Numerical Techniques 2024–2025

4. Spectral models

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Content of today

- Spectral decomposition: principle
- Discretization and truncation: FFT
- Accuracy of spectral derivatives
- Aliasing and nonlinearity
- Spectral models

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- Spectral decomposition: principle
- Discretization and truncation: FFT
- Accuracy of spectral derivatives
- Aliasing and nonlinearity
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Note: spectral decomposition plays an important role in

- (approximate) analytical solutions: see Dynamic Meteorology
- understanding the behaviour of numerical schemes: see previous lessons
- the development of spectral atmospheric models

Context

- Harmonic functions ($\sin x$, $\cos x$, $\exp ix$) have some interesting properties
  - periodic, wave-like
  - they don't change (a lot) when taking the derivative:

$$\frac{d}{dx}\sin kx = k\cos kx$$
$$\frac{d}{dx}\cos kx = -k\sin kx$$
$$\frac{d}{dx}\exp ikx = ik\exp ikx$$

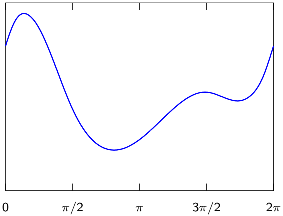
    We say that these functions are *eigenfunctions* of the differential operator

- Spectral decomposition allows us to use these properties for arbitrary functions!

- **Decomposition**
- Discretization
- Accuracy
- Aliasing
- Spectral models

Decomposition in harmonic functions

- Consider a periodic function $f(x)$ with period 2π:



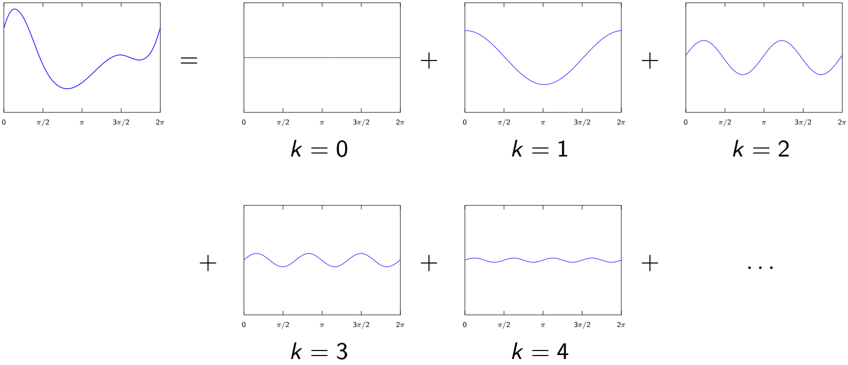
- Then we can *decompose* this function in harmonic functions with wavenumber $k = 0, 1, \ldots$:

$$f(x) = \sum_{k=0}^{\infty} a_k \cos(k\,x) + b_k \sin(k\,x)$$

Or, using the exponential notation for harmonic functions ($e^{i\theta} = \cos\theta + i\sin\theta$):

$$f(x) = \sum_{k=-\infty}^{\infty} \alpha_k \exp(i\,k\,x)$$

- For example:



(Think of distinguishing low and high tones in music. . .)

- Decomposition
- **Discretization**
- Accuracy
- Aliasing
- Spectral models

- On a computer, the function $f(x)$ needs to be discretized, and the infinite summation needs to be truncated:

$$f(x_j) = \sum_{k=-K}^{K} \alpha_k \exp(i\,k\,x_j)$$

- To uniquely determine the coefficients α_k, the number of gridpoints must be equal to the number of waves, i.e. $N = 2K + 1$, so $\Delta x = \pi/K$.

- For a uniform grid spacing, the highest resolvable wave has wavenumber K, i.e. period $2\Delta x$. We call this the Nyquist wavenumber. Waves with higher wavenumbers will be aliased (see further).

- Note that we now have information *between* gridpoints !?

- The Fourier coefficients are calculated with a Galerkin approach as

$$\alpha_k = \frac{1}{N} \sum_{j=1}^{N} f(x_j) e^{-ikx_j}$$

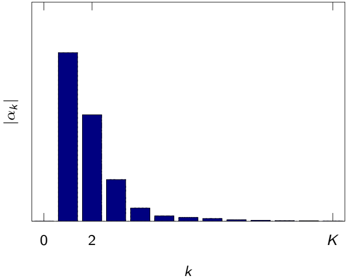
(note the symmetry with the composition formula).

