Diffusion

Learning Objectives

Following this lecture, students will be able to:

- Describe the differences between implicit and explicit numerical diffusion.
- Demonstrate that explicit numerical diffusion operators become increasingly scale selective as the diffusion operator's order increases.

Overview

Diffusion can be conceptualized as the spreading out, or smoothing, of atmospheric fields in all three spatial dimensions. Diffusion weakens or dampens gradients by reducing the magnitude of local maxima and minima (Fig. 1). Physical diffusion by turbulent eddies transports atmospheric fields. However, there are also two forms of artificial, or numerical, diffusion:

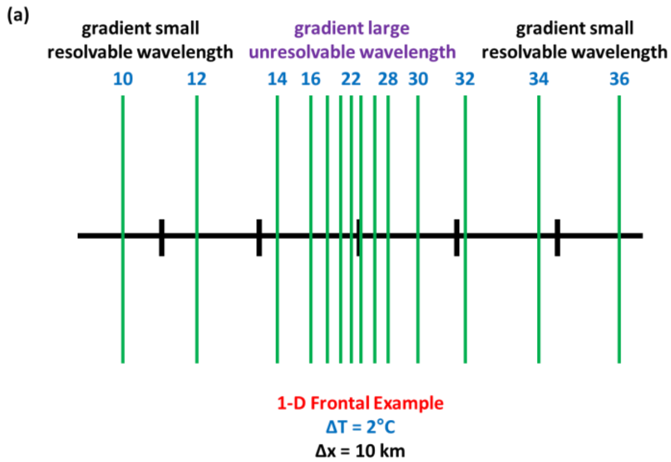
- **Implicit numerical diffusion**. This is identical to the idea of **implicit numerical damping** that we considered in an earlier lecture. Recall that specific characteristics of this damping, such as its scale selectivity and Courant number dependence, vary between finite-differencing schemes.

- **Explicit numerical diffusion**. This takes one of two forms:

    - The predictive equations for each model variable have an added explicit damping term, the properties of which (e.g., stability criteria, wavelength dependence, damping magnitude) vary between formulations. These terms are often solved implicitly because of the large damping coefficients used with such formulations.

    - Most physical diffusion occurs on the subgrid-scale, such that explicit numerical diffusion formulations are also used to parameterize the associated vertical transports in the substrate (soil) and atmospheric boundary layer.

This lecture focuses on explicit numerical diffusion in the content of explicit damping terms added to the model predictive equations. Though this diffusion is non-physical, such formulations can improve model forecasts if they help to dampen poorly resolved, shorter-wavelength features while largely not affecting better resolved, longer-wavelength phenomena.



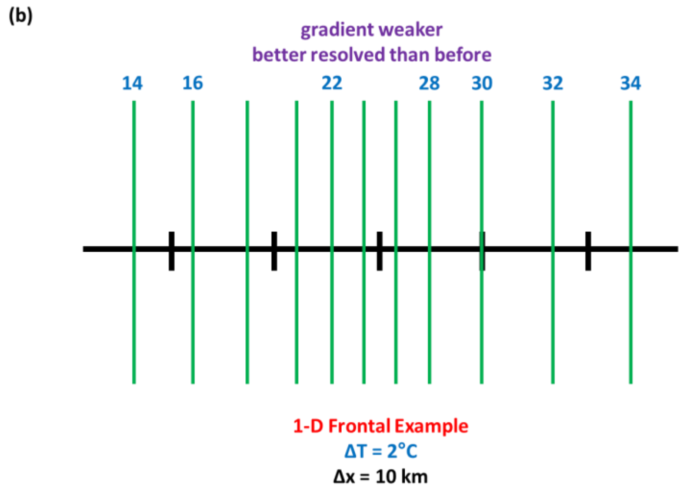


Figure 1. An idealized diffusion conceptualization. In panel (a), a sharp horizontal gradient in temperature exists in the middle of the grid. In panel (b), diffusion has weakened this gradient and reduced the magnitude of the local temperature minimum and maximum present in panel (a).

Numerical Formulation for Explicit Diffusion

A generalized explicit numerical diffusion term is given by:

$$\frac{\partial h}{\partial t} = \left(-1\right)^{\frac{n}{2}+1} K_n \nabla^n h$$

Here, h is any model dependent variable, n is the order of the diffusion operator (n = 0, 2, 4, 6…), and K_n is the diffusion (or damping) coefficient.

