

TOPICS IN COMPUTATIONAL MECHANICS

MEK4250

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Abstract

In this document we consider the different topics in computational mechanics covered in the course MEK4250. A lot of emphasis is put on showing the well-posedness of the various variational and finite element formulations of the problems. Error estimation methods are given for the various problems. This document is hopelessly void of any mathematical rigour.

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Chapter 1

Weak Formulation And Finite Element Error Estimation

Problem. Formulate a finite element method for the Poisson problem with a variable coefficient $\kappa: \Omega \rightarrow \mathbb{R}^{d \times d}$. Show that the Lax–Milgram theorem is satisfied. Consider extensions to e.g. the convection-diffusion and the elasticity equation. Derive *a priori* error estimates for the finite element method in the energy norm. Describe how to perform an estimation of convergence rates.

1.1 Finite Element Formulation

The Poisson problem is formulated as:

$$-\nabla \cdot (\kappa \nabla u) = f \text{ in } \Omega, \tag{1.1}$$

$$u = u_0 \text{ on } \Gamma_D, \tag{1.2}$$

$$-\kappa \nabla u \cdot n = g \text{ on } \Gamma_N. \tag{1.3}$$

Here u denotes the unknown field. We associate to this strong formulation of the problem, the bilinear operator $a: \hat{V} \times V \rightarrow \mathbb{R}$, and the linear operator $L: \hat{V} \rightarrow \mathbb{R}$ as

follows:

$$a(u, v) := \langle -\nabla \cdot (\kappa \nabla u), v \rangle, \quad (1.4)$$

$$L(v) := \langle f, v \rangle. \quad (1.5)$$

Weak Formulation

We can therefore consider instead the *weak formulation* of the Poisson problem, which is: Find $u \in V$ such that

$$a(u, v) = L(v) \text{ for all } v \in \hat{V}. \quad (1.6)$$

We need to place some requirements to the spaces V and \hat{V} in order to satisfy the boundary conditions. However, one requirement we impose immediately is that $v = 0$ on Γ_D for all $v \in \hat{V}$. What these spaces should be is not immediate from the current formulation. Throughout the following, $\langle \cdot, \cdot \rangle$ denotes the L^2 inner product on V . Expanding a using among others the Gauss–Green lemma yields:

$$a(u, v) = \langle -\nabla \cdot (\kappa \nabla u), v \rangle = -\langle \kappa \Delta u, v \rangle \quad (1.7)$$

$$= \langle \kappa \nabla u, \nabla v \rangle - \int_{\partial\Omega} -v\kappa \frac{\partial u}{\partial x} \cdot n \, dS. \quad (1.8)$$

The boundary integral above can be rewritten using the partitioning of the boundary:

$$\int_{\partial\Omega} -v\kappa \frac{\partial u}{\partial x} \cdot n \, dS = - \int_{\Gamma_D} v\kappa \frac{\partial u}{\partial x} \cdot n \, dS + \int_{\Gamma_N} -v\kappa \frac{\partial u}{\partial x} \cdot n \, dS. \quad (1.9)$$

Applying the boundary conditions over respective boundaries and condition on \hat{V} we get in total that:

$$a(u, v) = \langle \kappa \nabla u, \nabla v \rangle - \int_{\Gamma_N} gv \, dS. \quad (1.10)$$

Since the boundary term in a is independent of u we decide to transfer this term to L :

$$a(u, v) = \langle \kappa \nabla u, \nabla v \rangle, \quad L(v) = \langle f, v \rangle + \int_{\Gamma_N} gv \, dS. \quad (1.11)$$

We now have what we need to determine the spaces \hat{V} and V . Note that we in the weak form only require u and v to be once differentiable. Furthermore, we require u to reduce to u_0 on Γ_D by the boundary conditions, while we need v to vanish identically at Γ_D . We therefore decide on the test and trial spaces

$$V = H_g^1(\Omega) := \{u \in H^1(\Omega) : u = g \text{ on } \Gamma_D\} \subseteq H^1(\Omega), \quad (1.12)$$

$$\hat{V} = H_0^1(\Omega) := \{u \in H^1(\Omega) : u = 0 \text{ on } \Gamma_D\} \subseteq H^1(\Omega). \quad (1.13)$$

