Numerical Solution of Initial Boundary Value Problems

Jan Nordström
Division of Computational Mathematics
Department of Mathematics

Linköping University

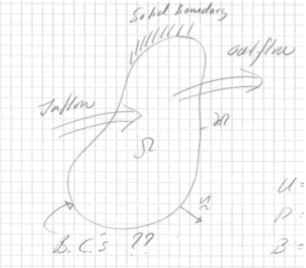
General structure and overview

- Relate the PDE to the numerical approximation.
- Semi-discrete approximation in space, time continuous.
- 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 $A + A^T$?
- Summation-by-parts and weak boundary conditions.
- ~~Multi-block, finite volume + discontinuous Galerkin techniques.~~
- The nonlinear incompressible Navier-Stokes equations.
- The coupling of different types of PDE's.

Additional read-up

- 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.

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 (10) 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.

Why is (iii) important? Consider the perturbed problem

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

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

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

(12)-(10) $\Rightarrow W = V - U$, P = linear operator.

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

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

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

Apply (iii) 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).

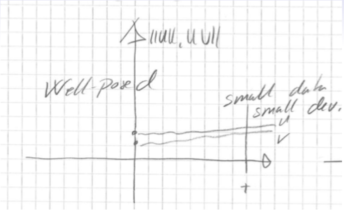


Figure: A good numerical approximation possible. Choice of numerical method next step.

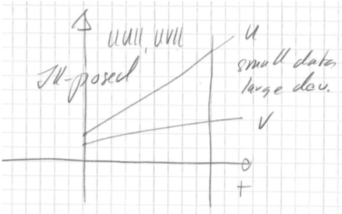


Figure: A good numerical approximation NOT possible. Modify the problem (in practice change boundary conditions).

Examples:

Existence

$$u_x = 0 \qquad u = constant$$
$$u(0) = a$$
$$u(1) = b \qquad a \neq b \Rightarrow \text{too many b.c.'s !}$$

Uniqueness

$$u_{xx} = 0 \qquad u = c_1 + c_2 x$$
$$u(0) = a \qquad u = a + c_2 x \quad \Rightarrow \text{too few b.c.'s !}$$

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.!

Boundary conditions

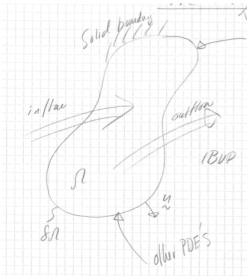


Figure: Where? How many? What form?

$$U_t + P(U, \frac{\partial}{\partial x})U = F(x,t), \quad x \in \Omega,\ t \geq 0$$

$$LU = g(x,t) \quad x \in \delta\Omega,\ t \geq 0$$

$$u = f(x) \quad x \in \Omega,\ t = 0$$

IBVPs "Roughly Speaking"

$$P + (L) \to \tilde{P}, \quad F + (g) \to \tilde{F}$$
$$\Rightarrow$$

$$U_t + \tilde{P}U = \tilde{F}$$
$$U(x,0) = f$$

$\tilde{P}$ = generalized operator, $\tilde{F}$ = generalized data.

Eigenvalue analysis, associate $\tilde{P}$ with a matrix:

$$\tilde{P} = X(\Lambda^R + i\Lambda^I)X^{-1}$$

- Hyperbolic: $\Lambda^R \approx 0$ (Euler, Maxwell, Wave propagation)
- Parabolic: $\Lambda^R > 0$ (damping, heat, diffusion)
- Incompletely Parabolic: $\Lambda^R \geq 0$ (N-S, mixed systems)
- Well-posed: $|\Lambda^R| < \infty$

Conflicting demands on the boundary operator

- (i) Must choose L such that $P + L = \tilde{P}$ = bounded operator.
- (ii) Must choose L such that we have data $LU - g = 0$.

$\rightarrow$ (i) and (ii) often in conflict $\leftarrow$

$$Ex: \quad U = U_\infty, \quad U_x = 0, \quad \alpha U + \beta U_x = \alpha U_\infty$$

Figure: Examples of boundary conditions that could be chosen.

