Chapter 5. Basics of Higher-order Discretization Methods

Chap. 5-1. Comparison of Discretization Methods_Revisited

- ***Discretization Methods Available***
  - **FDM (Finite Difference Method)**
    - Direct discretization of the differential form by assuming point-wise values defined at each grid point

$$\frac{\partial q}{\partial t}+\frac{\partial f(q)}{\partial x}=0 \xrightarrow[\text{with } h(=\Delta x),\Delta t]{q_j,\,f_j \text{ at } x=x_j} \frac{dq_j}{dt}+\frac{\sum_q c_{jq} f_{j+q}}{h}=0 \text{ plus a suitable time-discretization}$$

    - Simple, efficient and easy to discretize
    - One-dimensional (or dimension-by-dimension) interpolation and transformation to computational coordinate are essential. → not suitable to complex geometry
  - **FVM (Finite Volume Method)**
    - Integration of the differential form of conservation laws over finite computational cell
    - Apply control volume analysis to each computational cell defined by (Δx, Δt) using cell-averaged quantities.

$$\frac{\partial q}{\partial t}+\frac{\partial f(q)}{\partial x}=0 \xrightarrow[\text{over } (h,\Delta t)]{\text{integration}} \int_{t^n}^{t^n+\Delta t}\int_{x_{j-1/2}}^{x_{j+1/2}}\left(\frac{\partial q}{\partial t}+\frac{\partial f(q)}{\partial x}\right)dxdt=0 \xrightarrow[\text{cell-averaged quantities}]{\text{discretized form using}}$$

$$\frac{q_j^{n+1}-q_j^n}{\Delta t}+\frac{F_{j+1/2}\left(q_{j-p}^n,\ldots,q_{j+q}^n\right)-F_{j-1/2}\left(q_{j-p-1}^n,\ldots,q_{j+q-1}^n\right)}{h}=0 \text{ or } \frac{dq_j}{dt}=L(q_{j-p-1}^n,\ldots,q_{j+q}^n)$$

$$\text{with } \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} q\left(x,t^n\right)dx=q_j^n,\quad \frac{1}{\Delta t}\int_{t^n}^{t^n+\Delta t} f\left(q\left(x_{j+1/2},t\right)\right)dt=F_{j+1/2}$$

Chap. 5-1. Comparison of Discretization Methods_Revisited

- **FVM (Finite Volume Method) (cont'd)**
  - Purely local analysis without assuming any grid structure or the shape of computational cell → suitable to complex geometry
  - Cell-wise interpolation for high-order accuracy → not flexible on general unstructured grids
- **FEM (Finite Element Method)**
  - Weak formulation (or weighted-residual formulation) from the differential form of conservation laws over each computational element
  - Local expansion of solution using basis functions followed by orthogonal projection of the residual (or error) to test function space

$$\frac{\partial q}{\partial t}+\frac{\partial f(q)}{\partial x}=0 \xrightarrow{\int_{T_k}(\ldots)\phi_i dx=0} \frac{\partial}{\partial t}\int_{T_k} q\phi_i dx+\int_{\partial T_k} f\phi_i dx-\int_{T_k} f\frac{d\phi_i}{dx}dx=0 \text{ on } T_k \quad \text{for } \phi_i,\ 1\le i\le ndof(n)$$

$\rightarrow$ approximate $q(x,t)$ on T_k using basis functions, $q(x,t)\cong\sum_{i=1}^{ndof(n)} q_k^{(i)}(t)\phi_i(x)$

$\rightarrow$ evaluate temporal and spatial integral terms by numerical quadrature

  - Local formulation without assuming any grid structure or the shape of computational cell → suitable to complex geometry
  - Local expansion of solution with multiple DOFS → flexible for higher-order approximation on general unstructured grids
  - Uncertainty on conservative and accurate treatment of the boundary integral

Chap. 5-1. Comparison of Discretization Methods_Revisited

- **Value of high-order accuracy** (~ O(h^n) with n > 2)
  - Ex) Behavior of computed solutions by changing order-of-polynomial approximation(N) mesh size(K)
    - $\frac{\partial q}{\partial t} + a\frac{\partial q}{\partial x} = 0$ with $x \in [0, 2\pi]$, $a = -2\pi$, $q_0(x) = q(x,0) = \sin(\frac{2\pi}{\lambda}x)$

