Summation by Parts for Finite Difference Method

Mathematical Modeling: Final project

Singyuan Yeh
Advisor: Chunhao Teng, Taichia Lin

Institute of Applied Mathematical Sciences
National Taiwan University

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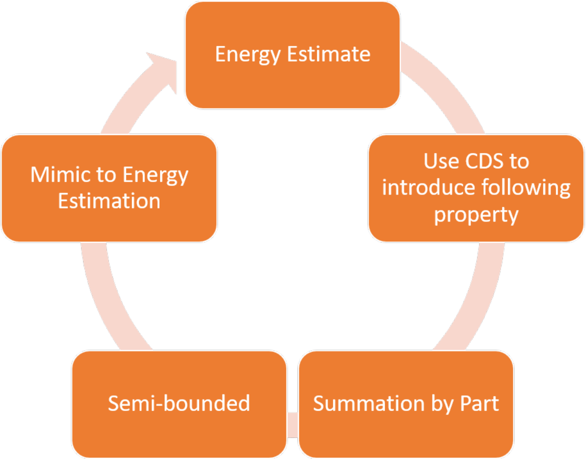
Outline

1. Introduction
2. Difference Operator D for Bounded Domain
   - Introduction to energy estimation
   - Central Difference Scheme (CDS)
   - Definition of semi-bounded
   - Relation between semi-bounded and energy estimation
3. Difference Operator D for Unbounded Domain
   - Operator D with interior second order and boundary first order: CDS
   - Operator D with interior forth order and boundary second order
   - Numerical result
4. Literature Review of Strand [2]
   - Check second order on boundary points
   - A necessary and sufficient form of operator D
   - Obtain the component of operator D
5. Summary

- In my thesis, I want to simulate the black holes formation, but I cannot make it converge. The problem seems to occur at boundary. Fortunately, I chanced to heard this SBP method in Prof. Teng class. Prof. Deng gave me lots of advice and reference. Although the problem not solved completely, this method make my simulation a big improvement. Therefore, I want to investigate this method more deeper.
- In this report, it can divided two part, the first part is introduction to difference operator for bounded domain, which has an intersection of our class. The main idea of this part is how to construct a difference operator mimics to energy estimation, which is called semi-bounded. The second part is literature review. I follow the method in Strand [2] to **verify** the particular accuracy operator.


Energy Estimate
Use CDS to introduce following property
Summation by Part
Semi-bounded
Mimic to Energy Estimation

Introduction to energy estimation

In this report, the uniform grid with step size h

$$x_i = ih,\ j = 0, 1, \cdots\ ,$$

is used.

Example

Consider the transport equation

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0\ , & \text{if } x \in [0,1], t > 0 \\ u(x,0) = f(x)\ , & \text{if } x \in [0,1], t = 0 \\ u(0,t) = g(t)\ , & \text{if } x = 0, t > 0 \end{cases}$$

Define $E(t) = \int_0^1 u^2(x,t)\ dx$. We know the energy estimate method,

$$\begin{aligned} \frac{1}{2}\frac{dE}{dt} &= \int_0^1 uu_t\ dx = -\int_0^1 uu_x dx = \frac{1}{2}(u^2(0,t) - u^2(1,t)) \\ &= \frac{1}{2}(g^2(t) - u^2(1,t)) \end{aligned} \tag{1}$$

In discrete space sense, we consider the following

$$\begin{cases} \frac{dv_0}{dt} + \frac{v_1 - v_0}{h} = -\tau(v_0 - g(t)) \\ \frac{dv_i}{dt} + \frac{v_{i+1} - v_{i-1}}{2h} \\ \frac{dv_N}{dt} + \frac{v_N - v_{N-1}}{h} = 0 \end{cases}$$

Then, rewrite in matrix form

$$\frac{d}{dt}\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_N \end{bmatrix} = \frac{-1}{h}\begin{bmatrix} -1 & 1 & & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 1 \end{bmatrix}\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_N \end{bmatrix} - \tau\begin{bmatrix} 1 & 0 & \cdots \\ 0 & 0 & \\ \vdots & & \ddots \end{bmatrix}\begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_N \end{bmatrix}$$

$$= -Dv - \tau(e_0 {e_0}^T v) = -(D + \tau I_-)v \ ,$$

where $I_- = e_0 {e_0}^T$ and $e_0 = [1 \ 0 \ \cdots \ 0]^T$. By the way, $I_+ = e_N {e_N}^T$ and $e_N = [0 \ \cdots \ 0 \ 1]^T$.

