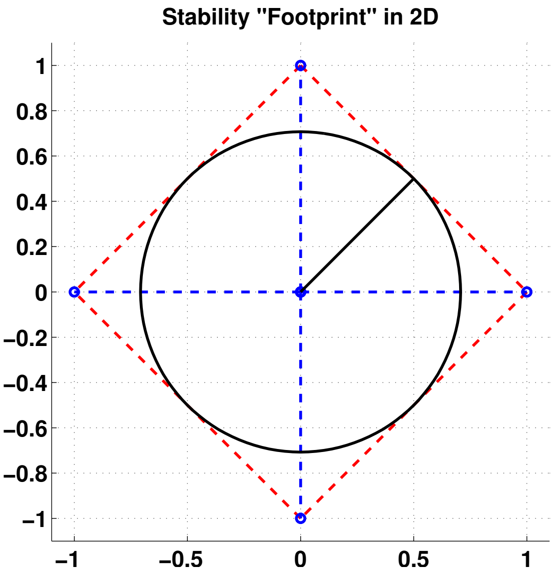
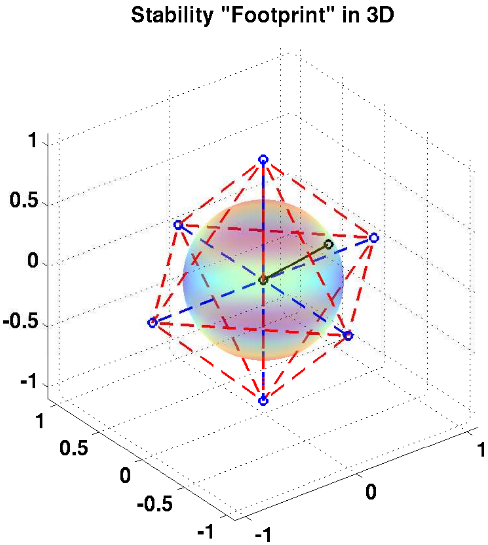
Second-Order Equations in 2D and 3D



Second-Order Equations in 2D and 3D



Second-Order Equations in 2D and 3D

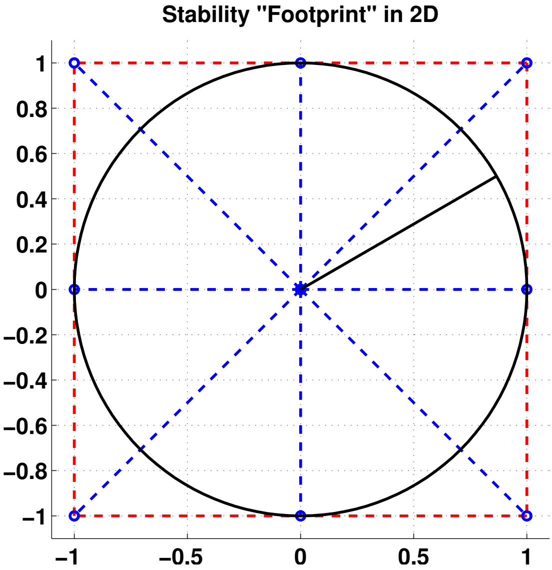
These restrictions can be improved to $a\lambda \leq 1$, by modifying the schemes, here in 2D:

$$\delta_t^2 v_{\ell,m}^n = \frac{1}{4}a^2 \Big[\delta_x^2 (v_{\ell,m+1}^n + 2v_{\ell,m}^n + v_{\ell,m-1}^n) + \delta_y^2 (v_{\ell+1,m}^n + 2v_{\ell,m}^n + v_{\ell-1,m}^n) \Big]$$