- Efficient algorithms exist to perform the spectral decomposition (i.e. calculate the coefficients α_k), or the spectral composition (i.e. determine the values $f(x_j)$ from the coefficients α_k) in $O(N \log N)$ operations:

Fast Fourier Transforms (FFT)

The Fourier spectrum

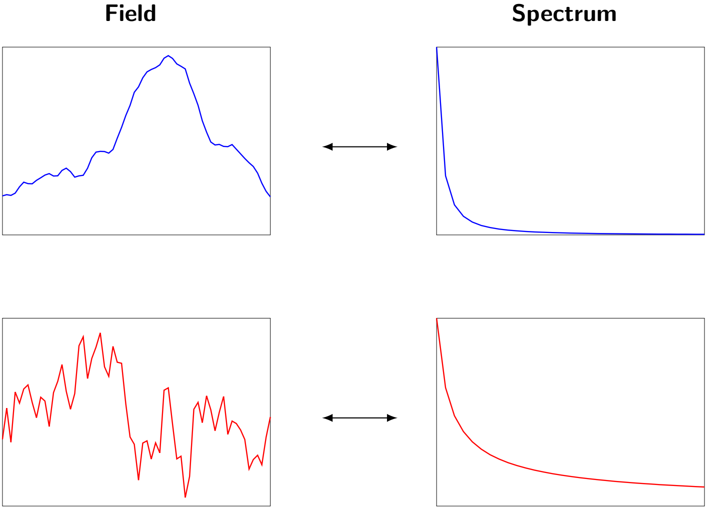
- When plotting the spectral coefficients α_k against the wavenumbers, one obtains the *spectrum* of the function $f(x)$:



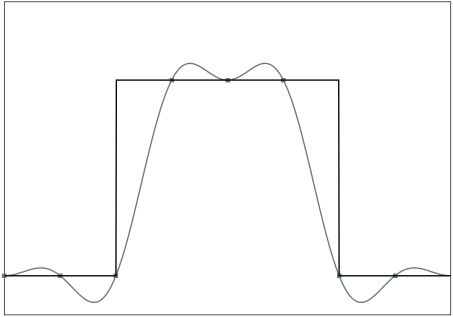
- The spectrum is a measure for the energy distribution over the different scales. For many physical variables, the spectrum quickly decreases for large wavenumbers.

Relation between the smoothness and the spectrum

- The spectrum of a smooth function decays quickly
- Rougher functions have a wider spectrum



- When modeling a *discontinuity* with harmonic functions, the approximation will contain *overshoots*



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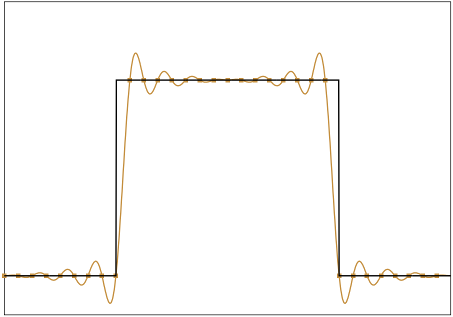

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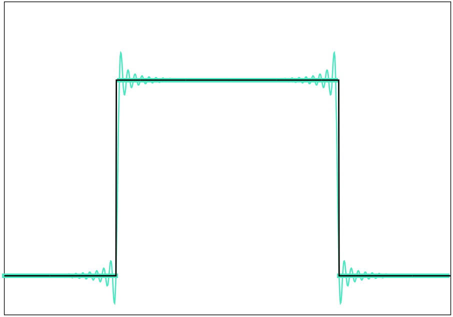

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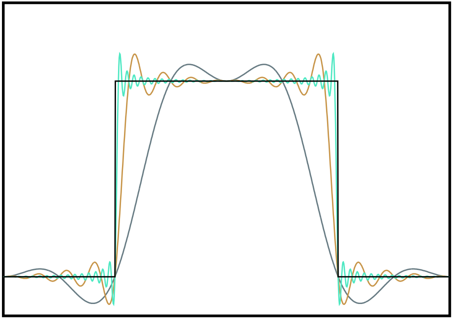


- These overshoots don't disappear when going to a higher resolution. They even get worse!

