Chapter 7. Introduction to Spectral Methods

Reference: Durran Chapter 4. Haltiner and Williams Chapter 6.

7.1. Introduction

- Grid points method – evaluates spatial derivatives using Tayler series expansion
- Galerkin method (a super set of spectral method) represents dependent variables as the sum of a set of functions with pre-specified space structure (basis-function). 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 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

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

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 set of finite basis functions →

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

(4) leads to

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

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

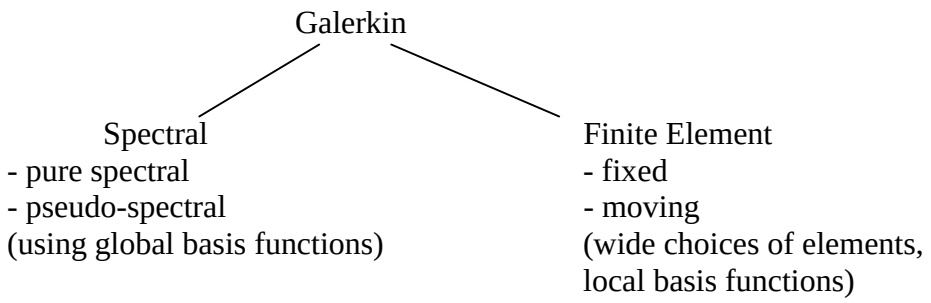
7.3. Choices of basis functions

- 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.

<u>Two main branches of Galerkin methods</u>:



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:

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

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 meet these requirements:

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

and the series (7) becomes

$$f(x_j) = f_j = \sum_{n=1}^{N} F_n e^{i\frac{2\pi n}{N\Delta x} j\Delta x} = \sum_{n=1}^{N} F_n e^{i2\pi nj/N} \qquad \text{for } j = 1, 2, \ldots, N \tag{9}$$

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

The inverse of (9) is

$$F_n = \frac{1}{N}\sum_{j=1}^{N} f_j e^{-i2\pi nj/N} \qquad \text{for } n=1, 2, \ldots, N \tag{10}$$

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

(9) and (10) defines the finite or discrete Fourier transforms, which are the discretized 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 of 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 Δx (k_n 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

$$\frac{dU_n}{dt}e^{inkx} + cinkU_n e^{inkx} = 0 \qquad \text{for n=1, …, N} \tag{16}$$

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

Finite difference is usually used for the time derivative. After U_n is obtained, u(x,t) is obtained from (8). Note for simple linear equation such as (11), (13) needs to be evaluated on at the output times. The inverse transform for U_n needs to be performed once at the initial time.

Notes:

Galerkin method leads naturally to energy conservation (see discussion in pages 186-187 of Haltiner and Williams), and the time integration of ODE is also subject to stability condition.

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

Equivalent of (15):

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

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, unless 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 practical 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:

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

(uv) is then expanded in a spectral series:

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

where

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

We end up solving the following ODE's:

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

With this method, there are 2x(N) 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).

7.6. Advantages and Disadvantages of Spectral Method

Advantages

- Derivatives computed exactly
- 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 missing, 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)
- Conserves energy naturally (see Haltiner and Williams section 6.3)

Disadvantages

- More complicated to implement
- Can't represent physical processes in spectral space
- Hard to parallelize on distributed memory computers
- Basis function global, not well suited for handling localized features and/or sharp gradients (remember the Gibbs phenomenon). FEM and those based on local basis functions usually do better
- Expensive for high resolutions. E.g., the operation count for FFT is proportional to N ln(N) instead of N as for grid point method – a reason why grid point method is reviving for global models.