Finite Element Formulation

In order to compute with these spaces, we need to introduce a basis. However, the spaces might be infinite dimensional, so we approximate by finite subspaces \hat{V}_h and V_h respectively¹. Since we have $\hat{V} \subseteq V$ we have $\hat{V}_h \subseteq V_h$, and we therefore use the same basis vectors for both test and trial functions. We seek a solution $u = \sum_i c_i \varphi_i$ such that

$$\sum_{i=1}^N c_i a(\varphi_i, \varphi_j) = L(\varphi_j) \text{ for } j = 1, \dots, M \quad (1.14)$$

where N, M denotes the dimensions of V_h, \hat{V}_h respectively. This determines a linear system

$$\mathbf{A}\mathbf{c} = \mathbf{b} \quad (1.15)$$

where the matrix entries are determined as follows:

$$A_{i,j} = a(\varphi_i, \varphi_j), \quad b_j = L(\varphi_j). \quad (1.16)$$

1.2 Well Posedness of Weak Formulation

In this section we discuss whether the problem in its weak formulation is in fact well posed. Does there exist a solution, and if it does, is this solution unique? The Lax–Milgram theorem provides sufficient conditions for this problem to be well posed, and hence the solution to exist and be unique. We verify the three properties in turn:

¹Much of the finite element theory amounts to determining what the error in this specific approximation is.

Boundedness of a : Let $u, v \in H^1(\Omega)$. Then we have

$$a(u, v) = \langle \kappa \nabla u, \nabla v \rangle \underset{\text{Using the Cauchy-Schwartz inequality}}{\leq} \overbrace{\|\kappa\|}^{\text{subordinate matrix norm}} \|\nabla u\|_0 \|\nabla v\|_0 = \|\kappa\| \|u\|_1 \|v\|_1 \quad (1.17)$$

This is close to proving boundedness of a , however, I do not know how to deal with the $\|\kappa\|$. However, for $\kappa = 1$ this proves the claim.

Coercivity of a : Let $u \in H^1(\Omega)$ and consider the following:

$$\|u\|_1^2 \stackrel{\text{def}}{=} \|u\|_0^2 + \|\nabla u\|_0^2 \underset{\text{Using the Poincaré inequality on } H_0^1(\Omega)}{\geq} (C^2 + 1) \|\nabla u\|_0^2 \quad (1.18)$$

This shows that $a(u, u) (C^2 + 1)^{-1} \|u\|_1^2$ in the case where $\kappa = 1$ identically.

Boundedness of L :

$$L(v) = \langle f, v \rangle + \int_{\Gamma_N} g v \, dS \quad (1.19)$$

Using Cauchy-Schwartz on both terms yields

$$\leq \|f\|_0 \|v\|_0 + \|g\|_{L^2(\Gamma_N)} \|v\|_{L^2(\Gamma_N)}; \quad (1.20)$$

Using the fact that v is defined on the entirety of Ω , the L^2 norm is certainly larger over the whole domain

$$\leq \|f\|_0 \|v\|_0 + \|g\|_{L^2(\Gamma_N)} \|v\|_0; \quad (1.21)$$

Using that the H^1 norm greater than or equal to the L^2 norm

$$\leq (\|f\|_0 + \|g\|_{L^2(\Gamma_N)}) \|v\|_1, \quad (1.22)$$

$$= D \|v\|_1. \quad (1.23)$$

This proves the boundedness of L .

This means that the weak formulation of the Poisson problem satisfies the Lax-Milgram theorem, hence is well posed. In addition, the solution u satisfies

$$\|u\|_1 \leq \frac{(C^2 + 1)^{-1}}{\|\kappa\|} \|f\|_{-1}. \quad (1.24)$$

1.3 Extensions to Other Problems

Recall that the equation of linear elasticity is given as

$$-2\mu(\nabla \cdot \varepsilon(u)) - \lambda \nabla(\nabla \cdot u) = 0 \quad (1.25)$$

where $\varepsilon(u) := (\nabla u + (\nabla u)^T)/2$ is the strain tensor. Ignoring the second term, first term is supposedly a Poisson-equation². However, in order to check whether we can apply the results found for the abstract Poisson-problem we need to determine what the $\nabla(\nabla \cdot u)$ in the second term is. The Helmholtz decomposition theorem states that any u in $L^2(\Omega)$ can be decomposed into a curl-free part ψ and a divergence-free part φ :

$$u = \psi + \varphi \quad (1.26)$$

where $\nabla \cdot \varphi = 0$ and $\nabla \times \psi = 0$. In the light of this, we can consider the two special cases where either φ or ψ are zero.