- Decomposition
- Discretization
- **Accuracy**
- Aliasing
- Spectral models

- Let us consider $\psi(x)$ on a domain $0 \leq x \leq 2\pi$, then

$$\psi(x) = \sum_{k=-\infty}^{\infty} \alpha_k e^{ikx}$$

and

$$\frac{\partial \psi}{\partial x} = \sum_{k=-\infty}^{\infty} ik\alpha_k e^{ikx}$$

Accuracy of spectral derivatives

- If we discretize the function and truncate the Fourier series, the error of the representation of the derivative is given by

$$E = \sum_{|k|>K} ik\alpha_k e^{ikx}$$

- If the p-th order derivative is continuous and all the lower order derivatives are continuous, it's possible to show that

$$|\alpha_k| \leq \frac{C}{|k|^p}$$

for a finite C (cfr. decaying spectrum).

Accuracy of spectral derivatives

- Remember that the maximum wavenumber K is related to the grid distance Δx:

$$K \sim \frac{1}{\Delta x}$$

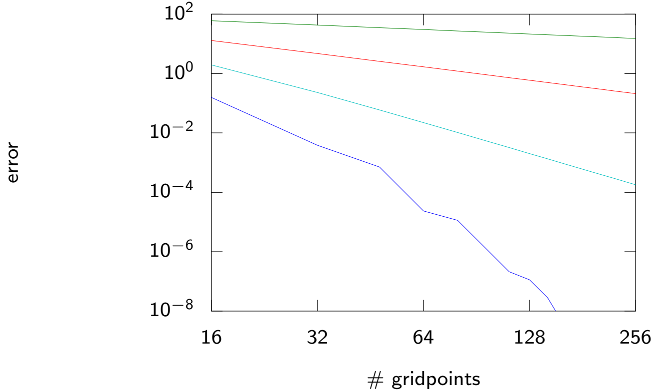
- So the error on the derivative is bound by

$$|E| \leq \tilde{C}\,(\Delta x)^{p-2}$$

with $\tilde{C}$ a finite constant.

- This means that
  - the order of accuracy of the spectral method is determined by the smoothness of ψ
  - if ψ is infinitely differentiable then the spatial derivatives are represented by infinite-order accuracy !

Comparison of spectral derivatives with 1st, 2nd and 4th order schemes:



Consequence for time differencing

- We need to choose a smaller time step than for centered space differencing. For instance for a mode with $\kappa = ck$, we have seen before that the stability requirement is $|\kappa \Delta t| \leq 1$. For the $2\Delta x$-mode, this corresponds to:

$$\left| \frac{c\Delta t}{\Delta x} \right| \leq \frac{1}{\pi}$$

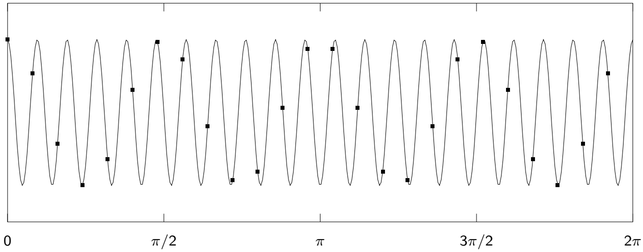
- For leapfrog time integration with centered differences:

second-order	$\left\lvert \frac{c\Delta t}{\Delta x} \right\rvert \leq 1$
fourth-order	$\left\lvert \frac{c\Delta t}{\Delta x} \right\rvert \leq 0.73$
sixth-order	$\left\lvert \frac{c\Delta t}{\Delta x} \right\rvert \leq 0.63$
$\vdots$	
∞-order	$\left\lvert \frac{c\Delta t}{\Delta x} \right\rvert \leq \frac{1}{\pi}$

- There is no such thing as a free lunch. . .

- Decomposition
- Discretization
- Accuracy
- **Aliasing**
- Spectral models

- Sampling a wave with wavenumber $k = 21$ on a grid with $K = 12$, so $N = 2K + 1 = 25$ gridpoints:



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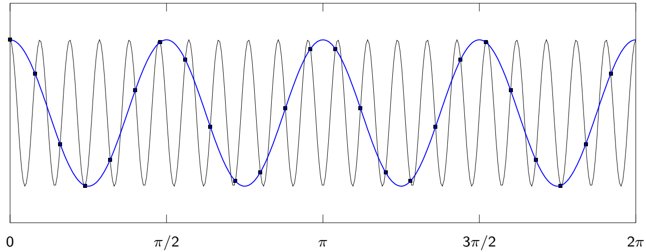
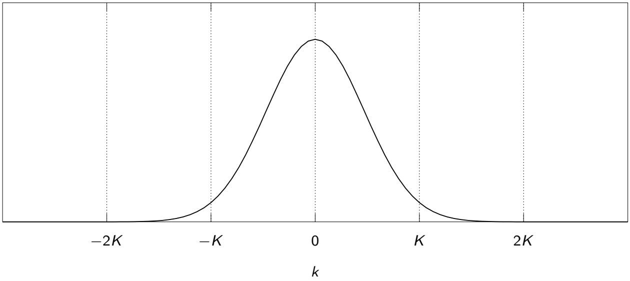


- These points lie exactly on a wave with wavenumber $k' = 4$. So the high-frequency wave *appears* as a lower frequency wave; this is *aliasing*.

- A different way to interpret aliasing is by considering the spectrum as periodic:



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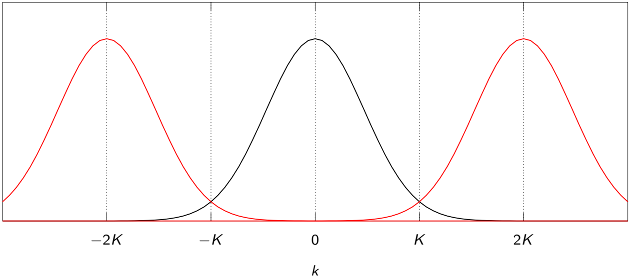

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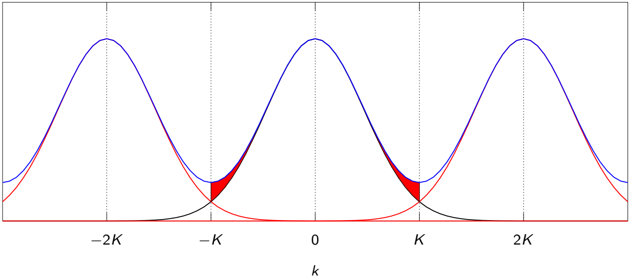

- The part of the spectrum that is truncated ($|k| > K$) 'contaminates' the part where $|k| < K$.

- Aliasing mainly poses problems when multiplying fields: let $\phi_1(x) = e^{i\,k_1 x}$ and $\phi_2(x) = e^{i\,k_2 x}$. Then

$$\phi_1(x)\phi_2(x) = e^{i(k_1+k_2)x}$$

- A multiplication of two fields changes the wavenumber. If $|k_1 + k_2| > K$, aliasing will occur.

- Besides aliasing, there is an additional problem with nonlinearity in spectral space. Take, for instance, the advection equation with a nonconstant speed:

$$\frac{\partial \phi(x,t)}{\partial t} + c(x,t)\frac{\partial \phi(x,t)}{\partial x} = 0$$

with

$$\phi(x,t) = \sum_{k_1=-K}^{K} \hat{\phi}_{k_1}(t) e^{ik_1 x} \qquad\qquad c(x,t) = \sum_{k_2=-K}^{K} \hat{c}_{k_2}(t) e^{ik_2 x}$$

- Then the equation for each wave component $\hat{\phi}_k(t)$ is:

$$\frac{d\hat{\phi}_k}{dt} + \sum_{\substack{k_1 + k_2 = k \\ |k_1|, |k_2| \le K}} i\, k_1\, \hat{c}_{k_2}\, \hat{\phi}_{k_1} = 0$$

- In other words, one has to consider *all possible combinations* of k_1 and k_2 that may contribute to each wave component.

- For instance, to write the equation for the spectral coefficient $\hat{\phi}_2$ of a wave with wavenumber $k = 2$, one has to consider
  - $\hat{c}_0\hat{\phi}_2$
  - $\hat{c}_1\hat{\phi}_1$
  - $\hat{c}_2\hat{\phi}_0$
  - $\hat{c}_3\hat{\phi}_{-1}$
  - ...
- We say that multiplication is *not local* in spectral space.

