

NTNU

PROJECT

Least Squares Finite Element Method

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Abstract

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The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Notation

CONVENTION	we let subscript h denote the discretized variables
u	Solution of the pde
$\mathbf{w} = [w_1 \ w_2]$	Negative gradient of u
$\mathbf{u} = [\mathbf{w} \ u]^T$	Solution to the first order transformation
R_g	Lifting function
$\tilde{\mathbf{u}} = \mathbf{u} - R_g$	Solution to the first order transformation minus the lifting function
\mathbf{b}	Two dimensional vector field
f	loading function
$\mathbf{f} = (0, 0, f)$	loading function for the first order transformation
\mathcal{L}, \mathcal{B}	Linear operators
(\cdot, \cdot)	Inner product
$a(\cdot, \cdot)$	Bilinear form obtained from standard galerkin approach
$Q(\cdot, \cdot)$	Bilinear form obtained from the least squares approach
$\mathring{a}(\cdot, \cdot)$	Bilinear form obtained from the combined GLS-method
$F(\cdot)$	Linear form obtained from the least squares approach
$\tilde{F}(\cdot)$	Linear form obtained from the least squares approach including BC's
$\mathring{F}(\cdot)$	Linear form obtained from the combined GLS-method
$\mathcal{F}(\cdot, \cdot)$	non-linear functional
\mathcal{J}	Jacobian of \mathcal{F}
Linear Algebra	A good idea to denote matrices with an underscore ?
A	The stiffness matrix
G	The gradient matrix
F	The vector obtained from the linear functional F
B_1	The diagonal matrix with the first component of b evaluated in each node
B_2	The diagonal matrix with the second component of b evaluated in each node

F	The diagonal matrix with the loading function evaluated in each node
W	The diagonal matrix with the GLL-weights
L	The matrix with the derivative of the lagrange functions evaluated in each node
Φ	$W \otimes WL$
Ψ	$WL \otimes W$

Chapter 1

Theory

1.1 Informal introduction to least-squares

The least-squares finite element method is a numerical method with similarities to mixed Galerkin. However it has a fundamentally different approach regarding the definition of the bilinear functional. Let us look at a system of first order differential equations on the form

$$Au = f \text{ in } \Omega \quad (1.1)$$

$$u = g \text{ on } \partial\Omega. \quad (1.2)$$

Where A is a partial differential operator defined as

$$A = \sum_{i=1}^n A_i \frac{\partial}{\partial x_i} + A_0. \quad (1.3)$$

n being the number of dimensions of the domain Ω . If u happens to be a vector function of say k dimensions then A_i will be a matrix with k columns and k or more rows. Let us initially assume without loss of generality that $g = 0$. Further we require $f \in L_2(\Omega)$ and choose $V = \{v \in L_2(\Omega) | v = 0 \text{ on } \partial\Omega\}$. A residual is defined

$$R(v) = Av - f, \quad (1.4)$$

and a functional

$$J(v) = \frac{1}{2} \|R(v)\|_0^2. \quad (1.5)$$

The solution u and its gradient needs to be in L^2 for the functional to make sense, hence u is restricted to the space $H_0^1(\Omega)$. The homogeneous boundary condition is now baked into the definition of the search space. By minimizing J we obtain

$$\lim_{t \rightarrow 0} \frac{d}{dt} J(u + tv) = \int_{\Omega} (Av)^T (Au - f) d\Omega = 0, \quad \forall v \in V. \quad (1.6)$$

We can now write a variational formulation of the least-squares method: Find $u \in V$ such that

$$Q(u, v) = F(v), \quad \forall v \in V, \quad (1.7)$$

where

$$Q(u, v) = (Au, Av), \quad (1.8)$$

$$F(v) = (f, Av). \quad (1.9)$$

Notice that the bilinear form Q is symmetric, this is an important advantage least-squares has over regular Galerkin methods. The bilinear form that surged from a first-order problem by the least-squares leads us to a variational formulation similar to the one obtained from a second order problem by regular FEM. Generally the bilinear form from least-squares will correspond to a bilinear form of a problem of twice the order obtained using FEM. **Bold statement?** In order to avoid problems of large complexity a higher order PDE should therefore be transformed to a system of first order PDE's (similar to a mixed Galerkin approach) before defining the least squares functional. [1]