      - With periodic BC and a fixed time step for all cases, computed results shows

        i) $\|q - q_h\|_2 = O(h^{N+1}) \le C(T)h^{N+1} \simeq (c_1 + c_2 T)h^{N+1}$ with T = target time

        ii) computational cost $= C(T)K(N+1)^2$ with $h = \frac{2\pi}{K}$, N = order-of-approximation

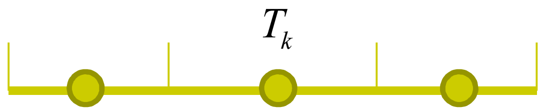
      - Comparison of computed results reveals that higer-order approximation is beneficial for the cases requiring i) highly accurate solutions, ii) long-time integrations

N \ K	2	4	8	16	32	64
1	1.00	2.19	3.50	8.13	**19.6**	54.3
2	2.00	3.75	**7.31**	15.3	38.4	110.
4	**4.88**	8.94	20.0	45.0	115.	327.
8	15.1	32.0	68.3	163.	665.	1271.
16	57.8	121.	279.	664.	1958.	5256.

< Scaled computation cost >

Chap. 5-1. Comparison of Discretization Methods_Revisited

- ***Strategy for High-Order Accuracy***
  - **One unknown (or one DOF) per one cell approach**
    - Within a cell T_k, approximate the exact solution $q(x)$ as a polynomial $q_k(x)$ by using Taylor expansion with neighboring computational cells (or grid points)



    - n^{th}-order polynomial approximation within T_k

$$q_k(x) = q_k + \sum_{l=1}^{n} c_l(q_{j-a}, q_{j-a+1}, \cdots, q_{j+b-1}, q_{j+b})\, x^l, \quad x_{k-1/2} \le x \le x_{k+1/2} \text{ with } a+b=n$$

      - FDM: direct Taylor expansion, compact difference
      - FVM: TVD-MUSCL, ENO/WENO, MLP reconstruction
    - Cell-interface values estimated from $q_k(x)$ are used to evaluate a numerical flux.

    \+ Relatively simple, easy to understand, and suitable for coding

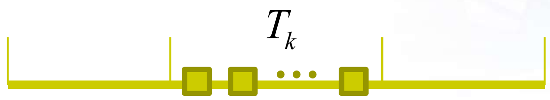
    − Non-local computational stencil

    As a result, when $q_k(x)$ is higher than linear polynomial,
    - Hard to treat boundary conditions, hard to handle 3-D complex geometry, and hard to exploit parallel computations
  - **Multiple DOFs per one cell approach**
    - Within an element T_k, approximate the exact solution $q(x)$ as a polynomial $q_k^h(x)$ by a linear combination of local shape functions (or basis functions).

Chap. 5-1. Comparison of Discretization Methods_Revisited

- **Multiple DOFs per one cell approach (cont'd)**
  - n^{th}-order polynomial approximation within T_k

$$q_k^h(x) = \sum_{l=1}^{n+1} q_k^{(l)} \phi_l(x), \quad x_{k-1/2} \le x \le x_{k+1/2}$$



    - Each coefficient $q_k^{(l)}$ is regarded as an unknown or a degree of freedom (DOF).
  - Finite element discretization based on weighted residual formulation is commonly adopted to determine the evolution of $q_k^{(l)}$.

\+ Highly local construction → compact stencil

As a result,

- Only nearest elements sharing a common cell interface/vertex are necessary → amenable to parallel computation
- Easy to implement boundary conditions
- Easier to tackle 3-D complex geometry

\- More mathematical background and more efforts to implement it into a code

\- More delicate numerical treatment for temporal and spatial integral terms

\- More data storage and/or more computational costs in general

→ Overcome via computational techniques such as parallel computing or *h/p* adaptation

Chap. 5-2. Basic Formulation

- ***Discretization of 1-D SCL,*** $\mathbf{q_t + f_x(q) = 0}$
  - **Weighted residual formulation**
    - Approximate solution of $q(x,t)$ within the cell $T_k = [x_{k-1/2}, x_{k+1/2}]$