Consider the zeroth-order (n = 0) diffusion, i.e.,

$$\frac{\partial h}{\partial t} = -K_0 h$$

This defines a diffusion that is applied directly to *h*. It acts uniformly over all wavelengths. Such uniform damping is typically not employed by numerical models except near lateral boundaries.

Consider the second-order ($n = 2$) diffusion, i.e.,

$$\frac{\partial h}{\partial t} = K_2 \nabla^2 h$$

This defines a diffusion that acts on the Laplacian of *h*. Recall that the Laplacian of a field has the opposite sign of the field itself. As a result, where *h* is a local maximum, $\nabla^2 h$ is negative and *h* thus decreases with time. Conversely, where *h* is a local minimum, $\nabla^2 h$ is positive and *h* thus increases with time. In both cases, the diffusion operator reduces the magnitude of the gradient in *h*.

This diffusion formulation is weakly scale selective, wherein shorter wavelengths are modestly dampened more than are longer wavelengths. As compared to a second-order diffusion, higher-order formulations are generally more scale-selective, damping shorter wavelengths (e.g., sharper gradients) more so than longer wavelengths.

Since the Laplacian's magnitude is greatest at local maxima or minima, the second-order diffusion operator does not introduce new maxima or minima to the field, a desirable trait. This is not true for higher-order diffusion operators, which can introduce new extrema. However, there are methods (e.g., flux limiter methods) that can mitigate this drawback.

Horizontal Diffusion and Linear Numerical Stability

Let us consider the linear stability of a second-order diffusion operator computed using the forward-in-time, second-order centered-in-space differencing scheme, i.e.,

$$\frac{h_x^{t+1} - h_x^t}{\Delta t} = K_2 \left(\frac{h_{x+1}^t + h_{x-1}^t - 2h_x^t}{(\Delta x)^2} \right)$$

As before, assume a wave-like solution for *h* of the form:

$$h = \hat{h} e^{i(kx - \omega t)} = \hat{h} e^{\omega_I t} e^{i(kx - \omega_R t)}$$

where $\omega = \omega_R + i\omega_I$. If we substitute this solution for *h*, expand the resulting exponential functions, and divide through by a common factor of $\hat{h} e^{\omega_I t} e^{i(kx - \omega_R t)}$, we obtain:

$$e^{\omega_I \Delta t} e^{-i\omega_R \Delta t} - 1 = \frac{K\Delta t}{(\Delta x)^2}\left(e^{ik\Delta x} + e^{-ik\Delta x} - 2\right)$$

We can use Euler's relations to rewrite the complex exponentials. Doing so, we obtain:

$$e^{\omega_I \Delta t}\left(\cos(\omega_R \Delta t) - i\sin(\omega_R \Delta t)\right) - 1 = \frac{K\Delta t}{(\Delta x)^2}\left(2\cos(k\Delta x) - 2\right)$$

Splitting this equation into its real and imaginary components, we obtain:

$$e^{\omega_I \Delta t}\cos(\omega_R \Delta t) - 1 = \frac{K\Delta t}{(\Delta x)^2}\left(2\cos(k\Delta x) - 2\right) \qquad \text{(real)}$$

$$-i\sin(\omega_R \Delta t) e^{\omega_I \Delta t} = 0 \qquad \text{(imaginary)}$$

Recall that to evaluate the linear stability of this equation, we need to eliminate ω_R from this system of equations, leaving only ω_I or, more specifically, $e^{\omega_I \Delta t}$.

Because the exponential function in the imaginary equation never equals zero, $\sin(\omega_R \Delta t)$ must equal 0 for that equation's equality to hold. The only values of ω_R that result in $\sin(\omega_R \Delta t) = 0$ are 0 (such that $\omega_R \Delta t = 0$) and $\Delta t/\pi$ (such that $\omega_R \Delta t = \pi$). It can be shown that $\omega_R = \Delta t/\pi$ is a version of the $\omega_R = 0$ case, allowing us to focus on the $\omega_R = 0$ case.