Choose positive definite matrix $H = diag([\frac{1}{2}\ 1\ \cdots\ 1\ \frac{1}{2}])$. Then, define matrix Q as following

$$Q := hHD = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & & \\ -\frac{1}{2} & 0 & \ddots & \\ & \ddots & \ddots & \frac{1}{2} \\ & & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$$= \begin{bmatrix} -\frac{1}{2} & & & & \\ & 0 & & & \\ & & \ddots & & \\ & & & 0 & \\ & & & & \frac{1}{2} \end{bmatrix} + \begin{bmatrix} 0 & \frac{1}{2} & & \\ -\frac{1}{2} & 0 & \ddots & \\ & \ddots & \ddots & \frac{1}{2} \\ & & -\frac{1}{2} & 0 \end{bmatrix} := Q_S + Q_A\ , \tag{2}$$

where Q_S is symmetric matrix and Q_A is anti-symmetric i.e. $Q_A + {Q_A}^T = 0$. Hence, matrix Q satisfy $Q + Q^T = -I_- + I_+$.

Definition of semi-bounded

Note that the good property of matrix Q

$$hv^T HDv = v^T Q_s v + v^T Q_A v = \frac{1}{2}({v_0}^2 - {v_N}^2) \tag{3}$$

Hence, this idea gives the generalization property:

Remark

If exist positive definite matrix H such that difference operator D satisfy

$$(v, Dv)_{h,H} := v^T HDv \leq \alpha \|v\|^2 \ , \tag{4}$$

we call operator D is semi-bounded. The H-norm $(\cdot, \cdot)_H$ will be introduced later.

Now, we can compute it directly

$$\frac{dv}{dt} + Dv = -\tau(v_0 - g(t))e_0$$
$$hv^T H \frac{dv}{dt} + hv^T HDv = -\tau(v_0 - g(t))v^T He_0 h$$

Hence,

$$\frac{1}{2}\frac{d}{dt}(v^T hHv) = \frac{1}{2}({v_0}^2 - {v_N}^2) - \tau(v_0 - g(t))h \tag{5}$$

The above equation mimics to energy estimation (1).

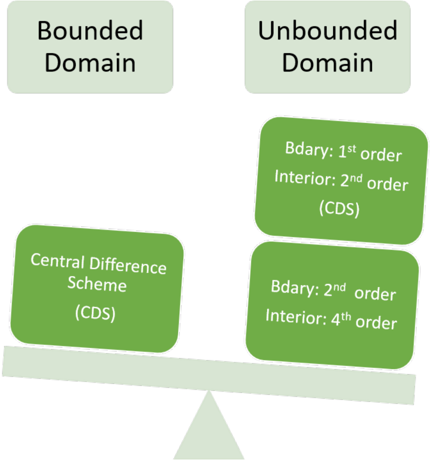
Remark

If the operator D is to approximate $\frac{d}{dx}$, then we have to find positive definite matrix H such that

$$HD = Q_S + Q_A$$

Then, operator is semi-bounded (4).

Next, we want to find high order semi-bounded operator D to $\frac{d}{dx}$.


Bounded Domain
Unbounded Domain
Bdary: 1st order
Interior: 2nd order
(CDS)
Central Difference Scheme
(CDS)
Bdary: 2nd order
Interior: 4th order

Central Difference Scheme: Outflow Problem

Example

Consider the outflow problem

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0 \ , & \text{if } x > 0, t > 0 \\ u(x,0) = f(x) \ , & \text{if } x > 0, t = 0 \\ u(0,t) = g(t) \ , & \text{if } x = 0, t > 0 \end{cases}$$

By above discussion (previous section), the interior second order and boundary first order SBP difference operator is as following

$$D = \begin{bmatrix} -1 & 1 & & \\ -\frac{1}{2} & 0 & \frac{1}{2} & \\ & \ddots & \ddots & \ddots \end{bmatrix}$$