Nonlinearity

- For instance, to write the equation for the spectral coefficient $\hat{\phi}_2$ of a wave with wavenumber $k = 2$, one has to consider
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  - $\hat{c}_2\hat{\phi}_0$
  - $\hat{c}_3\hat{\phi}_{-1}$
  - $\ldots$
- We say that multiplication is *not local* in spectral space.
- For a grid with N gridpoints, this means that multiplication in spectral space takes $\mathcal{O}(N^2)$ operations, while in gridpoint space, it only takes $\mathcal{O}(N)$ operations.

Nonlinearity

- Note that 'multiplication' and 'taking derivative' behave oppositely in gridpoint and in spectral space:

operation	Gridpoint space	Spectral space
multiplication	local	nonlocal
derivative	(weakly) nonlocal	local

- Make sure to perform the operations in the appropriate 'space'.

Avoiding aliasing

- Aliasing can be avoided by truncating the spectrum well before the Nyquist wavenumber K.

- For example, let $k_{max} = K/2$, then a multiplication will produce fields with a maximal wavenumber $2k_{max} = K$, and no aliasing will occur.

- The condition can even be relaxed to $k_{max} = 2K/3$. Why?
(hint: look at the interpretation of aliasing in terms of a periodic spectrum)

Check Durran's book for a mathematical derivation.

- Decomposition
- Discretization
- Accuracy
- Aliasing
- **Spectral models**

Spectral models: timestep layout

- Considering the advection equation

$$\frac{\partial \phi}{\partial t} + c\frac{\partial \phi}{\partial x} = \text{RHS}$$

- A typical timestep organization of a spectral model of this problem looks like

$$\left.\begin{array}{l}\text{1. Spectral truncation: } \hat{\phi}_k = \hat{c}_k = 0 \text{ for } k > 2K/3 \\ \text{2. Derivative of } \phi\text{: multiply } \hat{\phi}_k \text{ by } ik. \end{array}\right\} \text{Spectral space}$$

$$\left.\begin{array}{l}\text{3. Inverse FFT} \\ \text{4. Compute the product } c(x_j)\partial\phi(x_j)/\partial x \\ \text{5. Add addional forcings } \mathit{RHS} \text{ (physics parameterizations)} \\ \text{6. Forward FFT} \end{array}\right\} \text{Gridpoint space}$$

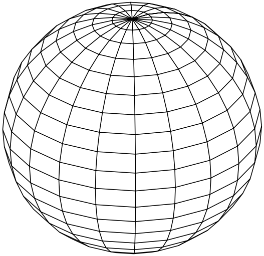
$$\left.\begin{array}{l}\text{7. Implicit time step scheme}\end{array}\right\} \text{Spectral space}$$

- Besides the accuracy and efficiency of the derivatives, there are other advantages of spectral models:
  - No **dispersion** (e.g. negative group speed!) due to spatial discretization.
  - The inversion of the differential operators like the Laplace operator ∇^2 (see Dyn. Met.), which appears in **implicit schemes**.

    In gridpoint space, this requires the inversion of a HUGE $(n_x n_y) \times (n_x n_y)$ sparse matrix.

    In spectral space, this matrix becomes diagonal, and its inversion is trivial. This means *implicit* time-integration schemes can be used much more easily.

- With a regular global grid, the spatial resolution is not uniform on the globe: near the **pole**, the resolution becomes very high ($\Delta x \to 0$).



  Note that stability (thus the timestep Δt) is determined by the *smallest* Δx across the domain.

- This so-called 'pole-problem' does not occur in a spectral model.

- In a spherical geometry, spectral decomposition looks like:

$$\psi(\lambda,\mu) = \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} \hat{\psi}_{m,n} Y_{m,n}(\lambda,\mu)$$

- The base functions Y are the eigenfunctions of the Laplace operator (*spherical harmonics*):

$$Y_{m,n}(\lambda,\mu) \equiv P_{m,n}(\mu) e^{im\lambda}$$

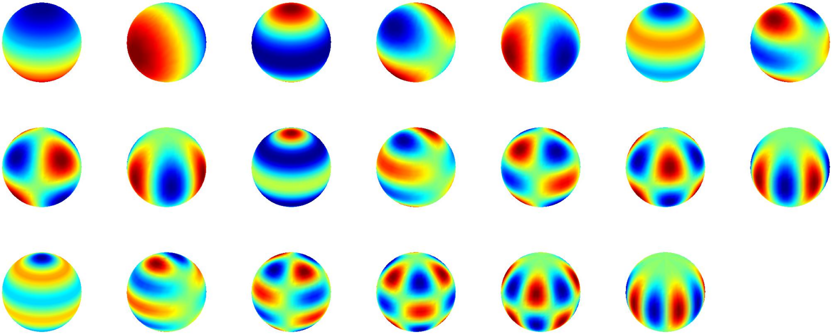
- The functions $P_{m,n}$ are the associated Legendre functions

