Diffusion

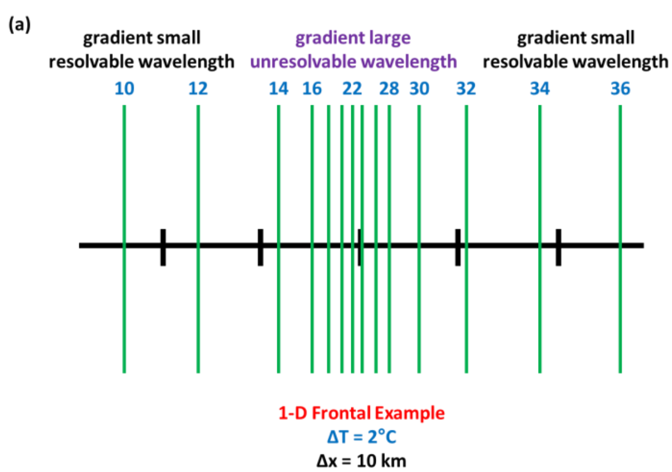
Numerical Diffusion

Diffusion can be viewed as the spreading out, or smoothing, of atmospheric fields in all three spatial dimensions. As a result, diffusion is often characterized by *damping*, as it weakens gradients by reducing the magnitude of local maxima and minima (Figure 1). Physical diffusion, driven by turbulent eddies, is an important transporter of atmospheric fields. However, there also exist two forms of artificial, or numerical, diffusion:

- **Implicit numerical diffusion**. This is manifest through damping properties possessed by certain finite differencing schemes, resulting in the model solution being damped over time (i.e., when $\left|e^{\omega_i t}\right| < 1$). Specific characteristics of this damping, such as its scale selectivity and Courant number dependence, vary between finite differencing schemes.

- **Explicit numerical diffusion**. This is manifest by adding an explicit damping term to the predictive equations for each model variable. Specific characteristics of this term, such as its stability, its wavelength dependence, the extent to which it dampens, and so on, vary between diffusion formulations and finite differencing schemes.

Implicit numerical diffusion was covered with linear numerical stability. As noted above, only selected finite differencing schemes are associated with implicit numerical diffusion. For example, the centered-in-time and second-order centered-in-space differencing schemes are not associated with implicit numerical diffusion, while the forward-in-time and Runge-Kutta 3 time differencing schemes are associated with implicit numerical diffusion. Specific details of the implicit numerical diffusion vary between differencing schemes. Please refer to the earlier lecture on linear numerical stability for specific examples.



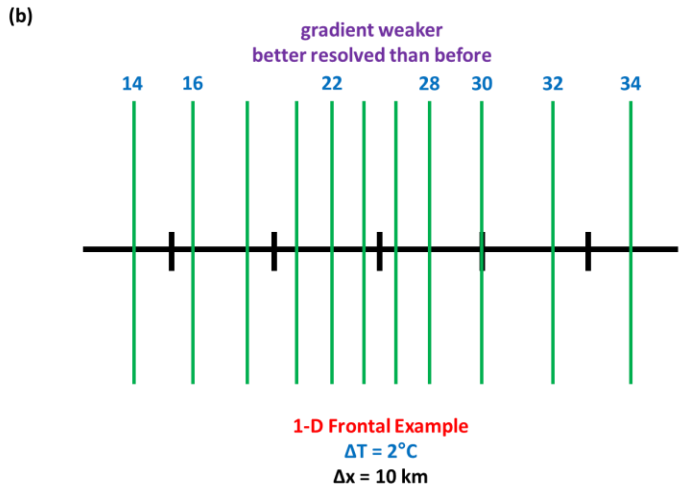


Figure 1. Conceptualization of diffusion, whether physical or artificial in nature. In panel (a), a sharp horizontal gradient in temperature exists in the middle of the grid. In panel (b), diffusion has weakened this gradient and reduced the magnitude of the local temperature minima and maxima that were present in panel (a).

