Numerical Solution of Initial Boundary Value Problems

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Overview

- Material: Notes + JNO + GUS + GKO + HANDOUTS.
- Homepage http://courses.mai.liu.se/FU/MAI0122/
- Notes at http://courses.mai.liu.se/FU/MAI0122/Lecture/
- Schedule: 6 lectures + 3 exercises + 3 seminars.
- Examination: 3 seminar presentations + 3 homeworks.
- Credit 3 points, European/Bologna system.
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Schedule

Times	Tuesday	Wednesday	Thursday	Friday
09:30-10:00		Seminar 1	Seminar 2	Seminar 3
10:00-10:15		Coffee/Tea	Coffee/Tea	Coffee/Tea
10:15-12:00	Lecture 1	Lecture 3	Lecture 5	Closure
12:00-13:15	Lunch	Lunch	Lunch	Lunch
13:15-15:00	Lecture 2	Lecture 4	Lecture 6	
15:00-15:15	Coffee/Tea	Coffee/Tea	Coffee/Tea	
15:15-16:30	Exercise 1	Exercise 2	Exercise 3	

Seminar preparation during exercises.

General structure and principles

"The Big Picture"

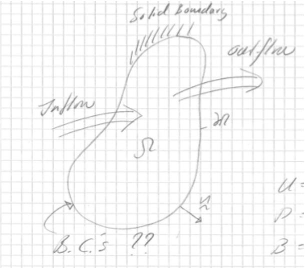
- Relate the PDE to the numerical approximation.
- Semi-discrete approximation in space, time is left continuous (until last lecture).
- Linear problems and smooth nonlinear problems.
- All approximations of the form: $U_t + AU = F$.
- What can we say about A based on knowledge of $A + A^T$?
- High order finite differences, the SBP-SAT technique.
- Extension to techniques for more complex geometries: multi-block, finite volume + dG techniques.

Course material

- Slides + possible additional handouts+references to relevant articles.
- JNO: A Roadmap to Well Posed and Stable Problems in Computational Physics, J. Nordström, Journal of Scientific Computing, Volume 71, Issue 1, pp. 365-385, 2017.
- GUS: High Order Difference Methods for Time Dependent PDE, Bertil Gustafsson, Springer-Verlag 2008.
- GKO: Time Dependent Problems and Difference Methods, Bertil Gustafsson, Heinz-Otto Kreiss, Joseph Oliger, John Wiley & Sons, 1995.

Lecture 1

Well posed problems



$$U_t + PU = F(x,t), \quad x \in \Omega,\ t \geq 0 \tag{1a}$$

$$BU = g(x,t) \quad x \in \delta\Omega,\ t \geq 0 \tag{1b}$$

$$u = f(x) \quad x \in \Omega,\ t = 0 \tag{1c}$$

U = dependent variable
P = differential operator in space
B = boundary operator

$$\text{data} \begin{cases} F = \text{forcing function} \\ g = \text{boundary data} \\ f = \text{initial data} \end{cases}$$

Equation (1) is Well-Posed if U exists and satisfies

$$||U||_I^2 \leq K\left(||f||_{II}^2 + ||F||_{III}^2 + ||g||_{IV}^2\right). \tag{2}$$

K independent of data F, f, g. A small K is good !

Why is (2) important? Consider the perturbed problem

$$V_t = PV + F + \delta F, \quad x \in \Omega,\ t \geq 0 \tag{3a}$$

$$BV = g + \delta g \quad x \in \Omega,\ t \geq 0 \tag{3b}$$

$$V = f + \delta f \quad x \in \Omega,\ t = 0. \tag{3c}$$

(3)-(1) $\Rightarrow W = V - U$, P = linear operator.

$$W_t + PW = \delta F, \quad x \in \Omega,\ t \geq 0 \tag{4a}$$

$$BW = \delta g \quad x \in \Omega,\ t \geq 0 \tag{4b}$$

$$W = \delta f \quad x \in \Omega,\ t = 0. \tag{4c}$$

Apply (2) to (4) $\Rightarrow$

$$||W||_I^2 \leq K\left(||\delta f||_{II}^2 + ||\delta F||_{III}^2 + ||\delta g||_{IV}^2\right). \tag{5}$$

$\therefore W = V - U$ small if $K, \delta f, \delta F, \delta g$ small!

Uniqueness follows directly from (5).

