Chapter 7. Introduction to Spectral Methods

Reference: Durran Chapter 4. Haltiner and Williams Chapter 6.
Temperton (2000).

7.1. Introduction

- Grid point method – evaluates spatial derivatives using Taylor series expansion
- Galerkin method (a superset of spectral method) represents dependent variables as the sum of a set of functions with pre-specified space structure (basis functions). We solve the equations (usually ODE's) for the coefficients of these functions.

7.2. Galerkin procedure

For equation

$$L(u) = f(x), \qquad a \le x \le b \tag{1}$$

where L is an operator involving partial derivatives of u.

Consider a set of linearly independent basis functions $\phi_j(x)$, so that

$$u(x) \approx \sum_{j=1}^{N} U_j \phi_j(x) \tag{2}$$

where U_j is the coefficient for basis function ϕ_j and U_j is usually independent of x (i.e., a function of t only for time dependent problems). The spatial dependency of u is represented by the basis functions.

The error of (2) satisfying (1) is

$$e \approx L\left(\sum_{j=1}^{N} U_j \phi_j(x)\right) - f(x). \qquad (3)$$

Galerkin procedure requires that the error be orthogonal to each basis function, or in another word, the error is a residual that cannot be expressed in terms of the given finite set of basis functions →

$$\int_a^b e_N \phi_i \, dx = 0 \qquad \text{for } i = 1, \ldots, N. \qquad (4)$$

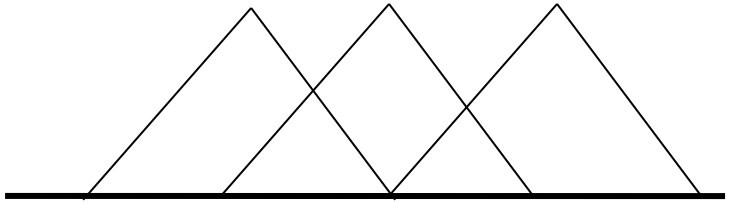
(4) leads to

$$\int_a^b \phi_i L\left(\sum_{j=1}^{N} U_j \phi_j(x)\right) dx - \int_a^b \phi_i f(x) dx = 0 \quad \text{for } i = 1, \ldots, N \qquad (5)$$

(5) is a set of N algebraic equations for U_j. When the operator L includes time derivatives, we have a set of coupled ODE's for U_j.

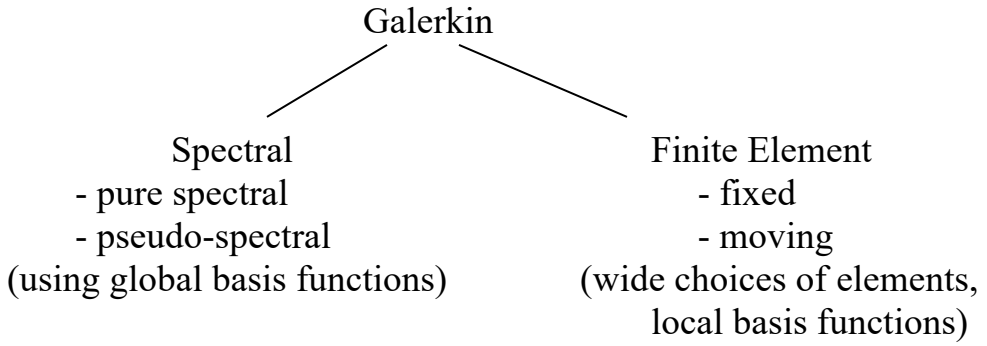
7.3. Choices of basis functions

- Spectral method uses orthogonal Fourier series (in term of sine-cosine or e^{-ikx}) as the basis function.
- Other local basis functions can be chosen, e.g., piecewise linear basis function



The latter gives rise to the finite element method.

Two main branches of Galerkin methods:



7.4. Discrete or Finite Fourier Transform

Before we look at the actual use of spectral method to solve PDE's, we need to review / introduce the discrete Fourier transform.

Assume we have a set of uniformly spaced grid points in 1-D:

$$x_j = j\,\Delta x, \qquad j = 0, 1, 2, \ldots, N \tag{6}$$

where $N\Delta x = L$.

We assume the functions we deal with are periodic with a period of L, which implies that $x = 0$ and $x = L = N\,\Delta x$ are equivalent points.