- (i) Assume that $\varphi = 0$. This means that $u = \psi$ consists only of the divergence free part. We then have that $\nabla(\nabla \cdot u) = 0$. Consequently, the second term vanishes in Equation (1.25).
- (ii) Assume that $\psi = 0$, i.e., u consists only of the curl free part. Then using the identity

$$\Delta u = \nabla(\nabla \cdot u) - \nabla \times (\nabla \times u) \quad (1.27)$$

we see that $u = \nabla(\nabla \cdot u)$. Hence, Equation (1.25) reduces to a Poisson problem.

In these two special cases, we have that the linear elasticity problem reduces to a Poisson problem of the form

$$-(\mu + \lambda) \Delta w = f. \quad (1.28)$$

for some source term f .

²This needs to be verified.

1.4 A Priori Error Estimates

In the following, we work over arbitrary test and trial spaces V , as these estimates are general.

Energy Norm

We now discuss some a priori estimates. Recall that any arbitrary inner product induces a norm by

$$\|x\| := \sqrt{\langle x, x \rangle}. \quad (1.29)$$

It turns out that the bilinear form a may, or may not, constitute an inner product. If it does, then we may talk about the norm induced by this bilinear form. We call this the *energy norm*. We first need to verify that a does indeed constitute an inner product. The only condition that is not trivial is the coercivity, however we already proved this for the Lax–Milgram theorem. We therefore define the energy norm

$$\|u\|_E := \sqrt{a(u, u)}. \quad (1.30)$$

Consider now the error $e := u - u_h$. Let $v \in \hat{V}$ be arbitrary. In the energy norm, we have

$$\|e\|_E^2 = a(e, e) = a(e, u - u_h) = a(e, u - v + v - u_h) \quad (1.31)$$

$$= a(e, u - v) + a(e, \underbrace{u_h - v}_{\in \hat{V}}) = a(e, u - v). \quad (1.32)$$

Using the Cauchy–Schwartz inequality, we have that

$$\|e\|_E^2 \leq \|e\|_E \|u - v\|_E \implies \|e\|_E \leq \|e - v\|_E \quad (1.33)$$

for all $v \in \hat{V}$. This does however not give any sharp bounds, so it is hard to quantify exactly what magnitude the error has. We can however combine this result with an interpolation error estimate:

$$\|e\|_E \leq \|u - \pi_{q,h}u\|_E \leq C(q) \|h^{q+1} D^{q+1}u\|. \quad (1.34)$$

Here, $\pi_{q,h}u$ denotes the q -th order interpolant to u , and h is the maximum mesh size.

Error estimate without coercivity of a

The symmetry of a is quite a strong requirement, and this is not always satisfied. In this section, we do *not* assume that a is symmetric. In the cases where a is bounded however we can consider the error in the vector space norm as follows. Let $v \in \hat{V}$ be arbitrary. Then using the coercivity of a we have:

$$\|e\|_V^2 \leq \frac{1}{\alpha} a(e, e) = \frac{1}{\alpha} a(e, u - v + v - u_h) \quad (1.35)$$

$$= \frac{1}{\alpha} a(e, u - v) \underbrace{\leq}_{\text{Using boundedness of } a} \frac{D}{\alpha} \|e\|_V \|u - v\|_V. \quad (1.36)$$

Dividing by $\|e\|_V$ and combining with an interpolation error estimate, as we did above,

$$\|e\|_V \leq \frac{DC(q)}{\alpha} \|h^{q+1} D^{q+1} u\|. \quad (1.37)$$

1.5 Error Approximation

In the following we assume we solve a constructed problem with known solution. Let N denote the number of basis elements over the domain. Then we can consider the error as a function of N . Using degree p elements over a mesh with maximal mesh size of h . Let u denote the analytic solution, and u_N the computed solution with N basis elements. Denote by e_N the error in the corresponding approximation. We wish to approximate the convergence rate β in the following:

$$\|e\|_V \leq \|h^\beta D^\beta u\|. \quad (1.38)$$

We can rewrite this as a linear equation in h with slope β and constant term $\log(D^\beta u)$. Computing e_N for various N we can find a linear regression line through the data and approximate β .