For $\omega_R = 0$, $\cos(\omega_R \Delta t) = 1$ and the real component of the equation becomes:

$$e^{\omega_I \Delta t} = 1 + 2\frac{K\Delta t}{(\Delta x)^2}\left(\cos(k\Delta x) - 1\right)$$

This defines the multiplicative change in amplitude in h that occurs with each time step during the model integration for the forward-in-time, second-order centered-in-space differencing scheme applied to a second-order diffusion operator.

The allowable values of $k\Delta x$ range from ~0 to π. For $\Delta x \sim 0$, $\cos(k\Delta x) \sim 1$ and $\cos(k\Delta x) - 1 \sim 0$. Thus, $e^{\omega_I \Delta t} = 1$ for all Δt and the solution is numerically stable. This is not realistic, however: Δx never approximately equals zero.

For $k\Delta x = \pi$, representing the $2\Delta x$ wave (since $\Delta x = L/2$), $\cos(k\Delta x) = -1$ and $\cos(k\Delta x) - 1 = -2$. In this case, the stability criterion takes the form:

$$e^{\omega_I \Delta t} = 1 - 4\frac{K\Delta t}{(\Delta x)^2}$$

Because K, Δt, and $(\Delta x)^2$ are all positive-definite, $e^{\omega_I \Delta t} < 1$. However, $e^{\omega_I \Delta t} < -1$ can still occur, defining exponential growth with a change in the wave's phase. (Note that all negative values define a change in the wave's phase; only values smaller than -1 denote exponential growth.)

From this, we can assess the stability criterion: simply let $e^{\omega_I \Delta t} = -1$, change the equality to an inequality (less than or equal to), and rearrange to obtain:

$$-1 \geq 1 - 4\frac{K\Delta t}{(\Delta x)^2} \qquad \text{becomes} \qquad \frac{K\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$$

We can also determine a criterion to prevent the wave from changing phase; simply let $e^{\omega_I \Delta t} = 0$ and rearrange to obtain:

$$0 \geq 1 - 4\frac{K\Delta t}{(\Delta x)^2} \qquad \text{becomes} \qquad \frac{K\Delta t}{(\Delta x)^2} \leq \frac{1}{4}$$

For $\frac{K\Delta t}{(\Delta x)^2} \leq \frac{1}{4}$, the diffusion term is stable with no change in phase. Because Δt and Δx cannot be 0, however, there will always be some damping of the wave's amplitude even if this criterion is met (i.e., from the equation at the top of this page, $e^{\omega_I \Delta t}$ can never exactly be equal to 1).

If one instead plugs in different values for Δx between $L/2$ and 0, the resulting stability criteria are less stringent than those above. Thus, since Δx cannot be 0, the $2\Delta x$ wave (with $\Delta x = L/2$) is the wavelength which limits numerical stability for this diffusion formulation.

Diffusion also may be formulated in the vertical, with an analogous stability term involving Δz (or the appropriate model vertical coordinate) that must be considered. The total linear stability of the model, then, is limited by the term of the primitive equations that requires in the smallest Δt for a given grid spacing (whether horizontal or vertical). This may change throughout the simulation's duration as the meteorology changes; thus, we typically choose a model time step well below the theoretical limits to avoid unnecessarily achieving numerical instability with the chosen model configuration.

Diffusion Scale Selectivity

Returning to our equation for $e^{\omega_I \Delta t}$, we can define a value of K that dampens the $2\Delta x$ wave entirely at each time step (i.e., $e^{\omega_I \Delta t} = 0$). This criterion is given by:

$$\frac{K\Delta t}{(\Delta x)^2} \leq \frac{1}{4}$$

If the inequality is replaced with an equal sign and the equation solved for *K*, we obtain:

$$K = \frac{(\Delta x)^2}{4\Delta t}$$

If we use this as our value for *K*, the stability equation becomes:

$$e^{\omega_I \Delta t} = 1 + \frac{1}{2}\left(\cos(k\Delta x) - 1\right)$$

If we substitute different wavelengths *L* for *k* in this equation, we can determine the wavelength-dependence, or scale-selectivity, of the damping function. This is depicted by the blue line in Fig. 2.