1.2 Formal formulation of least-squares

Let us look at a general boundary value problem where $f \in Y(\Omega)$, $g \in B(\partial\Omega)$, $\mathcal{B}: X(\partial\Omega) \rightarrow B(\partial\Omega)$ and $\mathcal{L}: X(\Omega) \rightarrow Y(\Omega)$. Find $u \in X(\Omega)$ such that

$$\mathcal{L}u = f \quad \text{in } \Omega \quad (1.10)$$

$$\mathcal{B}u = g \quad \text{on } \partial\Omega. \quad (1.11)$$

Whenever this BVP has a unique solution, a least-squares functional can be defined as

$$J(u; f, g) = \|\mathcal{L}u - f\|_Y^2 + \|\mathcal{B}u - g\|_B^2 \quad (1.12)$$

and the corresponding minimization problem is then given as

$$\min_{u \in X} J(u; f, g) \quad (1.13)$$

For any well-posed problem $\exists \alpha, \beta > 0$ such that

$$\alpha \|u\|_X^2 \leq J(u; 0, 0) = (\mathcal{L}u, \mathcal{L}u)_Y + (\mathcal{B}u, \mathcal{B}u)_B \leq \beta \|u\|_X^2. \quad (1.14)$$

The fact that our functional is norm-equivalent is of crucial importance to a successful LS-method. It is therefore important that the spaces X, Y and B is chosen such that the LS-functional defines a norm is equivalent to $\|\cdot\|_X$. **Need to show this ?** Minimizing this functional is equivalent to solving the Euler-Lagrange equations formulated as

$$\text{find } u \in X \text{ such that } Q(u, v) = F(v) \quad \forall v \in X \quad (1.15)$$

Where $Q(u, v)$ and $F(v)$ are defined as

$$Q(u, v) = (\mathcal{L}u, \mathcal{L}v)_Y + (\mathcal{B}u, \mathcal{B}v)_B, \quad (1.16)$$

$$F(v) = (f, \mathcal{L}v)_Y + (g, \mathcal{B}v)_B. \quad (1.17)$$

Notice that $Q(u, v)$ defines an inner product and $Q(u, u)^{1/2} = J(u; 0, 0)^{1/2}$ defines the corresponding norm.

In order to solve this numerically we define the function spaces X^h, Y^h and B^h and the corresponding variational formulation is then written as

$$\text{find } u^h \in X^h \text{ such that } Q(u^h, v^h) = F(v^h) \quad \forall v^h \in X^h. \quad (1.18)$$

[2]

1.2.1 Error analysis

Let u be the analytical solution of a problem of the type (1.11), u^h is our numerical solution to (1.18) and u_\perp^h is the orthogonal projection of u in X_h .

$$Q(u - u^h, u - u^h) = Q(u - u^h, u - u_\perp^h) + Q(u - u^h, u_\perp^h - u^h) \quad (1.19)$$

$$= Q(u - u^h, u - u_\perp^h) \quad (1.20)$$

$$\leq \beta \|u - u^h\|_{X_h} \|u - u_\perp^h\|_{X_h}. \quad (1.21)$$

The first equality is due to adding and subtracting u_\perp^h , because both u^h and u_\perp^h solves the variational formulation we can cancel the last term, and by using the norm-equivalency from (1.14) and Schwartz inequality we get the last expression. Now by applying the first inequality of (1.14) we end up with

$$\|u - u^h\|_{X_h} \leq \frac{\beta}{\alpha} \|u - u_\perp^h\|_{X_h} = \min_{w^h \in X_h} \frac{\beta}{\alpha} \|u - w^h\|_{X_h}. \quad (1.22)$$

Hence we can show that the Least squares method provides a convergence result of similar order as the Finite element method. **Add the convergence result of spectral methods**

1.3 Example - Poisson problem

The Poisson problem is defined as

$$-\Delta u = f \text{ in } \Omega \quad (1.23)$$

$$u = g \text{ on } \partial\Omega \quad (1.24)$$

Let us first consider the homogeneous case. The straight forward least-squares approach is to define $\mathbf{w} = -\nabla u$ and solve the system of equations

$$\mathbf{w} + \nabla u = 0 \text{ in } \Omega \quad (1.25)$$

$$\nabla \cdot \mathbf{w} = f \text{ in } \Omega \quad (1.26)$$

$$u = 0 \text{ on } \partial\Omega. \quad (1.27)$$

which can be written in the same form as (1.11) with $\mathbf{u} = \mathbf{w} \oplus u$, $\mathbf{f} = (0, 0, f)$, $g = 0$, $\mathcal{B} = (0, 0, 1)^T$ and \mathcal{L} given as

$$\mathcal{L} = \begin{bmatrix} 1 & 0 & \frac{\partial}{\partial x} \\ 0 & 1 & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & 0 \end{bmatrix} \quad (1.28)$$