      $q(x,t) \simeq q_k^h(x,t) = \sum_{l=1}^{ndof(n)} q_k^{(l)}(t)\phi_l(x)$, where $\{\phi_l\} \in V^n$ and $ndof(n) = \dim(V^n) = n+1$
      - Choice of the polynomial space V^n and basis function $\{\phi_l\}$ determines the nature of solution.
    - Approximate solution $q_k^h(x,t)$ does not satisfy the governing equation exactly.
      - Non-zero residual: $\frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0 \rightarrow \frac{\partial q_k^h}{\partial t} + \frac{\partial f_k^h(q_k^h)}{\partial x} = R(q_k^h)$
    - Minimize the residual, *R,* in the weighted integral sense over the test function space
      - $\int_{T_k} R(q_k^h) w_i(x) = 0$ over the whole domain $D = \bigcup_{i=1}^{N_{elem}} T_i$ for weighted functions $\{w_i(x)\}_{1 \le i \le ndof(n)}$
    - Choice of the weight function w_i determines the nature of the discretized equation.
      - Discrete Fourier spectral method: $w_j(x) = e^{-\hat{i}k_j x}$
      - Galerkin approximation: $w_i(x) = \phi_i(x)$

- ***Discontinuous Galerkin (DG) Method***
  - **Integration-by-parts over the cell T_k with a compactly supported $\phi_i(x)$**

    → a weak form: $\int_{T_k} R(q) w_i(x) = 0 \rightarrow \int_{T_k} \left(q_t + f_x(q)\right)\phi_i \, dx = \int_{T_k} q_t \phi_i \, dx + \int_{T_k} f_x \phi_i \, dx = 0$

    $$\rightarrow \frac{\partial}{\partial t}\int_{T_k} q\phi_i \, dx + \int_{\partial T_k} f \, \phi_i \hat{n} \, dx - \int_{T_k} f \frac{\partial \phi_i}{\partial x} dx = 0$$

Chap. 5-2. Basic Formulation

- **DG approach to treat the boundary integral**
  - Approximate solution allows to be discontinuous, in the sense of C^0, at the cell interface ∂T_k.
    $\rightarrow f$ is not uniquely determined at the cell interface.
  - If $\phi_i = 1,\ q_k^h(x,t) = \sum_{l=1}^{ndof(n)} q_k^{(l)}(t) f_l(x) = q_k^{(1)}(t)$. Thus, the weak form becomes $\frac{d\overline{q}_k^{(1)}}{dt} + f\big|_{k\pm 1/2} = 0$ or the finite volume discretization. → In order to maintain conservation at ∂T_k, f is approximated by a conservative numerical flux H from finite volume method.
    $$\frac{\partial}{\partial t}\int_{T_k} q\phi_i\,dx + \int_{\partial T_k} H(q_-,q_+)\phi_i\,dx - \int_{T_k} f\frac{\partial \phi_i}{\partial x}dx = 0 \quad \text{with}$$
    - q_- : the value of q at the boundary ∂T_k obtained from $q(x)$ of the cell T_k

      q_+ : the value of q at the boundary ∂T_k obtained from $q(x)$ of the adjacent cell sharing ∂T_k
- **Spatial approximations**

$$\frac{\partial}{\partial t}\int_{T_k} q_k^h\phi_i\,dx + \int_{\partial T_k} H_k^h(q_{k-}^h,q_{k+}^h)\phi_i\,dx - \int_{T_k} f_k^h(q_k^h)\frac{\partial \phi_i}{\partial x}dx = 0$$

$$\rightarrow \frac{\partial}{\partial t}\int_{T_k}\left(\sum_{l=1}^{ndof(n)} q_k^{(l)}(t)\phi_l\right)\phi_i\,dx + \int_{\partial T_k} H_k^h(q_{k-}^h,q_{k+}^h)\phi_i\,dx - \int_{T_k} f_k^h(q_k^h)\frac{\partial \phi_i}{\partial x}dx = 0$$

$$\rightarrow \frac{\partial}{\partial t}\left(\sum_{l=1}^{ndof(n)} q_k^{(l)}(t)\int_{T_k}\phi_l\phi_i\,dx\right) + \int_{\partial T_k} H_k^h(q_{k-}^h,q_{k+}^h)\phi_i\,dx - \int_{T_k} f_k^h(q_k^h)\frac{\partial \phi_i}{\partial x}dx = 0$$

Thus, we have $\sum_{l=1}^{ndof(n)}\left(\int_{T_k}\phi_i\phi_l\,dx\right)\frac{\partial q_k^{(l)}}{\partial t} + \int_{\partial T_k} H_k^h(q_{k-}^h,q_{k+}^h)\phi_i\,dx - \int_{T_k} f_k^h(q_k^h)\frac{\partial \phi_i}{\partial x}dx = 0.$