The same process can be used to determine the multiplicative change in *h* that occurs with each time step for the forward-in-time, second-order centered-in-space differencing scheme applied to fourth- and sixth-order diffusion operators. Second-order centered-in-space finite difference approximations for the fourth and sixth partial derivatives, respectively, are given by the following equations:

$$\frac{\partial^4 h}{\partial x^4} = \frac{(h_{x+2} + h_{x-2}) - 4(h_{x+1} + h_{x-1}) + 6h_x}{(\Delta x)^4}$$

$$\frac{\partial^6 h}{\partial x^6} = \frac{(h_{x+3} + h_{x-3}) - 6(h_{x+2} + h_{x-2}) + 15(h_{x+1} + h_{x-1}) - 20h_x}{(\Delta x)^6}$$

The resulting equations for $e^{\omega_I \Delta t}$ with these diffusion formulations are given by:

$$e^{\omega_I \Delta t} = 1 + 2\frac{K\Delta t}{(\Delta x)^4}\left(-\cos(2k\Delta x) + 4\cos(k\Delta x) - 3\right)$$

$$e^{\omega_I \Delta t} = 1 + 2\frac{K\Delta t}{(\Delta x)^6}\left(\cos(3k\Delta x) - 6\cos(2k\Delta x) + 15\cos(k\Delta x) - 10\right)$$

Using these equations, values of *K* that result in $e^{\omega_I \Delta t} = 0$ for the $L = 2\Delta x$ wave may be obtained for these diffusion formulations and the chosen differencing scheme. These are given by:

$$K = \frac{(\Delta x)^4}{16\Delta t} \qquad \text{(fourth-order diffusion)}$$

$$K = \frac{(\Delta x)^6}{64\Delta t} \qquad \text{(sixth-order diffusion)}$$

If we use these as our values for K, the stability equations become:

$$e^{\omega_I \Delta t} = 1 + \frac{1}{8}\left(-\cos(2k\Delta x) + 4\cos(k\Delta x) - 3\right)$$

$$e^{\omega_I \Delta t} = 1 + \frac{1}{32}\left(\cos(3k\Delta x) - 6\cos(2k\Delta x) + 15\cos(k\Delta x) - 10\right)$$

Substituting different wavelengths L for k in these equations allows us to determine the wavelength dependence or scale selectivity of the fourth- and sixth-order diffusion formulations. These are depicted by the red and green lines, respectively, in Fig. 2. For all diffusion functions, the damping magnitude decreases as the wavelength increases. The rate at which it does so is largest for higher-order diffusion operators. Thus, we prefer higher-order diffusion operators so long as their weaknesses (e.g., creating new extrema) can be mitigated by some means.