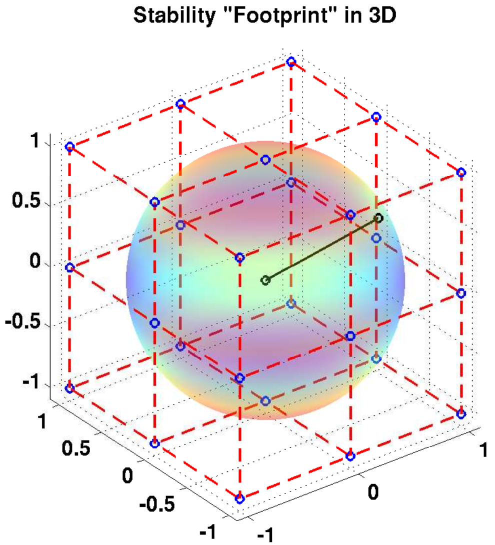
Further, ADI schemes can be developed, *e.g.*

$$\begin{aligned} \left[1 - \frac{1}{4}k^2 a^2 \delta_x^2\right] \tilde{v}_{\ell,m}^{n+1/2} &= \left[1 + \frac{1}{4}k^2 a^2 \delta_y^2\right] v_{\ell,m}^n \\ \left[1 - \frac{1}{4}k^2 a^2 \delta_y^2\right] \tilde{v}_{\ell,m}^{n+1} &= \left[1 + \frac{1}{4}k^2 a^2 \delta_y^2\right] \tilde{v}_{\ell,m}^{n+1/2} \\ v_{\ell,m}^{n+1} &= 2\tilde{v}_{\ell,m}^{n+1} - v_{\ell,m}^{n-1} \end{aligned}$$

Second-Order Equations in 2D and 3D



Second-Order Equations in 2D and 3D



Second-Order Equations in 2D and 3D

If we look at the amplification factors corresponding to the finite difference scheme for the wave equations, we have

$$g_{\pm} = \left[\left[1 - a^2\lambda^2 \left(\sin^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\phi}{2}\right)\right)\right] \pm ia\lambda \left(\sin^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\phi}{2}\right)\right)^{1/2}\right]^2$$

Comparing this with

$$e^{ia\,(\xi_1^2+\xi_2^2)^{1/2}\,k}$$

we can identify the phase velocity, $\alpha(\xi_1, \xi_2)$, from the expression

$$\sin\left[\frac{1}{2}\alpha(\xi_1,\xi_2)k\,(\xi_1^2+\xi_2^2)^{1/2}\right] = a\lambda \left(\sin^2\left(\frac{h\xi_1}{2}\right) + \sin^2\left(\frac{h\xi_2}{2}\right)\right)^{1/2}$$

Second-Order Equations in 2D and 3D

With a little bit of help from Taylor, we identify

$$\alpha(\xi_1, \xi_2) = a\left[1 - \frac{h^2|\xi|^2}{24}\left(\cos^4\beta + \sin^4\beta - a^2\lambda^2\right) + \mathcal{O}\left(h^4|\xi|^4\right)\right]$$

where

$$|\xi| = (\xi_1^2 + \xi_2^2)^{1/2}, \quad \beta = \tan^{-1}(\xi_1/\xi_2)$$

This shows that the **phase error** depends on the direction of propagation $\bar{\mathbf{n}} = (\cos\beta, \sin\beta)$.

In most computations this distortion is not visible, unless the grid is very coarse (h large).

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2nd Order Eqns. in 2D and 3D — Numerical Dispersion

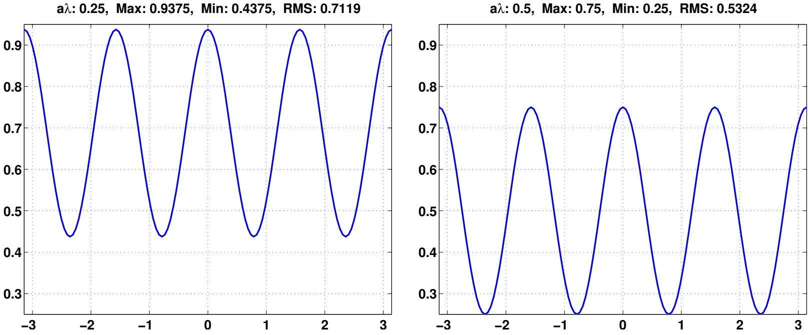


Figure: LEFT: The numerical dispersion factor $(\cos^4\beta + \sin^4\beta - a^2\lambda^2)$ for angles in $[-\pi, \pi]$ for $a\lambda = \frac{1}{4}$. The RMS-deviation is 0.71. RIGHT: $a\lambda = \frac{1}{2}$, with RMS-deviation at 0.53.