Moreover the positive definite matrix is

$$H = \begin{bmatrix} \frac{1}{2} & & \\ & 1 & \\ & & \ddots \end{bmatrix}$$

Operator with interior forth order and boundary second order

Consider the outflow problem, the following is the operator with interior forth order and boundary second order which given by Gustafsson [1].

$$D = \frac{1}{h}\begin{bmatrix} \frac{-24}{17} & \frac{59}{34} & \frac{-4}{17} & \frac{-3}{34} & & & & \\ \frac{-1}{2} & 0 & \frac{1}{2} & 0 & & & & \\ \frac{4}{43} & \frac{-59}{86} & 0 & \frac{59}{86} & \frac{-4}{43} & & & \\ \frac{3}{98} & 0 & \frac{-59}{98} & 0 & \frac{32}{49} & \frac{-4}{49} & & \\ & & \frac{1}{12} & \frac{-2}{3} & 0 & \frac{2}{3} & \frac{-1}{12} & \\ & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}$$

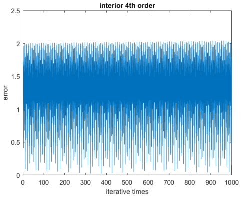
and positive definite matrix

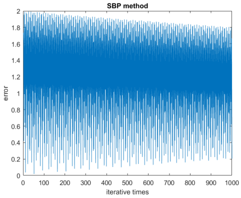
$$H = \begin{bmatrix} \frac{17}{48} & & & & & \\ & \frac{59}{48} & & & & \\ & & \frac{43}{48} & & & \\ & & & \frac{49}{48} & & \\ & & & & 1 & \\ & & & & & \ddots \end{bmatrix}$$

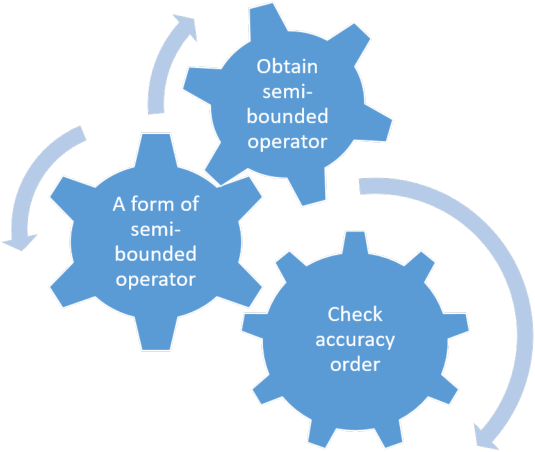
Numerical result

I want to use the following periodic system to explain the difference between origin method and SBP method, but I **FAILED**. I use operator D with interior forth order and boundary second order which mentioned above and the other is operator with interior forth order and boundary is first order and second order, which is origin method. Moreover, I use forth order Runge Kutta to evolve the system. I originally thought the original method will unstable in long time, but by the following figure, it is not significant.

$$\begin{cases} \frac{\partial u}{\partial t} - \frac{\partial u}{\partial x} = 0 \ , & \text{if } x \in [0, 2\pi], t > 0 \\ u(x, 0) = \sin(x) \ , & \text{if } x \in [0, 2\pi], t = 0 \\ u(2\pi, t) = u(0, t) \ , & \text{if } t > 0 \end{cases}$$






Obtain semi-bounded operator
A form of semi-bounded operator
Check accuracy order

A excuses for my lazy

Before the following discussion, let me make it clear that I am not going to prove the general case (for all accuracy order τ) because the space is limited. Therefore, I just **verify** the operator D with interior forth order and boundary second order satisfy the theorem and proposition in Strand [2].