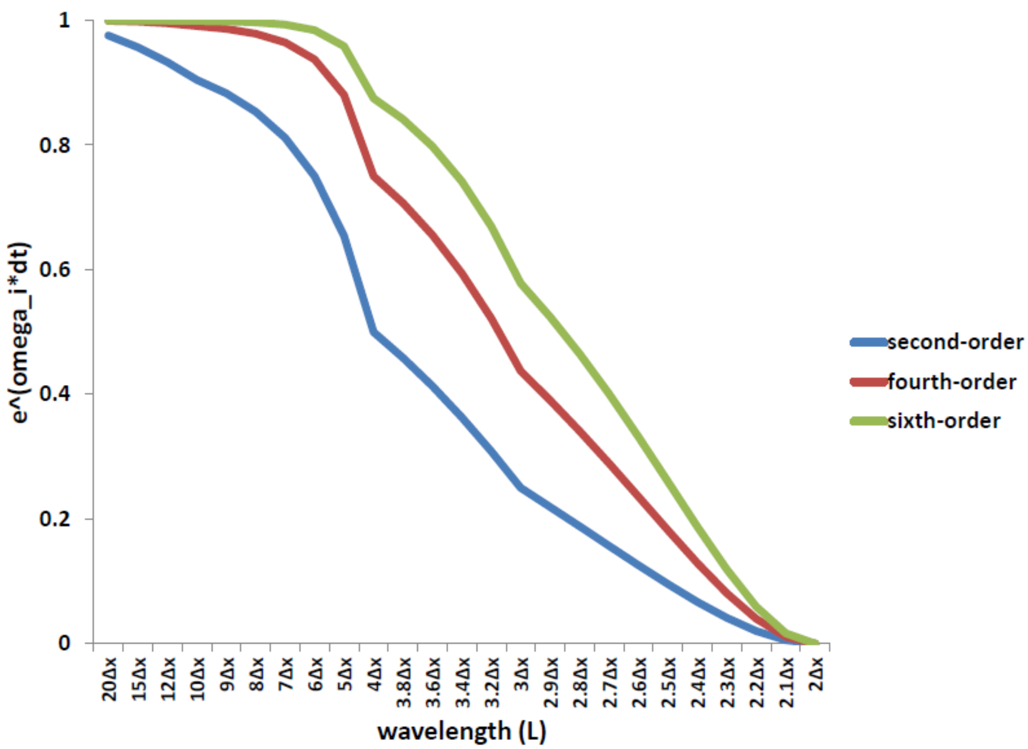


Figure 2. Depiction of damping magnitude per time step, $e^{\omega_I \Delta t}$, as a function of wavelength for second-, fourth-, and sixth-order diffusion operators using the forward-in-time, second-order centered-in-space finite differencing scheme. Note that for each diffusion operator, the value of K is chosen such that the $2\Delta x$ wave is entirely dampened at each time step. Adapted from Warner (2011), their Fig. 3.34.

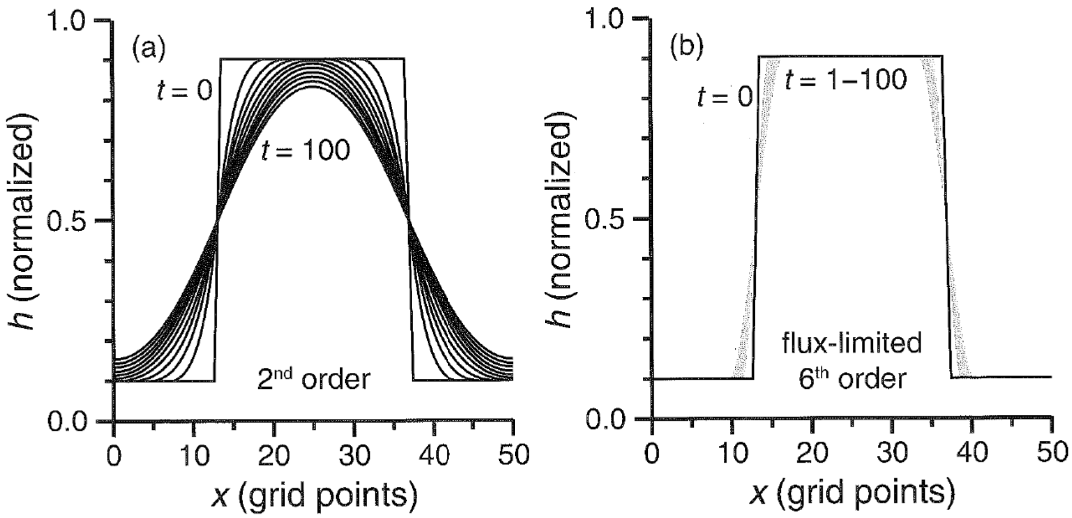


Figure 3. In each panel, the influence of diffusion – second-order in panel (a), sixth-order with a flux limited in panel (b) – upon an initial square wave over 100 model time steps is depicted. Note that the value of *K* for each diffusion operator is chosen such that the $2\Delta x$ wave is entirely dampened at each time step. As the second-order diffusion operator is less scale-selective than is the sixth-order diffusion operator, its effects upon the square wave extend across the wave rather than being localized to its sharp edges. Reproduced from Warner (2011), their Fig. 3.35.

The scale-selectivity of the second-order and sixth-order diffusion formulations is demonstrated in Fig. 3 using a one-dimensional model. There is no advection in this model; only diffusion acts on the initial square wave that extends over twenty-five grid points. The value of the diffusion coefficient *K* is chosen so that the $2\Delta x$ wave is entirely dampened at each time step by the diffusion formulation, and the model is integrated forward for 100 time steps.

The square wave has highest amplitude at two wavelengths: that of the wave itself ($25\Delta x$ given no corresponding negative portion of the wave) and that of the discontinuities along the edge of the wave ($\sim 2\Delta x$). The less-scale-selective second-order diffusion operator dampens both wavelengths, reducing the gradient's magnitude along the wave's edges and the wave's amplitude. The more-scale-selective sixth-order diffusion operator – which includes a flux-limiter correction term as noted above – also reduces the gradient's magnitude along the wave's edges, albeit to less extent than the second-order diffusion operator. The change in the wave's amplitude is negligible, a desirable trait since it is reasonably well resolved by the model grid.