Definitions and concepts

$$\begin{aligned} u_t &= Pu + F, \;\; 0 \le x \le 1, \; t \ge 0 \\ Bu &= g \;\; x = 0, 1 \\ u &= f \;\; 0 \le x \le 1 \end{aligned} \tag{1}$$

Define scalar products and norms

$$(u, v) = \int_0^1 u^* H v dx, \quad \|u\|^2 = (u, u)$$

where $H(x)$ positive definite Hermitian matrix.

Definition: Let V be space of differentiable functions satisfying the homogeneous boundary condition $Bu = 0$. The differential operator P is semi-bounded if for all u in V

$$(u, Pu) \le \alpha \|u\|^2, \;\; \alpha = const.$$

If a solution exists, semi-boundedness guarantees well-posedness since

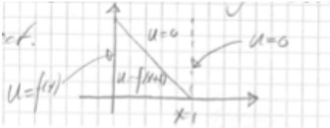
$$\frac{d}{dt}\|u\|^2 = 2(u, u_t) = 2(u, Pu) \leq 2\alpha\|u\|^2$$

Existence?

$$u_t = u_x, \;\; 0 \leq x \leq 1, \, t \geq 0$$
$$u(0,t) = u(1,t) = 0$$
$$u(x,0) = f, \;\; 0 \leq x \leq 1$$

$$2(u, Pu) = u^2|_0^1 = 0, \;\; \therefore \text{ P is a semi-bounded operator}$$

However, the boundary condition at $x = 0$ is not correct since $u = f(x+t)$ if $x + t \leq 1$ and zero otherwise.



$\therefore$ No existence, we must restrict semi-boundedness.

Definition: P is maximally semi-bounded if it is semi-bounded in V but not in any space with less number of boundary conditions.

In our example V is too "small" for allowing existence, must be made "bigger" by dropping b.c. at $x = 0$.

$V = \{u(x), u(0) = 0, u(1) = 0\} \Rightarrow (u, Pu) = 0, V$ "too small".

$V = \{u(x), u(1) = 0\} \Rightarrow (u, Pu) = -\frac{u(0)^2}{2} \leq 0, V$ "perfect".

$V = \{u(x)\} \Rightarrow (u, Pu) = \frac{u(1)^2}{2} - \frac{u(0)^2}{2}, V$ "too large".

Definition: The IBVP (1) is well-posed if for $F = g = 0$, a unique (i) solution exists (ii) satisfying

$$\|u\|^2 \leq k^2 e^{2\alpha t} \|f\|^2 \qquad \text{(iii)}$$

K, α are constants independent of the data f.

Definition: The IBVP (12) is strongly well-posed if a unique (i) solution exists (ii) satisfying

$$\|u\|_I^2 \leq k^2 e^{2\alpha t} \left(\|f\|_I^2 + \int_0^t \left[\|F\|_I^2 + \|g\|_{II}^2 \right] d\tau \right) \qquad \text{(iii)}$$

k, α are constants independent of the data F, f, g.

Note that different norms exist in (iii).

Boundary conditions

Where? How many? Of what form?

$$u_t + au_x = 0; \;\; 0 \le x \le 1; \;\; t \ge 0$$

1. Physical intuition

"Information comes from left." $a > 0$ b. at $x = 0$.
"Information comes form right." $a < 0$ b.c. at $x = 1$.

2. The energy-method

$$\frac{d}{dt}\|u\|^2 = au^2_{x=0} - au^2_{x=1}$$

$a > 0 \Rightarrow$ growth term removed/limited by b.c. at $x = 0$.
$a < 0 \Rightarrow$ growth term removed/limited by b.c. at $x = 1$.

3. Laplace/Normal mode theory (not in this course).

$$u_t = \epsilon u_{xx}, \;\; 0 \leq x \leq 1, \;\; t \geq 0$$

1. Physical intuition
"heat everywhere?" $\Rightarrow$ b.c. at $x = 0, 1$.

2. The energy method

$$\frac{d}{dt}||u||^2 + 2\epsilon||u_x||^2 = 2\epsilon u u_x \mid_0^1 = \epsilon \begin{bmatrix} u \\ u_x \end{bmatrix}^T \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{\lambda=\pm 1} \begin{bmatrix} u \\ u_x \end{bmatrix} \Bigg|_0^1$$

Always one negative eigenvalue, always one growth term at each boundary. $\Rightarrow$ b.c. at $x = 0, 1$.