We define the search space $X = H^1(\Omega; \text{div}) \times H_0^1(\Omega)$ and the solution space $Y \times B = [L^2(\Omega)]^3 \times L^2(\Omega)$ and the functional can then be defined as in (1.12). The variational formulation of the problem can be stated. Find $\mathbf{u} \in X$ such that

$$Q(\mathbf{u}, \mathbf{v}) = F(\mathbf{v}) \quad \forall \mathbf{v} \in X. \quad (1.29)$$

We require that $\mathbf{f} \in Y$. Should I state the numerical variational formulation instead??

Notice that the spaces X and Y chosen as described above fulfill the condition (1.14).

1.4 Example - Diffusion convection reaction problem

The diffusion convection problem to be analyzed is given as

$$-\mu \Delta u + \mathbf{b} \cdot \nabla u + \sigma u = f \text{ in } \Omega \quad (1.30)$$

$$u = g \text{ on } \partial\Omega \quad (1.31)$$

where $\mathbf{b} = [b_1, b_2]$ is a vector field, and σ is some reaction constant. By following the same approach as for the Poisson problem we end up with \mathcal{L} on the form

$$\mathcal{L} = \begin{bmatrix} 1 & 0 & \frac{\partial}{\partial x} \\ 0 & 1 & \frac{\partial}{\partial y} \\ \mu \frac{\partial}{\partial x} - b_1 & \mu \frac{\partial}{\partial y} - b_2 & \sigma \end{bmatrix} \quad (1.32)$$

which leads to a similar but slightly different linear system than the one created by the Poisson problem.

1.5 Boundary conditions

1.5.1 non-homogeneous Dirichlet boundary conditions

If $g \neq 0$ then we simply define a lifting function $R_g \in X$ such that $R_g(\partial\Omega) = g(\partial\Omega)$. By defining $\tilde{\mathbf{u}} = \mathbf{u} - R_g$ we can replace \mathbf{u} in the variation formulation and get

$$Q(\tilde{\mathbf{u}} + R_g, \mathbf{v}) = F(\mathbf{v}) \quad (1.33)$$

$$Q(\tilde{\mathbf{u}}, \mathbf{v}) + Q(R_g, \mathbf{v}) = F(\mathbf{v}) \quad (1.34)$$

$$Q(\tilde{\mathbf{u}}, \mathbf{v}) = F(\mathbf{v}) - Q(R_g, \mathbf{v}) \quad (1.35)$$

$$Q(\tilde{\mathbf{u}}, \mathbf{v}) = \tilde{F}(\mathbf{v}) \quad (1.36)$$

1.5.2 non-homogeneous Neumann boundary conditions

Because of the geometry of our problem and the fact that we define the flux as an extra variable we can transform the Neumann conditions to a Dirichlet condition on the flux.

$$\frac{\partial u}{\partial \mathbf{n}} = h \text{ on } \partial\Omega \quad (1.37)$$

$$\nabla u \cdot \mathbf{n} = h \quad (1.38)$$

$$\mathbf{w} \cdot \mathbf{n} = -h. \quad (1.39)$$

Let us define \hat{x} and \hat{y} as the unit vectors in each direction. Notice that for the west ($x = 0$) and east ($x = 1$) edges the normal vector $\mathbf{n} = \pm\hat{x}$, and at the north ($y = 1$) and south ($y = 0$) edges $\mathbf{n} = \pm\hat{y}$. This way we can write the Neumann conditions as a

Dirichlet condition on the first and second component of $\mathbf{w} = [w_1 \ w_2]$.

$$w_1 = \pm h \text{ for } y = 0 \text{ and } y = 1 \quad (1.40)$$

$$w_2 = \pm h \text{ for } x = 0 \text{ and } x = 1 \quad (1.41)$$

Chapter 2

New Theory

2.1 Using least-squares method to gain stability

With regular Galerkin approach for the diffusion-transport equation you end up with the variational formulation

$$a(u, v) = (f, v) \quad \forall v \in V. \quad (2.1)$$

where V is some closed subspace of H^1 , and the bilinear functional is given as

$$a(u, v) = \mu \int_{\Omega} \nabla u \cdot \nabla v \, d\Omega + \int_{\Omega} v(b \cdot \nabla u) \, d\Omega \quad (2.2)$$