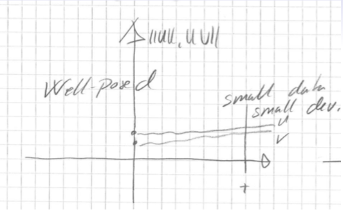


Figure: A good numerical approximation possible. Choice of numerical method next step.

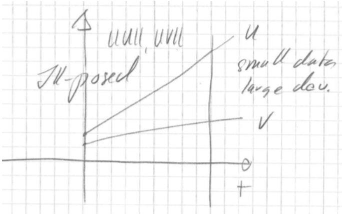


Figure: A good numerical approximation NOT possible. Change problem, in practice boundary conditions

Existence

$$u_x = 0 \qquad\qquad u = constant$$

$$u(0) = a$$

$$u(1) = b \qquad\qquad a \neq b \;\Rightarrow \text{too many b.c.'s !}$$

Uniqueness

$$u_{xx} = 0 \qquad\qquad u = c_1 + c_2 x$$

$$u(0) = a \qquad\qquad u = a + c_2 x \quad \Rightarrow \text{too few b.c.'s !}$$

Boundedness

$$u = a + c_2 x \;\; \text{no bound} \Rightarrow \text{too few b.c.'s !}$$

Example

$$u_t = -u_x, \quad x \geq 0, t \geq 0$$
$$Bu = g, \quad x = 0, t \geq 0$$
$$u(x,0) = 0, \quad x \geq 0, t = 0$$

$$P = -\frac{\partial}{\partial x}, B = 1 + \beta\frac{\partial}{\partial x}$$

$$\text{Laplace} \Rightarrow s\hat{u} + \hat{u}_x = 0 \Rightarrow \hat{u} = c_1 e^{-sx}$$

$$\text{i) } \beta = 0, \quad c_1 = \hat{q} \Rightarrow \hat{u} = \hat{q}e^{-sx}, \quad \underline{\text{Well posed}}$$

$$\text{ii) } \beta \neq 0 \quad c_1(1-\beta s) = \hat{q} \Rightarrow \hat{u} = \frac{\hat{q}}{1-\beta s}e^{-sx}, \quad \underline{\text{Ill posed}}$$

Nonlinear problems

(see Kreiss and Lorenz 1989)

- Linearization principle: A non-linear problem is well-posed at u if the linear problem obtained by linearizing all the functions near u are well-posed.
- Localization principle: If all frozen coefficient problems are well-posed, then the linear problem is also well-posed.

$$
\begin{aligned}
U_t + UU_x &= 0, \quad \text{Nonlinear} \\
U_t + \bar{U}(x,t)U_x &= 0, \quad \text{Linear} \\
U_t + \bar{U}U_x &= 0, \quad \text{Frozen coefficients}
\end{aligned}
$$

Note: Principles valid if no shocks present.

Summary of well-posedness

A problem is well-posed if

- A solution exists (correct number of b.c.)
- The solution is bounded by the data (correct form of b.c.).
- The solution is unique (follows from bound).

A nonlinear problem is related to well-posedness through the Linearization and Localization principles .

If a problem is not well-posed, do NOT discretize. Modify first to get well-posedness. In practice, change b.c.!

Initial value problems for periodic solutions using Fourier transforms

Consider the Cauchy problem on $-\infty \leq x \leq \infty$

$$U_t = P(\partial/\partial x)U + F \tag{6a}$$

$$U(x, 0) = f(x). \tag{6a}$$

Definition: The problem (10) is well-posed if there is a unique solution satisfying

$$||u||^2 \leq k^2 e^{2\alpha t}\left(||f||^2 + \int_0^t ||F||^2 dt\right), \tag{7}$$

where k, α are bounded constants.