To write a Fourier series for a function $f(x)$ whose values are given only at N grid points requires only N Fourier coefficients. For generality, $f(x)$ is allowed to be complex. The series is

$$f(x_j) = f_j = \sum_{n=1}^{N} F_n e^{ik_n x_j} \tag{7}$$

where F_n are the coefficients of the Fourier components, or the spectral coefficients.

The values of k_n should be properly chosen so that the Fourier components satisfy the periodic condition, and for computational reasons, equally spaced. The following set of values meets these requirements:

$$k_n = \frac{2\pi n}{N\Delta x} \quad n=1, 2,\ldots, N \tag{8}$$

and the series (7) becomes

$$f(x_j) = f_j = \sum_{n=1}^{N} F_n e^{i\frac{2\pi n}{N\Delta x} j\Delta x} = \sum_{n=1}^{N} F_n e^{i\frac{2\pi nj}{N}} \quad \text{for j =1, 2, …, N} \qquad (9)$$

(9) is an expression of f_j in terms of a series of Fourier components.

The inverse transform of (9) is

$$F_n = \frac{1}{N}\sum_{j=1}^{N} f_j e^{-i\frac{2\pi nj}{N}} \qquad \text{for } n\text{=1, 2, …, } N \qquad (10)$$

(10) gives us the spectral coefficients from the grid point values f_j.

(10) defines the finite or discrete Fourier transform and (9) the corresponding inverse transform, which are the discrete analogues of the standard Fourier transform and its inverse. The integral in the continuous transforms are replaced by sums in the discrete expressions.

(10) can be proven by substituting it into (9) and recognizing the orthogonality among the basis functions.

7.5. Spectral Method as Applied to 1-D advection Equation

In this section, we use the discrete Fourier transforms to solve PDE's

We look at linear and nonlinear1-D advection equations:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0\,, \tag{11}$$

and

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0\,. \tag{12}$$

Consider linear advection equation (11) first.

For a periodic domain L:

$$u(x,t) = \sum_{n=1}^{N} U_n(t) e^{inkx}\,, \tag{13}$$

where the basis functions are

$$\phi_n(x) = e^{inkx}\,, \tag{14}$$

for $k = \frac{2\pi}{L}$, $L = N\Delta x$, $x = j\,\Delta x$ ($k_n = \frac{2\pi n}{N\Delta x}$ in the previous section = $n\,k$ here).

Substitute (13) into (11) →

$$\sum_{n=1}^{N}\left[\frac{dU_n}{dt}e^{inkx} + cinkU_n e^{inkx}\right] = 0 \tag{15}$$

Because of the linear independence or by requiring the error be orthogonal to each basis function [Eq.(5)], we have

$$\frac{dU_n}{dt} + cinkU_n = 0 \quad \text{for } n=1, \ldots, N, \qquad (16)$$

which is a set of N ODE's for coefficients U_n.

Finite difference is usually used for the time derivative. After U_n at the future time t is obtained, $u(x, t)$ is obtained from (13), or inverse discrete Fourier transform (IDFT). Note for simple linear equation such as (11), (13) needs to be evaluated at the output times only when the physical u is needed. The inverse transform needs to be performed once at the initial time to obtain initial U_n. In practice, physical parameterizations usually require physical quantity u every time step so the inverse transform is needed every step.

Steps to integrate equation (11) using spectral method with Fourier basis functions:

1) Perform discrete Fourier transform (DFT, like Eq.10) on the initial condition $u(x_j, 0)$ to obtain spectral coefficients $U_n(0)$ at initial time.
2) Integrate Eq.(16) from time zero to a future time t to obtain coefficients $U_n(t)$.
3) When physical quantity u at the grid points are needed, perform IDFT (like Eq.13) to obtain $u(x_j, t)$.
4) Repeat steps 2 and 3 to integrate further in time.
5)

Now let's consider nonlinear advection equation (12).

Equivalent of (15):

$$\sum_{n=1}^{N} \frac{dU_n}{dt} e^{inkx} + \left(\sum_{n=1}^{N} U_n e^{inkx} \right) \left(\sum_{n=1}^{N} inkU_n e^{inkx} \right) = 0 \qquad (17)$$

The multiplication of two spectral series in the second term leads to N^2 terms!! And it is expensive to evaluate (note that for the linear equation, we do not need to evaluate this series every time step). We end up with equations for N^2 coefficients because wave interactions generate new waves.