We can define a new norm from this functional in the following manner

$$a(u, u) = \mu \int_{\Omega} \nabla u \cdot \nabla u \, d\Omega + \int_{\Omega} b \cdot (u \nabla u) \, d\Omega \quad (2.3)$$

$$= \mu \|\nabla u\|_0^2 + \frac{1}{2} \int_{\Omega} b \cdot \nabla u^2 \, d\Omega \quad (2.4)$$

$$= \mu \|\nabla u\|_0^2 - \frac{1}{2} \int_{\Omega} u^2 (\nabla \cdot b) \, d\Omega \quad (2.5)$$

$$(2.6)$$

Where we have used Greens theorem and the assumption that $u = 0$ on the boundary in the last equality. Let us assume that the divergence of our vector field can be bounded within some interval, say $\gamma_0 \leq \frac{1}{2} \nabla \cdot b \leq \gamma_1$, we can now make a lower and upper bound

for the bilinear form

$$\mu\|\nabla u\|_0^2 - \gamma_1\|u\|_0^2 \leq a(u, u) \leq \mu\|\nabla u\|_0^2 - \gamma_0\|u\|_0^2 \quad (2.7)$$

should I change signs in the equation??

It is clear that for small μ and large positive γ_1 the bilinear form is no longer coercive and thus our convergence requirements are no longer valid. Standard Galerkin method is therefore not a suited way to solve this type of problem.

Now remember from equation (1.14) that the least squares formulation guarantees us a coercive bilinear form, given that the BVP has a solution and that the search- and solution space are chosen correctly. For this particular problem we can find α, β such that $\alpha\|u\|_1^2 \leq Q(\mathbf{u}, \mathbf{u}) \leq \beta\|u\|_1^2$. Now, let us define $\mathring{a}(\cdot, \cdot)$ and $\mathring{f}(\cdot)$ as the as the linear combinations of the linear and bilinear form surging from standard Galerkin and least-squares method.

$$\mathring{a}(u, v) = a(u, v) + \delta Q(\mathbf{u}, \mathbf{v}) \quad (2.8)$$

$$\mathring{f}(v) = (f, v) + \delta F(\mathbf{v}) \quad (2.9)$$

Let us study the coerciveness of the bilinear form $\mathring{a}(\cdot, \cdot)$

$$\mathring{a}(u, u) \geq \mu\|\nabla u\|_0^2 + \gamma_0\|u\|_0^2 + \delta\alpha\|u\|_1^2 \quad (2.10)$$

$$\geq \mu\|\nabla u\|_0^2 + \gamma_0\|u\|_0^2 + \delta\alpha\|u\|_0^2 \quad (2.11)$$

$$\geq \mu\|\nabla u\|_0^2 + \mu\|u\|_0^2 \quad (2.12)$$

$$= \mu\|u\|_1^2 \quad (2.13)$$

Don't like the way Q has to be defined with \mathbf{u} In the third inequality we make the assumption that $\gamma_0 + \delta\alpha \geq \mu$ in other words δ , (the amount of smoothing from LS) has to be chosen such that $\delta \geq (\mu - \gamma_0)/\alpha$. Using (1.17) with homogeneous boundary conditions we obtain the identities $Q(\mathbf{u}, \mathbf{u}) = (\mathcal{L}\mathbf{u}, \mathcal{L}\mathbf{u})$ and $F(\mathbf{u}) = (\mathbf{f}, \mathcal{L}\mathbf{u})$ we can derive the following stability result for our discrete solution of the variational formulation,

$$\mathring{a}(u_h, u_h)_h \leq C \|f\|^2 \quad (2.14)$$

The proof for a similar method can be found in [3] Ch.12.