Herein, we focus upon explicit numerical diffusion, or that which arises due to the inclusion of an explicit diffusion term in a model's predictive equations. Though non-physical in nature, explicit numerical diffusion may nonetheless be beneficial if it can dampen shorter wavelength, poorly resolved phenomena while largely not affecting longer wavelength phenomena. Damping of short wavelength phenomena is desirable given the problems posed by such features – truncation error, linear numerical stability, numerical dispersion, and aliasing – discussed over the course of the semester to date.

Numerical Formulation for Explicit Diffusion

A generalized explicit numerical diffusion term is given by:

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

Here, h is any model dependent variable, n is the order of the diffusion operator ($n = 0, 2, 4, 6\ldots$), 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 within numerical models except perhaps near the 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 maximum, $\nabla^2 h$ is a minimum and, consequently, *h* decreases with time. Conversely, where *h* is a minimum, $\nabla^2 h$ is a maximum and, consequently, *h* increases with time. The net result of this diffusion operator, therefore, is to reduce the magnitude of the gradient in *h* between the aforementioned maximum and minimum.

This diffusion formulation is weakly scale-selective, wherein shorter wavelengths are modestly dampened more than are longer wavelengths. As the Laplacian's magnitude is greatest for maxima or minima in the field being diffused, it does not introduce new maxima or minima to the field, a desirable trait. As compared to a second-order diffusion formulation, higher-order formulations are generally more scale-selective, damping shorter wavelengths (e.g., sharper gradients) more so than longer wavelengths. However, they can introduce new extrema, although methods (e.g., so-called flux limiter methods) exist to mitigate this drawback.

Let us consider the linear stability of a second-order diffusion operator 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 with 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:

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

On the left-hand side of this equation, $e^{-i\omega_R \Delta t}$ can be rewritten using Euler's relations. For the right-hand side of this equation, Euler's relations result in $e^{ik\Delta x} + e^{-ik\Delta x} = 2\cos(k\Delta x)$. Substituting these, 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 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 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 cannot be equal to zero, $\sin(\omega_R \Delta t)$ must equal zero in order for the equality in that equation 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 just a special form of the $\omega_R = 0$ case. Thus, we focus upon 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.

From this result, the stability criteria for this equation may be obtained, as was done in the "Linear Numerical Stability" lecture notes. The $2\Delta x$ wave limits the linear stability of this diffusion operator. Two stability criteria, one ensuring that $e^{\omega_I \Delta t} \geq -1$ (numerically stable) and one ensuring that $e^{\omega_I \Delta t} \geq 0$ (numerically stable with no change in wave phase), exist. These can be obtained by substituting these inequalities into the above equations and solving.

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 plug in to this equation for *k* with values for wavelength *L*, we can determine the wavelength-dependence, or scale-selectivity, of the damping function. This is depicted by the blue line in Figure 2.

The same process as followed above can be used to determine the multiplicative change 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 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:

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

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

The resulting equations for $e^{\omega_I \Delta t}$ for the fourth- and sixth-order diffusion operators 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 operators and the chose 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:

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

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

Plugging in to these equations for *k* with values for wavelength *L* allows us to determine the wavelength-dependence, or scale-selectivity, of the fourth- and sixth-order damping functions. These are depicted by the red and green lines, respectively, in Figure 2.