Chapter 2

Discretization Of Convection-Diffusion

Problem. Derive a proper variational formulation of the convection-diffusion problem. Derive sufficient conditions that make the problem well posed. Discuss why oscillations appear for standard Galerkin methods and show how Stream-line diffusion / Petrov–Galerkin methods resolve these problems. Discuss also approximation properties in light of Cea's lemma.

2.1 Finite Element Formulation

The convection diffusion problem is given as:

$$-\mu \Delta u + \omega \cdot \nabla u = f \text{ in } \Omega, \quad (2.1)$$

$$u = g \text{ on } \Gamma_D. \quad (2.2)$$

Here u is the unknown, μ is the diffusivity, and ω is a velocity. We associate to this problem the bilinear operator $a: V \times \hat{V} \rightarrow \mathbb{R}$ and the linear operator $L: \hat{V} \rightarrow \mathbb{R}$ given

by

$$a(u, v) := \langle -\mu \Delta u, v \rangle + \langle \omega \cdot \nabla u, v \rangle; \quad (2.3)$$

$$L(v) := \langle f, v \rangle. \quad (2.4)$$

Weak Formulation

We can now consider the *weak formulation* of the Convection-Diffusion problem. That is: Find u in V such that:

$$a(u, v) = L(v) \text{ for all } v \in \hat{V}. \quad (2.5)$$

Again, we need to later properly determine the spaces V and \hat{V} , however, as always, we require $v = 0$ on Γ_D for all $v \in \hat{V}$. In order to get rid of the Laplacian term, we employ the Gauss–Green lemma, yielding:

$$a(u, v) = \langle \mu \nabla u, \nabla v \rangle - \underbrace{\int_{\Gamma_D} \mu \frac{\partial u}{\partial x} v \cdot n \, dS}_{\text{This is zero due to } v \in \hat{V}} + \langle \omega \cdot \nabla u, v \rangle \quad (2.6)$$

$$= \langle \mu \nabla u, \nabla v \rangle + \langle \omega \cdot \nabla u, v \rangle. \quad (2.7)$$

We again only require one derivative for u and v so we let

$$V = H_g^1(\Omega) \subseteq H^1(\Omega), \quad (2.8)$$

$$\hat{V} = H_0^1(\Omega) \subseteq H^1(\Omega), \quad (2.9)$$

as in the Poisson problem. We delay the finite element formulation until after the Streamline diffusion / Petrov–Galerkin method has been discussed.

We now need to verify that this abstract problem is well posed.

2.2 Well Posedness of Weak Formulation

While our problem is not *homogeneous* in the Dirichlet conditions, we can reduce it to a homogeneous problem. The reason for doing this is to employ the Poincaré

inequality, which only holds for $H_0^1(\Omega)$. Again, the Lax–Milgram theorem gives sufficient conditions for the problem being well posed. We have two cases for this specific problem: (i) Incompressible flow, $\nabla \cdot \omega = 0$; or (ii) compressible flow, $\nabla \cdot \omega \neq 0$. We deal with these two cases separately. Furthermore, for simplicity, we define

$$b(u, v) := \langle \mu \nabla u, \nabla v \rangle, \quad (2.10)$$

$$c_\omega(u, v) := \langle \omega \cdot \nabla u, v \rangle, \quad (2.11)$$

and note that $a(u, v) = b(u, v) + c_\omega(u, v)$.