Need to fix this Proof, not OK !! Proof:

$$\mathring{a}(u_h, u_h) = \mathring{f}(u_h) \quad (2.15)$$

$$= (f, u_h) + \delta(\mathbf{f}, \mathcal{L}\mathbf{u}_h) \quad (2.16)$$

$$\leq \|f\| \|u_h\| + \delta \|\mathbf{f}\| \|\mathcal{L}\mathbf{u}_h\| \quad (2.17)$$

$$\leq \|f\|^2 + \frac{1}{4} \|u_h\|^2 + \delta \|\mathbf{f}\|^2 + \frac{\delta}{4} \|\mathcal{L}\mathbf{u}_h\|^2 \quad (2.18)$$

$$= \|f\|^2 + \delta \|f\|^2 + \frac{1}{4} \mathring{a}(u_h, u_h). \quad (2.19)$$

Which Allows us to determine the constant $C = \frac{4}{3}(1 + \delta)$

2.1.1 estimation of the constant α

By performing the proof of the Poincaré inequality from [3] for our domain $\Omega = (0, 1)^2$ we end up with showing that $|v|_1 \leq \sqrt{2/3} \|v\|_1 \quad \forall v \in H_0^1$. By using this inequality twice we end up showing for the Poisson problem that

$$\|v\| \geq \frac{2}{3} \|v\|_1, \quad (2.20)$$

Hence $\alpha = \frac{2}{3}$. should find this constant for the difftrans problem

2.2 Nonlinear diffusion transport problem

Now let the vector field \mathbf{b} from the diffusion transport problem be a function of u .

$$-\mu \Delta u + \mathbf{b}(u) \cdot \nabla u = f \text{ in } \Omega \quad (2.21)$$

$$u = g \text{ on } \partial\Omega \quad (2.22)$$

This gives us a nonlinear variational formulation that does not allow us to solve our system of equations directly. In order to find a solution Newtons method was used. An important difference between standard Galerkin and least-squares, is that the linear functional $F(\cdot)$ will also be non-linear in the LS case.

Chapter 3

Implementation

All the implementation has been done in two dimensions on the unit square $(0,1)^2$. The goal of the implementation has been to show the strengths of the least-squares method. It is implemented with finite element and spectral basis functions and is compared to the results from standard Galerkin formulation. Finally the combined GLS-method described in chapter 2 is also tested against the separate methods. The problems solved are simply expansions of the Poisson problem (All problems have been implemented with non-homogeneous Dirichlet boundary conditions).

$$-\Delta u = f \text{ in } \Omega \tag{3.1}$$

Then by adding a transport term you obtain the diffusion transport equation

$$-\mu\Delta u + \mathbf{b} \cdot \nabla u = f \text{ in } \Omega \tag{3.2}$$

This can be further expanded by adding a reaction term

$$-\mu\Delta u + \mathbf{b} \cdot \nabla u + \sigma u = f \text{ in } \Omega \tag{3.3}$$

And as a final complication the vector field \mathbf{b} can be made dependent on u and hence give us the nonlinear diffusion transport reaction equation

$$-\mu\Delta u + \mathbf{b}(u) \cdot \nabla u + \sigma u = f \text{ in } \Omega \tag{3.4}$$

All the equations listed above are transformed into a first order system of PDE's

$$\mathcal{L}\mathbf{u} = \mathbf{f}. \quad (3.5)$$

The partial differential operator \mathcal{L} is the one stated in chapter 1.

3.1 The bilinear form obtained from least-squares

For the general problem (1.11) the functional Q will take the form

$$Q(u, v) = \int_{\Omega} (\mathcal{L}v)^T (\mathcal{L}u) d\Omega. \quad (3.6)$$

Implementing Q requires two sets of basis functions $\{N_i\}$ that describes the search and solution space. In this project assignment the search and solution space will be described by the same set of basis functions which will depend on the method applied. u is discretized as

$$u_h = \sum_{I=0}^K a_I N_I. \quad (3.7)$$

Where K denotes the number of discretization points, which is the same as the number of basis functions. **Is this statement OK?** Since equation (1.15) requires equality for all test functions in the search space we simply solve it for each basis function. We are therefore left with a system of K equations. Equation (3.6) can then be written for each test function as

$$Q(u_h, N_I) = \int_{\Omega} (\mathcal{L}N_I)^T (\mathcal{L}u_h) d\Omega \quad (3.8)$$

$$= \int_{\Omega} (\mathcal{L}N_I)^T (\mathcal{L} \sum_{J=1}^K a_J N_J) d\Omega \quad (3.9)$$

$$= \sum_{J=1}^K \int_{\Omega} (\mathcal{L}N_I)^T (\mathcal{L}a_J N_J) d\Omega \quad (3.10)$$

$$= \sum_{J=1}^K \int_{\Omega} (\mathcal{L}N_I)^T (\mathcal{L}a_J N_J) d\Omega \quad (3.11)$$

$$= \sum_{J=1}^K \int_{\Omega} (\mathcal{L}N_I)^T (\mathcal{L}N_J) d\Omega \cdot a_J. \quad (3.12)$$