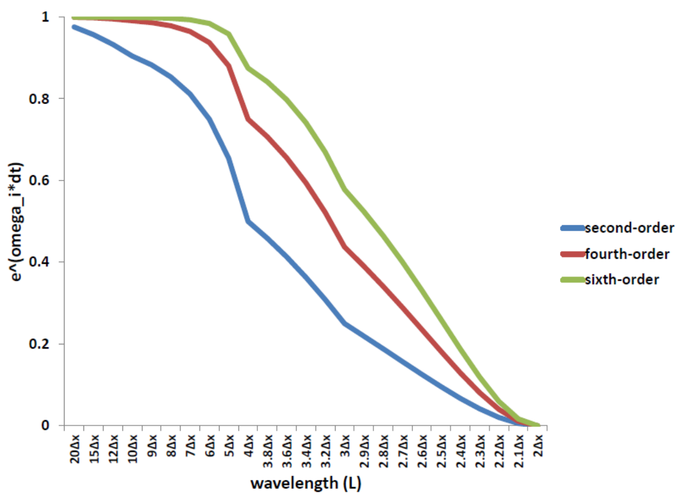


Figure 2. Depiction of damping magnitude per time step, $e^{\omega_I \Delta t}$, as a function of wavelength for second-, fourth-, and sixth-order diffusion operators using the forward-in-time, second-order centered-in-space finite differencing scheme. Note that for each diffusion operator, the value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

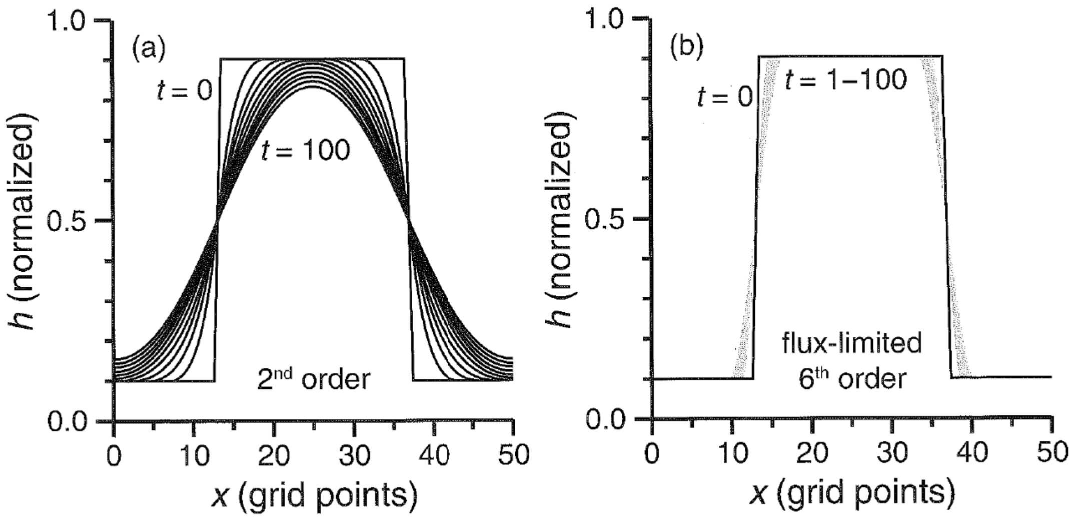


Figure 3. In each panel, the influence of diffusion – second-order in panel (a), sixth-order with a flux limited in panel (b) – upon an initial square wave over 100 model time steps is depicted. Note that the value of *K* for each diffusion operator is chosen such that the $2\Delta x$ wave is entirely 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 Figure 3.35.

For all damping functions, the magnitude of damping decreases as the wavelength increases. As the order of the diffusion operator increases, the extent to which longer wavelengths are dampened decreases. As a result, higher-order diffusion operators are preferable, so long as their weaknesses (e.g., creating new maxima or minima) can be mitigated by some means.

The scale-selectivity of the second-order and sixth-order diffusion operators is again demonstrated in Figure 3. A one-dimensional (in *x*) model, and thus diffusion formulation, is again utilized. There is no advection within this model; only diffusion acts upon the initial wave. In this example, the initial wave is given by a square wave, which generally is not present within atmospheric fields but possesses sharp horizontal gradients that help to illustrate the scale-selectivity of the applied diffusion operators. The initial square wave extends over twenty-five grid points. The value of the diffusion coefficient *K* is again chosen so that the $2\Delta x$ wave is entirely dampened at each time step, and the model is integrated forward for 100 time steps.