Chap. 5-2. Basic Formulation

- **Semi-discrete form with a matrix-vector notation**

$$\mathbf{M}_k \frac{d\mathbf{q}_k}{dt} = -\int_{\partial T_k} H_k^h(q_{k-}^h, q_{k+}^h)\,\mathbf{\Phi}\,dx + \int_{T_k} f_k^h(q_k^h)\frac{\partial \mathbf{\Phi}}{\partial x}dx,$$

where $\mathbf{M}_k = \left[\int_{T_k}\phi_i\phi_j\,dx\right]_{ndof(n)\times ndof(n)}$, $\mathbf{q}_k = \left[q_k^{(j)}(t)\right]_{ndof(n)}$, and $\mathbf{\Phi} = \left[\phi_i(x)\right]_{ndof(n)}$

- **Strong form by taking integration-by-parts once more**

$$\frac{\partial}{\partial t}\int_{T_k} q\phi_i\,dx + \int_{\partial T_k} H\phi_i\,dx - \int_{T_k} f\frac{\partial \phi_i}{\partial x}dx = 0 \;\rightarrow\; \int_{T_k}\left(\frac{\partial q_k^h}{\partial t} + \frac{\partial f_k^h}{\partial x}\right)\phi_i\,dx = \int_{\partial T_k}\left[f_k^h - H_k^h\right]\phi_i\,dx$$

or $$\mathbf{M}_k \frac{d\mathbf{q}_k}{dt} + \int_{T_k}\frac{\partial f_k^h}{\partial x}\mathbf{\Phi}\,dx = \int_{\partial T_k}\left[f_k^h - H_k^h(q_{k-}^h, q_{k+}^h)\right]\mathbf{\Phi}\,dx$$

  - Weighted residual is dependent on the choice of numerical flux H and test function ϕ_i
  - Smoothness of ϕ_i is not essential.
  - Various approaches to remove the boundary integral term
    - Collocation penalty approach, using Dirac delta functions $\phi_i(x) = \delta(x - y_i)$

Choice of Basis Function

- **Classification of polynomial basis functions**
  - (Option 1) Modal basis function to represent a specific solution distribution (or mode shape)
  - Solution of a singular Sturm-Liouville problem

$$(1-x^2)\frac{d^2\phi_n(x)}{dx^2} - 2x\frac{d\phi_n(x)}{dx} + n(n+1)\phi_n(x) = 0 \quad \text{for } x\in[-1,1],\ n\ge 0$$

Chap. 5-2. Basic Formulation

$\rightarrow\ \phi_n(x)=\dfrac{1}{2^n n!}\dfrac{d^n}{dx^n}[(x^2-1)^n]$ (Rodrigues' formula) gives a sequence of n^{th}-order Legendre ploynomials

as $\phi_0(x)=1,\ \phi_1(x)=x,\ \phi_2(x)=\dfrac{1}{2}(3x^2-1),\ \phi_3(x)=\dfrac{1}{2}(5x^3-3x),\ \phi_4(x)=\dfrac{1}{8}(35x^4-30x^2+3),\ldots$

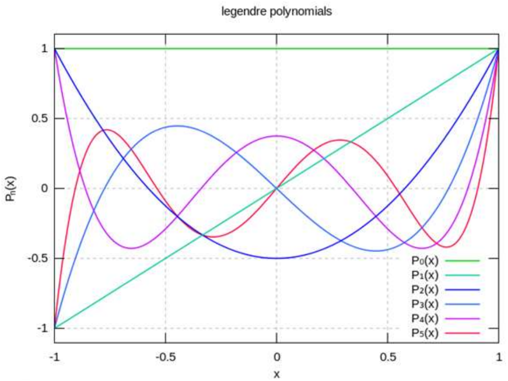
- Notable properties

  - Orthogonality: $\int_{-1}^{1}\phi_i\phi_j\,dx=\dfrac{2}{2i+1}\delta_{ij}$ and $\int_{-1}^{1}\phi_{j(\geq 1)}\,dx=0$ with $\phi_n(1)=1,\ \phi_n(-x)=(-1)^n\phi_n(x),\ n\geq 0$

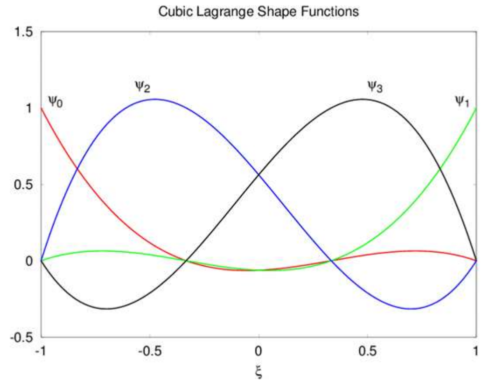
    $\rightarrow\ \mathbf{M}_k=[m_{ij}]$ with $m_{ij}=\int_{T_k}\tilde{\phi}_i\tilde{\phi}_j\,dx$ and $\tilde{\phi}=\phi/\|\phi\|$ becomes the identity matrix.