$$u_t + Au_x = 0, \;\; 0 \le x \le 1, \;\; t \ge 0, \;\; A = \begin{bmatrix} 1 & \alpha \\ \alpha & 1 \end{bmatrix}.$$

1. Physical intuition ?

2. The energy method

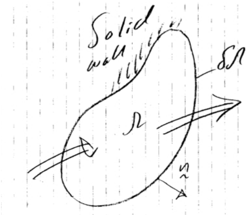
$$\frac{d}{dt}\|u\|^2 = u^T A u\Big|_1^0 = (X^T u)^T \Lambda (X^T u)\Big|_1^0$$

$$A = X\Lambda X^T, \;\; \Lambda = \begin{bmatrix} 1+\alpha & 0 \\ 0 & 1-\alpha \end{bmatrix}, \;\; X = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\begin{aligned} x = 0 \quad & (i) \;\; \alpha < -1 \;\; \Rightarrow \;\; 1 \text{ pos. eig.} \;\; \Rightarrow \;\; 1 \text{ b.c.} \\ & (ii) \;\; -1 < \alpha < 1 \;\; \Rightarrow \;\; 2 \text{ pos. eig.} \;\; \Rightarrow \;\; 2 \text{ b.c.} \\ & (iii) \;\; 1 < \alpha \;\; \Rightarrow \;\; 1 \text{ pos. eig.} \;\; \Rightarrow \;\; 1 \text{ b.c.} \end{aligned}$$

Minimal nr for maximal semi-boundedness and uniqueness !

The energy-method for choice of boundary conditions



A general conservation law in two dimensions can be written

$$u_t + (\underbrace{Au}_{F^I})_x + (\underbrace{Bu}_{G^I})_y = \epsilon \left[\underbrace{(C_{11}u_x + C_{12}u_y)}_{F^V}{}_x + \underbrace{(C_{21}u_x + C_{22}u_y)}_{G^V}{}_y \right].$$

$$u_t + (F^I)_x + (G^I)_y = \epsilon(F^V_x + G^V_y)$$

The matrices A, B, C_{ij} are assumed constant and symmetric.

Energy

$$\underbrace{\int_\Omega u^T u_t d\Omega}_{\frac{1}{2}\|u\|_t^2} + \underbrace{\int_\Omega u^T F_x^I + u^T G_y^V d\Omega}_{\frac{1}{2}(u^T A u)_x + \frac{1}{2}\left(u^T B u\right)_y} = \epsilon \underbrace{\int_\Omega u^T F_x^V + u^T G_y^V d\Omega}_{(u^T F^V)_x + (u^T G^V)_y - (u_x^T F^V + u_y^T G^V)}$$

Green - Gauss $\Rightarrow$

$$\|u\|_t^2 + \underbrace{\oint_{\partial\Omega} u^T A u dy - u^T B u dx = \oint_{\partial\Omega} (u^T F^V) dy - (u^T G^V) dx =}_{\text{Boundary Terms = BT}}$$

$$\underbrace{-2\epsilon \int_\Omega u_x^T F^V + u_y^T G^V d\Omega}_{\text{Dissipation = DI}}.$$

$$\mathrm{DI} = -2\epsilon \int_\Omega \begin{bmatrix} u_x \\ u_y \end{bmatrix}^T \underbrace{\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}}_{\text{must be} \geq 0} \begin{bmatrix} u_x \\ u_y \end{bmatrix} d\Omega \leq 0$$

$$\begin{aligned} \mathrm{BT} = &- \oint u^T (A dx - B dx) u - 2\epsilon u^T (F^V dy - G^V dx) = \\ &- \oint u^T \tilde{A} u - 2\epsilon u^T \left[\tilde{C}_x u_x + \tilde{C}_y u_y \right] ds \end{aligned}$$

$$\tilde{A} = (A, B) \cdot \vec{n}, \quad \tilde{C}_x = (C_{11}, C_{21}) \cdot \vec{n}, \quad \tilde{C}_y = (C_{12}, C_{22}) \cdot \vec{n}$$

Boundary Conditions? Where? How many? What form?