There are two primary wavelengths manifest through the initial square wave: 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 each of these wavelengths, resulting in both a weakening of the gradient across the edge of the square wave and a reduction in the amplitude of the wave itself. The more-scale-selective sixth-order diffusion operator – which includes a flux-limiter correction term as noted above – also weakens the gradient across the edge of the square wave, albeit to less extent than the second-order diffusion operator. The change in amplitude of the wave is negligible with this formulation, a desirable trait.

We can also consider the scale-selectivity of the second-, fourth-, and sixth-order diffusion operators in light of the one-dimensional advection example we have extensively considered thus far this semester. An initial Gaussian wave is advected at a constant U = 10 m s^{-1} over a domain containing 100 grid points (Δx = 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 within this example.

The influence of second-, fourth-, and sixth-order diffusion upon this solution is demonstrated in Figure 4. As the order of the diffusion operator increases, its scale-selectivity increases, such that its impact upon longer wavelength phenomena decreases. Though numerical dispersion is less evident in the second-order diffusion example, the amplitude of the primary wave is substantially reduced relative to both the physical wave and to that in the cases with higher-ordered diffusion operators. Thus, a trade-off exists, which motivates the use of more accurate finite differencing schemes that are less affected by numerical dispersion (among other attributes)!

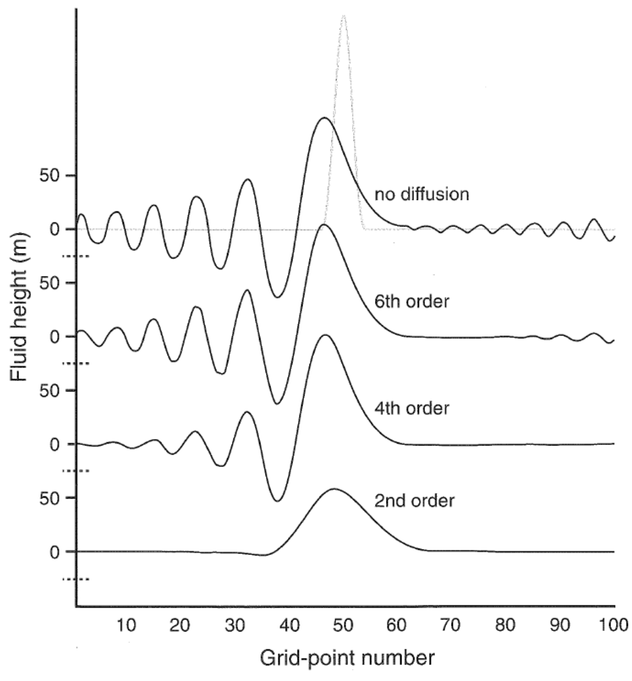


Figure 4. Fluid height h (m) after integrating the one-dimensional advection equation for 10,000 s on the model grid described in the text above, with a Courant number of 0.1, for integrations utilizing no explicit numerical diffusion (top), a sixth-order diffusion operator (middle-top), a fourth-order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

Horizontal Diffusion and Linear Numerical Stability

Diffusion terms influence linear numerical stability. To illustrate, let us analyze the stability of the second-order diffusion operator using a forward-in-time and second-order-accurate centered-in-space differencing scheme. Though this scheme is always numerically unstable when applied to advection terms, the same is not true for this diffusion operator.

$$\frac{\partial h}{\partial t} = K\frac{\partial^2 h}{\partial x^2} \quad \text{becomes} \quad \frac{h_x^{t+1} - h_x^t}{\Delta t} = K\left(\frac{h_{x+1}^t + h_{x-1}^t - 2h_x^t}{(\Delta x)^2}\right)$$

If we substitute for *h* with its wave-like solution given in our "Linear Numerical Stability" lecture, expand the resulting exponential functions, and divide through by a common factor, we obtain:

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

Euler's relations can be added to show that $e^{ik\Delta x} + e^{-ik\Delta x} = 2\cos(k\Delta x)$. Substituting into the above and rewriting the other exponential raised to the power of *i* using Euler's relations, 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 into its real and imaginary components, we obtain:

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

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

For a non-zero exponential function in the imaginary equation, the only values of ω_R that satisfy the equality 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 this latter case is just a special form of the $\omega_R = 0$ case, and so we focus upon this latter case here. For $\omega_R = 0$, $\cos(\omega_R \Delta t) = 1$ and the real component of the equation becomes:

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

The allowable values of $k\Delta x$ again 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 (given that $\Delta x = L/2$), $\cos(k\Delta x) = -1$ and $\cos(k\Delta x) - 1 = -2$. In this case, the stability criterion equation 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, $e^{\omega_I \Delta t} < 1$. But, it is possible for $e^{\omega_I \Delta t} < -1$, which defines exponential growth with a change in the phase of the wave. Note that any negative value defines a change in the phase of the wave; only negative values smaller than -1 denote exponential amplitude growth.

From this, we can assess the stability criterion; simply let $e^{\omega_I \Delta t} = -1$ and 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 would be less stringent than those above. Thus, since Δx cannot be 0, the $2\Delta x$ wave (with $\Delta x = L/2$) is that which limits numerical stability for this diffusion formulation. It can be shown that meeting this criterion produces little damping effect at large wavelengths relative to small wavelengths. This is actually a desirable attribute; the shortest wavelength features are those that are poorly resolved as it is, and damping them in whole or in part generally helps to keep them from compromising the quality of the simulation.

Diffusion also may be formulated in the vertical, with an analogous stability term 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 duration of the simulation as the meteorology changes; thus, we typically choose a model time step well below the theoretical limits so as to avoid unnecessarily achieving numerical instability with the chosen model configuration.

Practical Diffusion Applications

Figure 2 in the "Aliasing and Non-Linear Stability" notes demonstrates another utility of numerical diffusion – explicit, but in some applications also implicit – in mitigating the impacts of aliasing upon the model solution. Where aliasing results in an artificial buildup of wave energy at short, poorly resolved wavelengths, numerical diffusion dampens this accumulation. Though the kinetic energy spectrum deviates from that given by theory and observations at wavelengths below the effective model resolution when damping is applied, the model is less likely to become numerically unstable. As this is desirable, we choose the horizontal grid spacing of our model simulations in light of the resulting effective resolution. For example, to resolve thunderstorms, we require $\Delta x <$ 4 km with an effective resolution of < 28 km that is barely crude enough to encompass the area covered by larger thunderstorms.

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 at mountain top is often larger than that at the bottom of the mountain. Along a terrain-following surface, temperature would be a minimum at the top of the mountain and a maximum at the bottom of the mountain. Diffusion acting on the terrain-following surface would decrease the temperature at the bottom of the mountain and increase the temperature at the top of the mountain. This will locally increase the thickness of the column at mountain top, resulting in relatively low pressure at mountain top, into which air will converge due to friction. Diffusion calculated on horizontal surfaces would not lead to the development of this non-physical circulation.

In WRF-ARW, diffusion may be computed on either model coordinate or horizontal surfaces, as controlled by the diff_opt option. Where terrain gradients are small, diffusion along coordinate surfaces may not be overly problematic. Where terrain gradients are large, such as near mountains, diffusion should be computed along horizontal surfaces. The WRF-ARW default is second-order diffusion along model coordinate surfaces. However, a sixth-order diffusion operator is also available. For model simulations where $\Delta x \geq O(100 \text{ m})$, the diffusion coefficient K_n in the horizontal is determined from horizontal deformation. Vertical diffusion is handled, and thus K_n in the vertical is specified, by the chosen planetary boundary layer parameterization. More detail regarding explicit numerical diffusion within WRF-ARW may be found in Section 4.2 of the WRF-ARW Technical Document.