  - Recurrence:

$$(n+1)\phi_{n+1}(x)=(2n+1)x\phi_n(x)-n\phi_{n-1}(x),\ \frac{d\phi_{n+1}}{dx}=(n+1)\phi_n+x\frac{d\phi_{n-1}}{dx},\ \text{and}\ \frac{d\phi_{n+1}}{dx}-\frac{d\phi_{n-1}}{dx}=(2n+1)\phi_n,\ n\geq 1$$



< Example of modal basis functions >
(Legendre polynomials)



< Example of nodal basis functions >
(Cubic Lagrange polynomials)

- Legendre polynomial(ϕ_n) is a special case of the Jacobi polynomial($P_n^{(\alpha,\beta)}$) which is a solution of the general singular Sturm-Liouville problem.

Chap. 5-2. Basic Formulation

$$(1-x^2)\frac{d^2P_n^{(\alpha,\beta)}(x)}{dx^2}+[\beta-\alpha-(\alpha+\beta+2)x]\frac{dP_n^{(\alpha,\beta)}(x)}{dx}+n(n+\alpha+\beta+1)P_n^{(\alpha,\beta)}(x)=0 \text{ for } x\in[-1,1],\ n\geq 0,$$

and $(\alpha,\beta)>-1$ $\left(\text{or } \frac{d}{dx}\left[(1-x^2)w(x)\frac{dP_n^{(\alpha,\beta)}(x)}{dx}\right]+n(n+\alpha+\beta+1)w(x)P_n^{(\alpha,\beta)}(x)=0 \text{ with } w(x)=(1-x)^\alpha(1+x)^\beta\right)$

$\rightarrow P_n^{(\alpha,\beta)}(x)=\frac{(-1)^n}{2^n n!}\frac{1}{w(x)}\frac{d^n}{dx^n}[w(x)(1-x^2)^n]$ (Rodrigues' formula) or a form of hypergeometric function

- Notable properties
  - Orthogonality: $\int_{-1}^{1}P_i^{(\alpha,\beta)}P_j^{(\alpha,\beta)}w(x)\,dx=f(\alpha,\beta,i)\delta_{ij}$ with $P_n^{(\alpha,\beta)}(-x)=(-1)^n P_n^{(\alpha,\beta)}(x),\ n>0$
  - Recurrence: $xP_n^{(\alpha,\beta)}(x)=a_nP_{n-1}^{(\alpha,\beta)}(x)+b_nP_n^{(\alpha,\beta)}(x)+a_{n+1}P_{n+1}^{(\alpha,\beta)}(x)$ and

$$\frac{dP_n^{(\alpha,\beta)}}{dx}=\frac{(n+\alpha+\beta+1)}{2}P_{n-1}^{(\alpha+1,\beta+1)} \text{ with } a_n=a_n(\alpha,\beta,n),\ b_n=b_n(\alpha,\beta,n),\ n\geq 1$$

  - Jacobi polynomials contain other orthogonal polynomials as a special case, and they are quite useful for Gauss-like quadratures and construction of multi-dimensional basis.
    . $P_n^{(0,0)}(x)=\phi_n(x)$ (Legendre polynomials)
    . $P_n^{(-1/2,-1/2)}(x)=T_n(x)=con(n\theta)$ with $x=\cos\theta,\ -\pi\leq\theta\leq\pi$ (Chebyshev polynomials)

- (Option2) Nodal basis function
  - Lagrange polynomial by interpolating some selective points
    - $\phi_i(x)=\prod_{j=1}^{ndof(n)}\frac{x-x_j}{x_i-x_j}$ Thus, $\phi_i(x_j)=\delta_{ij}$ by definition.
    - $\mathbf{M}_k$ is not diagonalized.
    - Typically employed in flux reconstruction approach such as FR/CPR, ESFR