We can also consider how second-, fourth-, and sixth-order diffusion operators impact a model's forecast of one-dimensional linear advection. An initial Gaussian wave is advected at a constant $U = 10 \text{ m s}^{-1}$ over a domain containing 100 grid points ($\Delta x = 1$ km) until it returns to its original location. The time step is 10 s, such that the Courant number is 0.1. The centered-in-time, second-order centered-in-space finite differencing scheme is used to discretize the advection terms in this example. As the order of the diffusion operator increases, its scale-selectivity increases, such that its impact on longer wavelength phenomena decreases (Fig. 4). In other words, lower-order diffusion operators dampen all wavelengths to a greater extent than higher-order operators.

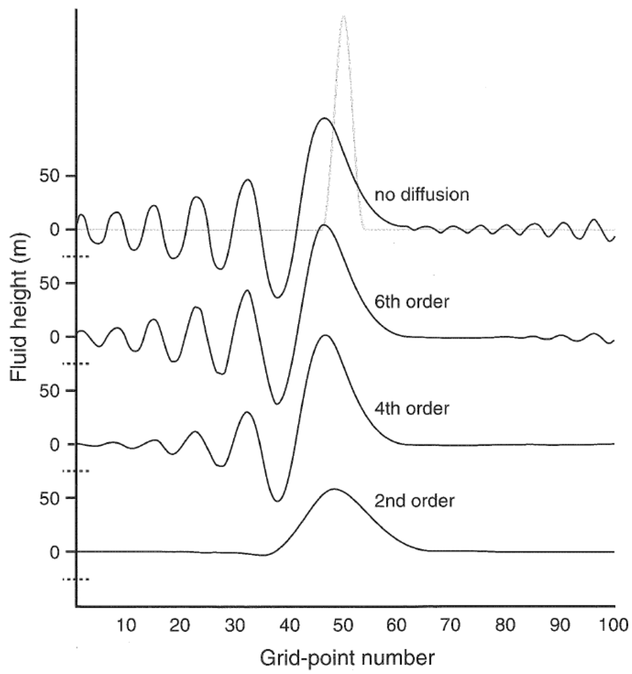


Figure 4. Fluid height *h* (m) after integrating the one-dimensional advection equation for 10,000 s on the model grid described in the text above, with a Courant number of 0.1, for integrations utilizing no explicit numerical diffusion (top), a sixth-order diffusion operator (middle-top), a fourth-order diffusion operator (middle-bottom), and a second-order diffusion operator (bottom). Reproduced from Warner (2011), their Fig. 3.26.

Practical Applications

Formally, diffusion operators should be evaluated on horizontal surfaces (e.g., constant height surfaces) rather than on model surfaces, which for most modern models follow the terrain. Let us consider the example of a mountain, where the temperature is often larger at the bottom rather than the top of the mountain. Along a terrain-following surface, temperature is a minimum at the mountain’s top and a maximum at the mountain’s base. Diffusion acting on the terrain-following surface would decrease the temperature at the mountain’s base and increase it at the mountain’s top. In thus, this would locally increasing the atmospheric thickness at the mountain’s top, resulting in relatively low pressure into which air will converge due to friction. Diffusion calculated on horizontal surfaces would not result in this non-physical circulation.

In WRF-ARW, horizontal diffusion may be computed on either terrain-following or horizontal surfaces, as controlled by the diff_opt namelist option. The WRF-ARW default is second-order diffusion along terrain-following surfaces; however, a sixth-order diffusion operator is also available. Diffusion along terrain-following surfaces is not overly problematic in the absence of sloped terrain, but diffusion should be computed along horizontal surfaces when terrain gradients are large.

Vertical diffusion in the WRF-ARW model, and most models, is handled by the chosen turbulence or boundary-layer parameterization. The methods for parameterizing vertical diffusion, manifest through turbulent vertical eddies, vary between parameterizations.

More detail regarding explicit numerical diffusion within WRF-ARW may be found in Section 4.2 of the WRF-ARW Technical Document.