$$P_{m,n}(\mu) = \left[\frac{2n+1}{2}\frac{(n-m)!}{(n+m)!}\right]^{\frac{1}{2}} \left(1-\mu^2\right)^{\frac{m}{2}} \frac{d^m}{d\mu^m} P_n(\mu)$$

where the functions P_n are Legendre polynomials

$$P_n(\mu) = \frac{1}{2^n n!}\frac{d^n}{d\mu^n}\left[(\mu^2-1)^n\right]$$

- Some spherical harmonics:



- Some properties of spherical harmonics:
  - orthogonality of associated Legendre functions

$$\int_{-1}^{1} P_{m,n}(\mu) P_{m,s}(\mu) d\mu = \delta_{n,s}$$

  - orthogonality of spherical harmonics

$$\frac{1}{2\pi} \int_{-1}^{1} \int_{-\pi}^{\pi} Y_{m,n}(\lambda, \mu) Y^{*}_{r,s}(\lambda, \mu) d\lambda d\mu = \delta_{m,r} \delta_{n,s}$$

  - Laplacian of spherical harmonics

$$\nabla^2 Y_{m,n} = -\frac{n(n+1)}{a^2} Y_{m,n}$$

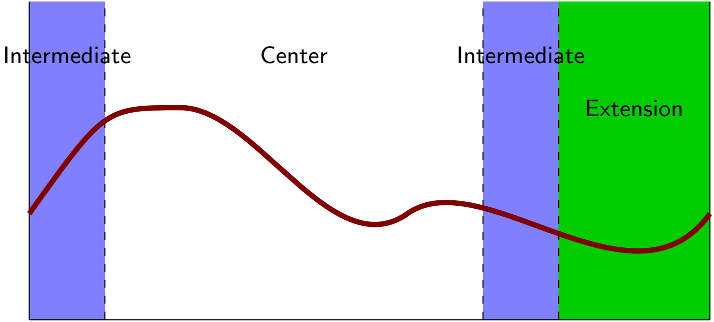
- Note that these properties have analogies in Fourier-space!

Spectral LAM

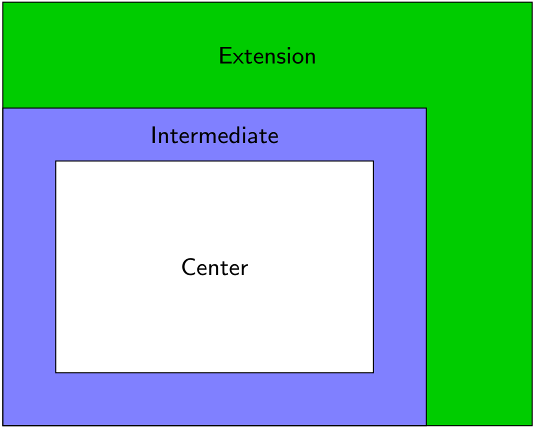
- In a spectral limited-area model (LAM) one has to
  - impose lateral boundary conditions
  - make the fields periodic to be able to apply the FFT's
- Remark: use of Chebyshev polynomials instead of harmonic functions could avoid need for periodization (student's project)

Spectral LAM: 1D

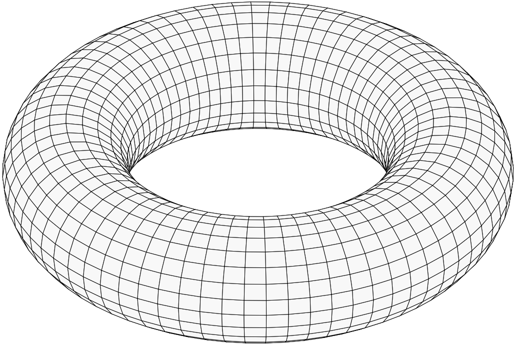
- A spectral limited area model (LAM) domain is organized in 3 zones:



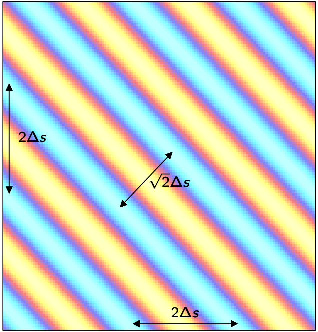
  - The Intermediate zone is used to apply lateral boundary conditions (see later).
  - In the extension zone, the fields are artificially extended such that they become periodic.
  - The center zone is the physical part of the model.