- (17) represents creation of new waves via nonlinear interaction
- Aliasing can be prevented by dropping waves numbers $n>N$ (spectral filtering)

The need to evaluate spectral series due to the nonlinear advection makes the spectral method unattractive for practical use, until the transform method was invented!

The other development that made spectral method practical is the Fast Fourier transform (FFT) algorithms.

Transform Method

In practice, the series multiplication in the nonlinear advection term is seldom directly evaluated. A transform method was invented that makes the use of spectral method in numerical models practical.

For the advection term $u\frac{\partial u}{\partial x}$, the spatial derivative is first evaluated at every grid point:

$$v = \frac{\partial u}{\partial x} = \sum_{n=1}^{N} inkU_n e^{inkx} \qquad (18)$$

(uv) together is then expressed as a single variable in a spectral series:

$$(uv) = \sum_{n=-N}^{N-1} V_n e^{inkx} \qquad \text{(Inverse Fourier transform)} \qquad (19)$$

where

$$V_n = \frac{1}{2N} \sum_{j=-N}^{N-1} (uv)_j e^{-inkx_j} \quad \text{(Fourier transform)} \tag{20}$$

We end up solving the following ODE's:

$$\frac{dU_n}{dt} + V_n = 0. \tag{21}$$

With this method, there are $2N$ operations for the advection term instead of N^2 for the true spectral method.

Note that it is (20) that is actually evaluated, not (19) because we need V_n in (21).

Steps to integrate nonlinear advection equation (12) using spectral method with Fourier basis functions:

1) Perform discrete Fourier transform (DFT, like equation 10) on the initial condition $u(x, 0)$ to obtain spectral coefficients $U_n(0)$ at initial time.
2) Calculate the spatial derivate of u at grid points, i.e., v_j, using Eq. (18).
3) Multiply u_j v_j to get $(uv)_j$ at grid points. Perform DFT on $(uv)_j$ to obtain spectral coefficients V_n .
4) Integrate Eq.(21) to obtain U_n at the next time step.
5) Perform IDFT (like Eq.19 but on U_n) to obtain u_j.
6) Repeat steps 2-5 to integrate the equation for more steps.
7) Given the next for step 5 every time step, physical quantity u at the grid points is available every time step.

7.6. Advantages and Disadvantages of Spectral Method

Advantages

- Derivatives computed exactly from the basis functions.
- Infinite convergence rate in space (in term of the order of accuracy)
- Can pick basis functions that are well-suited for the particular problem, e.g., spherical harmonics for flow on a sphere (the negative side is that one does not have complete freedom to choose the basis function – often subject to certain limitation such as the periodicity condition)
- Can obtain power spectra directly
- Can control aliasing, therefore NL instability easily
- Can apply spatial filters of very high order easily
- Often more accurate than FD method with the same number of degrees of freedom (grid points versus spectral components), especially relatively smooth fields (not containing many sharp gradients)
- Conserves energy naturally (see Haltiner and Williams section 6.3)

Disadvantages

- More complicated to implement
- Can't represent physical processes in spectral space (need to transform back and forth)
- Hard to (less efficient at least) parallelize on distributed memory computers – spectral transform does not scale linearly and involves global data.
- Basis functions are global, not well suited for handling localized features and/or sharp gradients (remember the Gibbs phenomenon). Finite element methods and those based on local basis functions usually do better in this aspect.
- Most global models since 70s until recently are spectral models.
- Spectral methods are expensive at high resolutions. The operation count for FFT is proportional to $N \ln(N)$ instead of N as for grid point method – one of the reasons (the dominance of distributed-memory parallel computers is another) why grid point method is coming back in fashion for global models.
- Few regional model uses spectral method because of the lack of natural periodic boundary condition (The regional spectral model, Juang and Kanamitsu 1994, of NCEP solves for the perturbation fields from the

global model in which it is nested, so that at the boundaries the perturbations are zero. Sine transform can then be used).

Juang, H. M. H. and M. Kanamitsu, 1994: The NMC regional spectral model. Mon. Wea. Rev., 122, 3-26.