As an example, consider

$$U_t + AU_x = BU_{xx}$$

where A, B = constant and symmetric. Fourier transform $\Rightarrow$

$$\hat{P}(i\omega) = -(i\omega A + \omega^2 B),$$

$$\hat{U}_t = \hat{P}(i\omega)\hat{U}, \;\; \hat{U}(0) = \hat{f}, \;\; \Rightarrow \hat{U} = e^{\hat{P}(i\omega)t}\hat{f}$$

<u>Theorem</u> (6) is well-posed if there are constants k, α such that

$$|e^{\hat{P}(i\omega)t}| \leq ke^{\alpha t}. \tag{8}$$

Proof:

$$||U||^2 = \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} |\hat{U}|^2 \leq \max(|e^{\hat{P}(i\omega)t}|^2) \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} |\hat{f}|^2 \leq k^2 e^{2\alpha t} ||f||^2.$$

Definition: The Petrovski condition is satisfied if the eigenvalues $\lambda(\omega)$ of $\hat{P}(i\omega)$ satisfy

$$\mathrm{Re}(\lambda(\omega)) \leq \alpha. \tag{9}$$

α = constant, independent of ω, $\alpha = 0$ if no zero order terms.

Theorem: The Petrovski condition is necessary for well-posedness. It is sufficient if there is a constant K and matrix T such that $T^{-1}\hat{P}T$ = diagonal and $||T^{-1}||||T|| \leq K$ for all ω.

Proof: The Petrovski condition leads to the estimate (8).

Periodic difference approximations

$$\frac{d}{dt}U_j = QU_j + F_j \tag{10a}$$

$$U_j(0) = f_j \tag{10b}$$

where U_j, F_j, f_j are vectors and Q is a matrix.

<u>Definiition:</u> The Petrovski condition is satisfied if the eigenvalues of the symbol $\hat{Q}(\xi)$ satisfy

$$\mathrm{Re}(\lambda(\xi, h)) \leq \alpha, \tag{11}$$

where $|\xi| = |\omega h| < \pi$.

Theorem: The problem (10) is stable in the semi-discrete sense if (11) is valid and $\hat{Q}$ can be diagonalized using a similarity transform with a bounded condition number.

Note similarity with PDE, the proofs are the same.

As an example, consider the heat equation.

$$\frac{d}{dt}U_j = QU_j = \frac{U_{j+1} - 2U_j + U_{j-1}}{h^2}$$
$$U_j = f_j.$$

Expand in Fourier-series

$$U_j = \frac{1}{\sqrt{2\pi}} \sum_{-\infty}^{\infty} \hat{U}_\omega e^{i\omega x_j}.$$

The problem separates into

$$\frac{d}{dt}\hat{U}_\omega = \hat{Q}\hat{U}_\omega \qquad \hat{U}_w = \hat{f}_\omega \qquad \Rightarrow \hat{U}_\omega = e^{\hat{Q}t}\hat{f}_\omega.$$

$\therefore$ Exactly as in continuous case.

Let $\omega h = \xi$. We have $Q = D_+D_- \Rightarrow$

$$\begin{aligned} Qe^{i\omega x_j} &= \frac{e^{i\omega x_{j+1}} - 2e^{i\omega x_j} + e^{i\omega x_{j-1}}}{h^2} \\ &= e^{i\omega x_j}\frac{(e^{i\xi} - 2 + e^{-i\xi})}{h^2} = e^{i\omega x_j}\frac{(e^{i\xi/2} - e^{-i\xi/2})}{h^2} \\ &= e^{i\omega x_j}\left(-4\frac{\sin{(\xi/2)}^2}{h^2}\right) = e^{i\omega x_j}\hat{Q}. \end{aligned}$$

- The Von Neumann condition on the time-step comes from the specific time-advancement scheme.
- The Petrovski, eigenvalue condition is more general, and fundamental.

Example of Von Neumann condition using Euler forward:

$$\begin{aligned} \hat{U}^{n+1} &= (1 + \Delta t \hat{Q})\hat{U}^n \\ &= \tilde{\hat{Q}}\hat{U}^n \end{aligned}$$

$$|\tilde{\hat{Q}}| \leq 1, \Rightarrow \quad \text{condition on time-step.}$$

Summary of theory for initial value problems

The continuous/semi-discrete problem is well-posed/stable if

- The Petrovski (Von Neumann) condition is satisfied.
- $\hat{Q} = T\Lambda T^{-1}$ can be diagonalized and $\|T^{-1}\|\|T\| \leq K$.

$\therefore$ Stability in semi-discrete form $\approx$ well-posedness for PDE.

Exercises/Seminars

- Discuss the difference between the Petrovski and Von Neumann condition.
- Discuss the use of energy-methods for periodic problems.
- Prove that the two bullets on previous slide lead to well-posedness and stability.
- Prove that no positive real parts in eigenvalues of A if $A + A^* \geq 0$.