2nd Order Eqns. in 2D and 3D — Numerical Dispersion

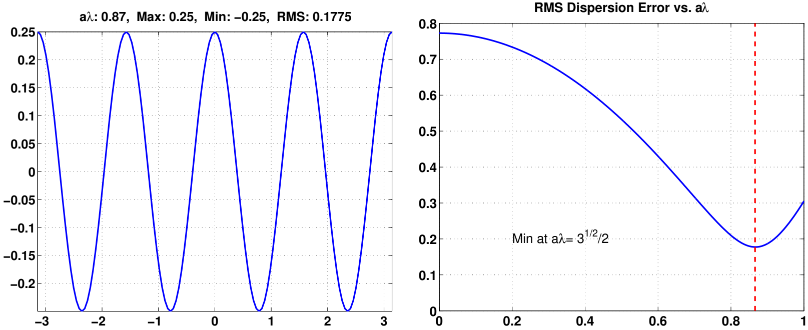


Figure: LEFT: The numerical dispersion factor $(\cos^4\beta + \sin^4\beta - a^2\lambda^2)$ for angles in $[-\pi, \pi]$ for $a\lambda = \frac{\sqrt{3}}{2}$. The RMS-deviation is 0.18. RIGHT: The RMS Dispersion Error vs. $a\lambda$ has a minimum at $\frac{\sqrt{3}}{2}$.

Example

We use the (2,4)-order scheme

$$\delta_t^2 v_{\ell,m}^n = \frac{1}{4}a^2\left[\delta_x^2(v_{\ell,m+1}^n + 2v_{\ell,m}^n + v_{\ell,m-1}^n) + \delta_y^2(v_{\ell+1,m}^n + 2v_{\ell,m}^n + v_{\ell-1,m}^n)\right]$$

to solve

$$u_{tt} = a^2(u_{xx} + u_{yy}), \quad x, y \in [-1, 1]$$

with

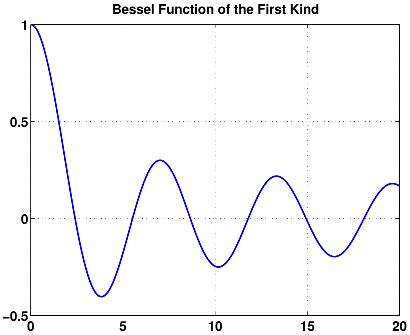
$$a = 1, \quad u(0,x) = J_0\left(3\sqrt{(x-1/2)^2 + (y-1/2)^2}\right), \quad u_t(0,x) = 0$$

and

$$\Delta x = \Delta y = h = 0.1, \quad \lambda = 0.9$$

Example

$J_0(r)$ is the Bessel function of the first kind



We use the exact solution

$$u(t,x,y) = \cos(3t)\, J_0\left(3\sqrt{(x-1/2)^2 + (y-1/2)^2}\right)$$

to prescribe boundary conditions.

Example

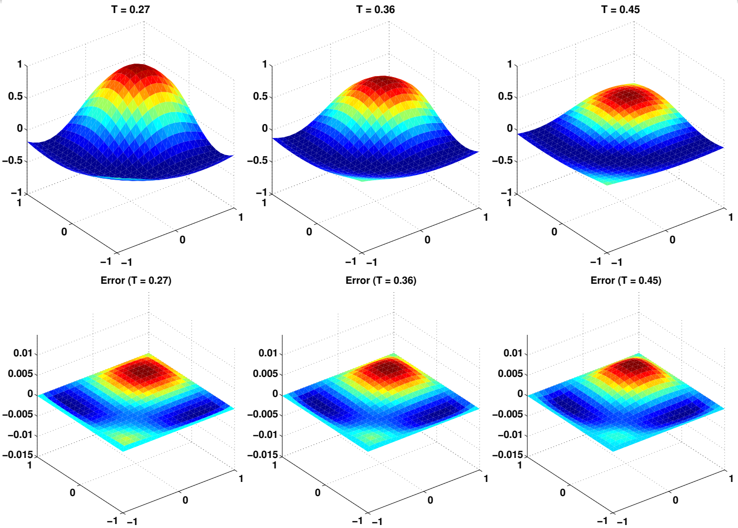


Figure: Snapshots of the solution and error at $T = 0.27$, $T = 0.36$, and $T = 0.45$. See also the movies **wave2d_soln.mpg**, and **wave2d_err.mpg**