$$\mathrm{BT} = -\oint \begin{bmatrix} u \\ \epsilon u_x \\ \epsilon u_y \end{bmatrix}^T \begin{bmatrix} \tilde{A} & \tilde{C}_x & \tilde{C}_y \\ \tilde{C}_x & 0 & 0 \\ \tilde{C}_y & 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ \epsilon u_x \\ \epsilon u_y \end{bmatrix} ds =$$

$$= -\oint \begin{bmatrix} W+ \\ W^0 \\ W^- \end{bmatrix}^T \begin{bmatrix} \Lambda^+ & 0 & 0 \\ & \Lambda^0 & 0 \\ 0 & 0 & \Lambda^- \end{bmatrix} \begin{bmatrix} W^+ \\ W^0 \\ W^- \end{bmatrix} ds.$$

- Number of boundary conditions = Number of negative entries in Λ^-.
- Where? On all points on boundary where negative eigenvalues exist.
- Form of boundary conditions? $W^- = RW^+ + g$ for a choice of R that leads to a bound. See JNO.

Summary of well-posedness for IBVP

- A maximally semi-bounded differential operator leads to well-posedness for homogeneous boundary conditions ($g = 0$) and non-zero initial data f and forcing function F.

- Strong well-posedness with ($g \neq 0$) require further analysis. Use the procedure in JNO (or Normal mode analysis).

- The choice of boundary conditions (choice of matrix R) is the crucial part in general.
- For the Euler and Navier-Stokes also problematic to integrate by parts. Splitting, change of variables and a particular choice of norm is probably necessary.

Semi-discrete approximations of IBVPs

$$\begin{aligned} \frac{d}{dt}u_j &= Qu_j + F_j, \quad j = 0 \ldots N \\ B_h u &= g \\ u_j(0) &= f_j, \quad j = 0 \ldots N \end{aligned} \tag{2}$$

$B_h u = g$ contains a complete set of boundary conditions, both for the IBVP and purely numerical ones.

The number of bondary conditions is equal to the number of linearly independent conditions. (No problem with existence).

The discrete scalar product and norm typically have the form

$$(u, v)_h = \sum_{j=1}^{N+1} \langle u_j, \tilde{H}_j v_j \rangle h, \quad \|u\|^2 = (u, u)_h$$

where $\tilde{H}_j$ positive definite symmetric matrix.

Definitions and concepts

Definition: Let V_h be the space of grid-vector functions u that satisfies $B_h u = 0$. The difference operator Q is semi-bounded if for all $u \in V_h$

$$(u, Qu) \le \alpha \|u\|_h^2$$

holds. α = bounded constant independent of V_h, h.

Definition: The problem (2) is stable for $F = g = 0$ if

$$\|u\|_h \le k e^{\alpha t} \|f\|_h$$

holds. k, α are constants independent of f, h.

Theorem: If Q is semi-bounded, then (2) is stable.

Note 1: No problem with existence and number of boundary conditions and maximal semi-boundedness.

Definition: The problem (2) is strongly stable if

$$\|u\|_h^2 \le k^2 e^{2\alpha t}\left(\|f\|_h^2 + \int_0^t \left(\|F\|_h^2 + \|g\|_B^2\right) d\tau\right). \quad (3)$$

k, α are bounded constants independent of F, f, g, h.

Why is (3) important?
The numerical error $e_j(t) = u_j(t) - u(x_j, t)$ satisfies

$$\begin{aligned} \frac{d}{dt} e_j &= Q e_j + \mathcal{O}(h^p), \quad j = 0 \ldots N \\ B_h e &= \mathcal{O}(h^q) \\ e_j(0) &= \mathcal{O}(h^r), \quad j = 0 \ldots N \end{aligned} \quad (4)$$

Now, apply (3) to (4) $\Rightarrow$

$$\|e\|_h^2 \le k^2 e^{2\alpha t}\left(\|\mathcal{O}(h^r)\|_h^2 + \int_0^t \left(\|\mathcal{O}(h^p)\|_h^2 + \|\mathcal{O}(h^q)\|_B^2\right) d\tau\right) \le \mathcal{O}(h^{min(p,q,r)}).$$

Definition: The problem (2) is time-stable or strictly-stable if the corresponding estimate for (1) with $F = g = 0$ has the estimate

$$||u|| \leq k_c e^{\alpha_c t} ||f||$$

and the estimate of (2) with $F = g = 0$ is

$$||u||_h \leq k_d e^{\alpha_d t} ||f||_h$$

where $\alpha_d \leq \alpha_c + O(h)$.

Not only the solution but also the time growth converges.