Check second order on boundary points

If operator approximate $\frac{d}{dx}$ of accurate order τ, then $Dv = \frac{dv}{dx} + O(h^\tau)$. Hence, if $deg(g(x)) \leq \tau$, then $D[g] - \frac{dg}{dx} = 0$.
Now, $\tau = 2$, let $g_j(x) = (x-4)^j$ for $j = 0, 1, 2$, and $h = 1$, $x = 0, 1, \cdots$. If $j = 0$, trivial.
If $j = 1$. Let

$$v^{(1)} = \begin{bmatrix} g_j(0) \\ g_j(1) \\ g_j(2) \\ g_j(3) \\ \vdots \end{bmatrix} = \begin{bmatrix} -4 \\ -3 \\ -2 \\ -1 \\ \vdots \end{bmatrix}, \text{ then } Dv^{(1)} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ \vdots \end{bmatrix} = [\frac{d}{dx}(x-4)]$$

If $j = 2$, by the similar work, let

$$v^{(2)} = \begin{bmatrix} 4^2 \\ 3^2 \\ \vdots \end{bmatrix}, \text{ then } Dv^{(2)} = 2\begin{bmatrix} -4 \\ -3 \\ \vdots \end{bmatrix} = [\frac{d}{dx}(x-4)^2]$$

Hence, the equality holds for $j = 0, 1, 2$, which imply second order accuracy on boundary points. Moreover, we will discuss more general form $Dv^{(j)} = jv^{(j-1)}$ in (7), later.

Now, we want to generalize the energy estimation (3) into a robust theorem in Strand [2]. Before that, for convenience, some notations are be introduced.

- The operator D be divided into 4 part

$$D = \begin{bmatrix} Q_{11} & Q_{12} \\ -C^T & \tilde{D} \end{bmatrix}, \text{ and } H = \begin{bmatrix} H_1 & O \\ O & I \end{bmatrix},$$

  where Q_{11} and H_1 are 4×4 matrix, and I is identity matrix. Moreover, by the same way, $v = [{v_I}^T \ {v_{II}}^T]^T$, where v_I is 4×1 matrix.

- The standard inner product is denoted by $(u, v) = \int_I u(x)v(x)dx$, and in the discrete sense is denoted by

$$(u, v)_h = \sum_{i=1}^{N} u_i v_i h \ ,$$

  where $u = (u_1, \cdots, u_N)$ and $v = (v_1, \cdots, v_N)$. Moreover, given a positive definite matrix H,

$$(u, v)_{h,H} = v^T H u$$

The following theorem give necessary and sufficient condition of operator D such that it satisfy semibounded condition $(v, Dv)_{h,H} = -\frac{1}{2}{v_0}^2$. This form is similar to (2) in bounded domain case.

Theorem

The operator satisfy $(v, Dv)_{h,H} = -\frac{1}{2}{v_0}^2$ if and only if it can be written as

$$hD = \begin{bmatrix} {H_1}^{-1}B & {H_1}^{-1}C \\ -C^T & \tilde{D} \end{bmatrix}, \tag{6}$$

where $B = B_S + B_A$, B_S is symmetric matrix and equal to $-\frac{1}{2}I_{-}$ and B_A is anti-symmetric.

Roughly proof: Since $\tilde{D}$ is anti-symmetric

$$\begin{aligned} -\frac{1}{2}{v_0}^2 &= (v, Dv)_{h,H} \\ &= {v_I}^T H_1 Q_{11} v_I + {v_I}^T H_1 Q_{12} v_{II} - {v_{II}}^T C^T v_I + {v_{II}}^T \tilde{D} v_{II} \\ &= {v_I}^T H_1 Q_{11} v_I + {v_I}^T (H_1 Q_{12} - C) v_{II} \end{aligned}$$

Hence, only if $H_1 Q_{11} = B$ and $H_1 Q_{12} = C$

Obtain the component of operator D

Before that, some notations have to be introduced, with $h = 1$, $x = 0, 1, \cdots$

$$v^{(j)} = [(x-4)^j] := \begin{bmatrix} e^{(j)} \\ f^{(j)} \end{bmatrix}, \text{ where } e^{(j)} = (-1)^j \begin{bmatrix} 4^j \\ \vdots \\ 1^j \end{bmatrix}, \text{ and } f^{(j)} = \begin{bmatrix} 0^j \\ 1^j \\ \vdots \end{bmatrix}$$

Since this is second order on boundary

$$[Q_{11} \ Q_{12}]e^{(j)} = je^{(j-1)} = Q_{11}e^{(j)} + Q_{12}f^{(j)} \text{ , where } j = 0, 1, 2, \text{ and } e^{(-1)} = 0 \quad (7)$$

which concept is the same as mention before.