Incompressible Flow

For the incompressible case, we have $\nabla \cdot \omega = 0$. In addition to this assumption, we also assume that the flow velocities are bounded, i.e., $D_\omega := \|\omega\|_\infty < \infty$. It can then be shown that the bilinear form $c_\omega(u, v)$ is *skew-symmetric*, that is

$$c_\omega(u, v) = -c_\omega(v, u). \quad (2.12)$$

We now show that the conditions in the Lax–Milgram theorem is satisfied.

Coercivity of a : Using the skew-symmetric property of $c_\omega(u, v)$, we get that $c_\omega(u, u) = -c_\omega(u, u)$ which implies that $c_\omega(u, u) = 0$. Therefore, we have

$$a(u, u) = b(u, u) + c_\omega(u, u) = b(u, u). \quad (2.13)$$

So, a is coercive, as

$$b(u, u) = \mu \int_{\Omega} (\nabla u)^2 d\Omega \geq \mu \left(\int_{\Omega} \nabla u d\Omega \right)^2 = \mu |u|_1^2. \quad (2.14)$$

Boundedness of a : Applying the Cauchy–Schwartz inequality we have

$$a(u, v) = \langle \mu \nabla u, \nabla v \rangle + \langle \omega \cdot \nabla u, v \rangle \quad (2.15)$$

$$\leq |\mu| \|\nabla u\|_0 \|\nabla v\|_0 + \|\omega \cdot \nabla u\|_0 \|v\|_0 \quad (2.16)$$

Using the assumption of bounded flow velocities; and that the problem has been reduced to homogeneous Dirichlet conditions — so we can apply the Poincaré inequality with domain dependent factor C_Ω — we get:

$$\leq |\mu| \|u\|_1 \|v\|_1 + D_\omega \|u\|_1 \|v\|_1 \quad (2.17)$$

$$\leq (\mu + D_\omega C_\Omega) \|u\|_1 \|v\|_1. \quad (2.18)$$

Consequently, a is bounded.

Boundedness of L : Applying the Cauchy–Schwartz inequality we get

$$L(u, v) = \langle f, v \rangle \leq \|f\|_0 \|v\|_0 \leq \|f\|_1 \|v\|_1. \quad (2.19)$$

The Lax–Milgram conditions are satisfied, hence the weak formulation of the convection-diffusion problem is well posed. In addition, the solution u satisfies

$$\|u\|_1 \leq \frac{\mu + D_\omega C_\Omega}{\mu} \|f\|_{-1}. \quad (2.20)$$

Compressible Flow

In the case where the flow is compressible, i.e., $\nabla \cdot \omega \neq 0$, we need to put some extra restrictions on the flow velocities ω in order to ensure well posedness. This is because in the general case, we have $c_\omega(u, u) \neq 0$. The coercivity of a was the only property where we assumed incompressibility, hence the two other properties remain the same.

Coercivity of a with compressible fluids: If $D_\omega C_\Omega \leq B\mu$ where $B < 1$ we obtain

$$a(u, u) = \langle \mu \nabla u, \nabla u \rangle + \langle \omega \cdot \nabla u, u \rangle \quad (2.21)$$

$$\geq \mu(1 - D_\omega) \|u\|_1^2, \quad (2.22)$$

however, it is not clear to me exactly how this result is obtained.

2.3 Oscillations in the Solution

Assume for now we are working with the one dimensional convection diffusion problem on a mesh with h denoting the largest mesh element. Solving this with first order Lagrangian elements corresponds to the central finite difference scheme

$$-\frac{\mu}{h^2}[u_{i+1} - 2u_i + u_{i-1}] - \frac{\omega}{2h}[u_{i+1} - u_{i-1}] = 0 \quad (2.23)$$

for $i = 1, \dots, N-1$, where N denotes the number of elements. Assume the boundary conditions are $u_0 = 0$ and $u_N = 1$. Examining the above expression we see that in the limit $\mu \rightarrow 0$ that the scheme reduces to

$$\frac{\omega}{2h}[u_{i+1} - u_{i-1}] = 0 \quad (2.24)$$

for $i = 1, \dots, N$ with $u_0 = 0$ and $u_N = 1$. Here we see that u_{i+1} is coupled to u_{i-1} but not u_i . This means that we may get a numerical solution consisting of two sequences $(u_{2i})_i$ and $(u_{2i+1})_i$ that have no relation to each other. This may very well cause oscillations in the solution.