Example:

$$\frac{d}{dt}u_j = D_o u_j, \;\; j = 0 \ldots N$$
$$u_{-1} = 2u_0 - u_1, \quad u_{N+1} = 0$$
$$u_j(0) = f_j, \;\; j = 0 \ldots N$$

The linear extrapolation at $j = 0$ give a one-sided approximation

$$(u_0)_t = (u_1 - u_0)/h.$$

Define a <u>new</u> scalar product:

$$(u, v)_h = \delta h u_0 v_0 + \sum_{j=1}^{N} u_j v_j h = u^T P v, \quad P = h\text{diag}(\delta, 1, 1, \ldots 1)$$
$$(u, Qu) = \delta u_0(u_1 - u_0) + u_1(u_1 - u_0)/2 \ldots = -\delta u_0^2 + u_0 u_1(\delta - 1/2)$$

The choice $\delta = 1/2 \Rightarrow (u, Qu) = -\delta u_0^2, \;\; \therefore \underline{Q = \text{ semi-bounded!}}$

Example:

Consider the Cauchy ($u(\pm\infty, t) = 0$) problem for

$$u_t + a u_x = 0, \quad a = a(x,t).$$

The energy method gives

$$\frac{d}{dt}\|u\|^2 = \int_{-\infty}^{\infty} a_x u^2 dx \leq |a_x|_\infty \|u\|^2.$$

$\therefore a\frac{\partial}{\partial x}$ is a semi-bounded operator for a well-posed problem.

A naive discretization using central difference operators yields $u_t + AQu = 0$ and

$$\frac{d}{dt}\|u\|_h^2 = -u^T(AQ + (AQ)^T)u \neq \int_{-\infty}^{\infty} a_x u^2 dx.$$

The skew-symmetry $Q + Q^T = 0$ does not help.

Go back to PDE

$$au_x = \alpha(au)_x + \beta au_x + \gamma a_x u = (\alpha + \beta)au_x + (\alpha + \gamma)a_x u$$

implies $\beta = 1 - \alpha, \gamma = -\alpha$.

The energy method again following the "advice" above leads to

$$\frac{1}{2}\frac{d}{dt}\|u\|^2 + \alpha u(au)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}(1 - 2\alpha)auu_x dx = \int_{-\infty}^{\infty} \alpha a_x u^2 dx.$$

The choice $\alpha = 1/2$ leads to

$$\frac{d}{dt}\|u\|^2 = \int_{-\infty}^{\infty} a_x u^2 dx,$$

which we of knew already. What about the semi-discrete case ?

Semi-discrete again (not so naive this time)

$$U_t + \frac{1}{2}Q(AU) + \frac{1}{2}AQU - \frac{1}{2}A_x U = 0.$$

The energy method yields

$$\begin{aligned} 2U^T U_t \Delta x &= -U^T(QA + AQ)U\Delta x + U^T A_x U \Delta x \\ &= \left[(QU)^T(AU) - (AU)^T(QU)\right]\Delta x + U^T A_x U \Delta x \\ &= U^T A_x U \Delta x. \end{aligned}$$

$$\left(\|U\|_h^2\right)_t = U^T A_x U \Delta x \leq \delta \|U\|_h^2 \to \int_{-\infty}^{\infty} a_x u^2 dx$$

$\therefore$ The approximation is semi-bounded..

$\therefore$ Convergence to the PDE result. (J. Nordström JSC 2006).

$\therefore$ The same technique must be used for nonlinear problems.

The relation between well-posedness and stability

Comparision		
Continuous		Semi-discrete
$U_t = PU$		$U_t = QU$
$LU = g$		$BU = g$
$U = f$		$U = f$
	Semi-boundness	
$\frac{1}{2}\|\|U\|\|_t^2$		$\frac{1}{2}(\|\|U\|\|_h)_t$
$= (U, PU)$		$=(U, QU)$
$\leq \alpha_c \|\|U\|\|^2$		$\leq \alpha_d \|\|U\|\|_h^2$
	Well-posedness and Stability	
$\|\|U\|\| \leq e^{\alpha_c t}\|\|f\|\|$		$\|\|U\|\|_h \leq e^{\alpha_d t}\|\|f\|\|_h$
	Time/Strict-Stability	
	$\alpha_c \leq \alpha_d + O(h)$	

End of Lecture 1