Extension
Intermediate
Center

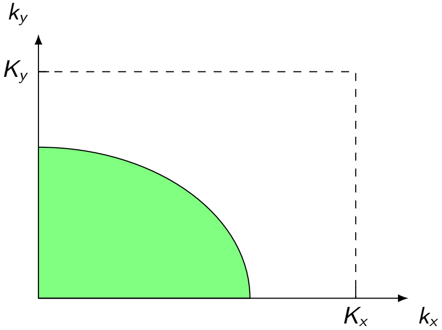
(. . . so in some sense we are working on a torus . . .)



- Avoiding aliasing: $k_{x,y} \leq 2K_{x,y}/3$
- In 2D, the resolution is not the same in all directions



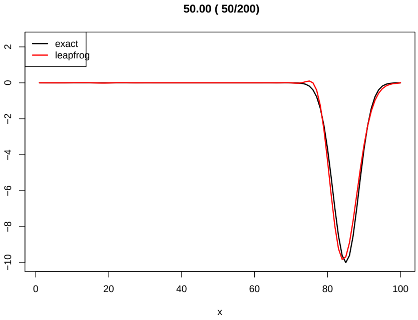
- Avoiding aliasing: $k_{x,y} \leq 2K_{x,y}/3$
- In 2D, the resolution is not the same in all directions
- This is solved by an *elliptic truncation* in spectral space

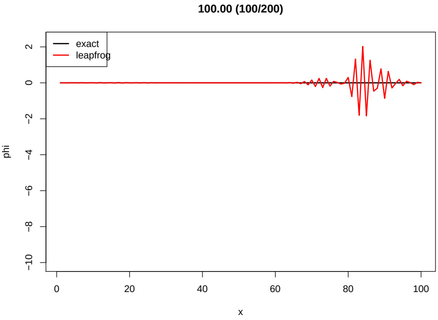


- A LAM needs lateral boundary conditions, usually provided by a global model running at lower resolution.

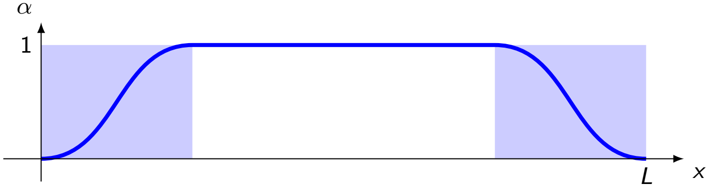
- When applying LBC's only at the boundary points, *spurious reflections* will arise due to inconsistency between boundary points and the internal points.

Example: a depression right before and after leaving a LAM domain:





- Davies' solution: apply the boundary conditions in a gentle way, i.e. through relaxation in the intermediate zone:



- Mathematically, the coupling looks like

$$\psi = \alpha\tilde{\psi} + (1 - \alpha)\psi_{LS}$$

where $\tilde{\psi}$ is the solution with periodic boundary conditions, and ψ_{LS} is the large-scale solution.

- This coupling is done *every time step*, but ψ_{LS} is interpolated in time because of data limits (e.g. 3h).

- This strategy can also be derived mathematically by starting from a modified equation:

$$\frac{\partial \psi}{\partial t}(x,t) + U\frac{\partial \psi}{\partial x}(x,t) = -K(x)\left[\psi(x,t) - \psi_{LS}(x,t)\right]$$

- The RHS represents a *relaxation term* which penalizes differences (at the boundary) between the LAM solution ψ and the large-scale solution ψ_{LS}. This scheme was proposed by Davies (1983).

- The function $K(x)$ ultimately determines the relaxation function $\alpha(x)$.

- Interested? See student's project.

Summary

- Concept of spectral decomposition
- Accuracy of derivatives is of infinite order
- Excellent for implicit times schemes!
- Aliasing due to nonlinearity (multiplication) and solution by truncating the spectrum
- Global spectral models with spherical harmonics
- Limited area models:
  - extension zone for periodization
  - relaxation zone for boundary conditions