Now, plug $Q_{11} = H_1 B = {H_1}^{-1}(B_S + B_A)$ and $Q_{12} = {H_1}^{-1}C$ into (7), and

$${H_1}^{-1}(B_S + B_A)e^{(j)} + {H_1}^{-1}Cf^{(j)} = je^{(j-1)}$$

Hence,

$$B_A e^{(j)} = jH_1 e^{(j-1)} - B_S e^{(j)} - Cf^{(j)} := d^{(j)} \quad (8)$$

Obtain the component of operator D

Now, we try $j = 1$. Since B_A is anti-symmetric,

$$d^{(1)} = B_A e^{(1)} = \begin{bmatrix} 0 & b_{01} & b_{02} & b_{03} \\ -b_{01} & 0 & b_{12} & b_{13} \\ -b_{02} & -b_{12} & 0 & b_{23} \\ -b_{03} & -b_{13} & -b_{23} & 0 \end{bmatrix} \begin{bmatrix} -4 \\ -3 \\ -2 \\ -1 \end{bmatrix} = - \begin{bmatrix} 3b_{01} + 2b_{02} + b_{03} \\ -4b_{01} + 2b_{12} + b_{13} \\ -4b_{02} - 3b_{12} + b_{23} \\ -4b_{03} - 3b_{13} + 2b_{23} \end{bmatrix}$$

$$= - \begin{bmatrix} 3 & 2 & 1 & & & \\ -4 & & & 2 & 1 & \\ & -4 & & -3 & & 1 \\ & & -4 & & -3 & -2 \end{bmatrix} \begin{bmatrix} b_{01} \\ b_{02} \\ b_{03} \\ b_{12} \\ b_{13} \\ b_{23} \end{bmatrix} \tag{9}$$

Since $j = 0, 1, 2$, there are 4×3 equations but only 6 unknown variable, it's overdetermined system.

Verify the equation (9)

In fact, matrix C and H are still unknown, but we don't find these two matrix here, because space is limited. However, we just want to verify above equation (9).

$$d^{(1)} = H_1 e^{(0)} - B_S e^{(1)} - C f^{(1)}$$

$$= \begin{bmatrix} \frac{17}{48} & & & \\ & \frac{59}{48} & & \\ & & \frac{43}{48} & \\ & & & \frac{49}{48} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} -\frac{1}{2} & 0 & \cdots & \\ 0 & 0 & & \\ \vdots & & \ddots & \\ & & & 0 \end{bmatrix} \begin{bmatrix} 4 \\ 3 \\ 2 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 & \cdots & & \\ 0 & \cdots & & \\ \frac{-1}{12} & 0 & \cdots & \\ \frac{2}{3} & \frac{-1}{12} & 0 & \cdots \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 2 \\ \vdots \end{bmatrix}$$

Hence, we can solve that

$$(b_{01}, b_{02}, b_{03}, b_{12}, b_{13}, b_{23}) = (\frac{59}{96}, \frac{-4}{48}, \frac{-3}{96}, \frac{59}{96}, 0, \frac{59}{96}) \ ,$$

which is equal to component of matrix B_A.

Summary

- We have to construct operator D is semi-bounded, to mimic the energy estimation.
- To construct semi-bounded operator D approximate $\frac{d}{dx}$ in bounded domain, we have to find positive definite matrix H, such that D forms as (2).

$$HD = Q_S + Q_A$$

- To construct semi-bounded operator D approximate $\frac{d}{dx}$ in unbounded domain, we have to find positive definite matrix H and $B = B_S + B_A$ such that D forms as (6).

$$hD = \begin{bmatrix} {H_1}^{-1}B & {H_1}^{-1}C \\ -C^T & \tilde{D} \end{bmatrix},$$

- After Following the Strand [2], the H and B can be constructed.

Reference

[1] Bertil Gustanfsson, *High Order Difference Methods for Time Dependent PDE*. Springer, (2008).

[2] Bo Strand, *Summation By Parts for Finite Difference Approximation for d/dx*, Journal of Computational Physics, (1994).