Finite Difference Upwinding

One remedy is to introduce the concept of *upwinding*. Instead of using a central finite difference scheme as above, one employs either a forward or a backward first order scheme, based on the velocity ω . That is:

$$u'(x_i) \approx \frac{1}{h}[u_{i+1} - u_i] \text{ if } \omega < 0, \quad (2.25)$$

$$u'(x_i) \approx \frac{1}{h}[u_i - u_{i-1}] \text{ if } \omega > 0. \quad (2.26)$$

This upwinding scheme can be seen as a special case of *artificial diffusion*, where one solves the “artificial” problem

$$-(\mu + \varepsilon) \Delta u + \omega \cdot \nabla u = f, \quad (2.27)$$

with $\varepsilon > 0$ some arbitrary real number. In particular, choosing $\varepsilon = h/2$ one regains the upwinding scheme mentioned above.

The fact that the finite element method coincides with the finite difference method in the case of one dimensional convection diffusion, and first order Lagrangian elements is not something that holds in general. Our question in the following is then: How do we implement artificial diffusion in our finite element method? This leads us to the Streamline diffusion / Petrov–Galerkin methods.

2.4 Streamline Diffusion / Petrov–Galerkin

Our goal here is to add artificial in a consistent way that does not changes the solution as h tends to zero. It turns out that naively adding artificial diffusion to our current finite element formulation does not give us what we want. We first examine why.

Naive Artificial Diffusion

Recall that our problem reads: Find $u \in V$ such that

$$\langle \mu \nabla u, \nabla v \rangle + \langle \omega \cdot \nabla u, v \rangle = \langle f, v \rangle \text{ for all } v \in \hat{V}. \quad (2.28)$$

Replacing μ by $\mu + \varepsilon$ yields a new bilinear operator \tilde{a} :

$$\tilde{a}(u, v) := \langle \mu \nabla u, \nabla v \rangle + \langle \varepsilon \nabla u, \nabla v \rangle + \langle \omega \cdot \nabla u, v \rangle. \quad (2.29)$$

This can be written succinctly as

$$\tilde{a}(u, v) = a(u, v) + \varepsilon \langle \nabla u, \nabla v \rangle. \quad (2.30)$$

If we let $\varepsilon = h/2$ we see that in the limit as $h \rightarrow 0$, we have $\tilde{a}(u, v) \rightarrow a(u, v)$, and the scheme is consistent in this sense. However, it is not *strongly consistent* as it does not satisfy the Galerkin-orthogonality as a does:

$$a(u - u_h, v) = 0 \text{ for all } v \in \hat{V}_h, \quad (2.31)$$

namely that this equation is zero for *all* discretizations, and not just in the limit.

We can however make the scheme strongly consistent by employing different spaces for the test functions and the trial functions.

Petrov–Galerkin method

The only difference between the Petrov–Galerkin and the standard Galerkin formulation is that the trial and test functions differ. In the standard Galerkin method, the same basis is used for both test and trial functions. In the Petrov-Galerkin method the test functions are tailored to ensure a strongly consistent scheme.

Finite Element Formulation

Letting \hat{V}_h and V_h denote the finite dimensional subspaces of \hat{V} and V respectively. Assume these are given by bases $(\psi_j)_{j=1}^M$ and $(\varphi_i)_{i=1}^N$. The finite element formulation then gives rise to a linear system

$$\mathbf{A}\mathbf{c} = \mathbf{b}, \quad (2.32)$$

where the matrix elements are given as

$$A_{i,j} = \langle \mu \nabla \varphi_i, \nabla \psi_j \rangle + \langle \omega \cdot \nabla \varphi_i, \psi_j \rangle, \quad (2.33)$$

$$b_j = \langle f, \psi_j \rangle. \quad (2.34)$$

How do we choose the basis $(\psi_j)_{j=1}^M$ such that we can add diffusion consistently? It turns out that setting

$$\psi_j := \varphi_j + \varepsilon \omega \cdot \nabla \varphi_j \quad (2.35)$$

does the trick.