The total system of equation for all test functions can then be written as a matrix equation

$$A^{LS} \mathbf{u} = F^{LS}. \quad (3.13)$$

Where $A_{I,J}^{LS} = \int_{\Omega} (\mathcal{L}N_I)^T (\mathcal{L}N_J) d\Omega$. Should somehow show the importance of this formula

Written explicitly for the **Poisson and diffusion transport equation** it will be a 3-by-3 matrix on the form

$$A_{I,J}^{LS} = \int_{\Omega} \begin{bmatrix} N_I N_J + \partial_x N_I \partial_x N_J & \partial_x N_I \partial_y N_J & N_I N_{J,x} \\ \partial_y N_I \partial_x N_J & N_I N_J + \partial_y N_I \partial_y N_J & N_I N_{J,y} \\ N_{I,x} N_J & N_{I,y} N_J & N_{I,x} N_{J,x} + N_{I,y} N_{J,y} \end{bmatrix} d\Omega \quad \text{where}$$

$\partial_x = \partial/\partial x$ for the Poisson problem and $\mu\partial/\partial x - b_1$ for the diffusion transport problem.

Similarly F_I will be given as

$$F_I = \int_{\Omega} (\mathcal{L}N_I)^T \vec{f} d\Omega = \int_{\Omega} \begin{bmatrix} \partial_x N_I \\ \partial_x N_I \\ 0 \end{bmatrix} f d\Omega \quad (3.14)$$

Notice that by doing the splitting of variables we obtain a system of equations three times as big as if we were to solve the equation directly.

3.2 Least squares with finite element basis functions

finite element space X_h^1 ? quadrature...

3.3 Least squares with spectral basis functions

The spectral implementation is done using Gauss Lobatto nodes and quadrature rule. The basis functions are then chosen as the lagrange functions based on the GL nodes. Notice that the discrete solution \mathbf{u}_h consist of the discretization of both u and $\mathbf{w} = -\nabla u$. is it clear what system I am talking of here?? \mathbf{u}_h can be structured block wise or

node wise. By choosing a block wise representation the final system of equations surging from the Poisson problem can be written as

$$\begin{bmatrix} A_{1,1} & A_{1,2} & A_{1,3} \\ A_{2,1} & A_{2,2} & A_{2,3} \\ A_{3,1} & A_{3,2} & A_{3,3} \end{bmatrix} \begin{bmatrix} u^h \\ w_1^h \\ w_2^h \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ 0 \end{bmatrix}.$$

Where each block $A_{m,n}$ corresponds to calculating element m, n in the matrix (3.1) for all combinations of I, J . In order to keep track of the indexing we use the expressions $I = i + jN$ and $J = k + lN$ where the helping indices denotes the position in x, y -coordinates. Let us take a closer look at element $A_{1,3}$ in order to achieve a more compact notation.

$$(A_{1,3})_{I,J} = \int_{\Omega} N_I N_{J,x} d\Omega \quad (3.15)$$

$$= \int_{\Omega} l_i(x) l_j(y) l'_k(x) l_l(y) d\Omega \quad (3.16)$$

$$= \sum_{\alpha} \sum_{\beta} w_{\alpha} w_{\beta} l_i(x_{\alpha}) l_j(y_{\beta}) l'_k(x_{\alpha}) l_l(y_{\beta}). \quad (3.17)$$

The sum is obtained by using Gauss Lobatto quadrature rule. Now notice that the lagrange polynomials $l_j(y_{\beta})$ are non-zero only when $\beta = j$, this implies that for the non-zero terms in the sum we have $\beta = j = l$, and $\alpha = i$. With these considerations the double sum above simplifies to

$$(A_{1,3})_{I,J} = w_i w_j l'_k(x_i) \quad (3.18)$$

Remember that $I = i + jN$ and $J = k + lN$, with N being the number of nodes in each spacial direction. This means that $A_{1,3}$ will consist of blocks where i and k goes from 1 to N while j and l are constant within each block. Since we require that $j = l$ we can immediately conclude that $A_{1,3}$ is nonzero only in the blocks along the diagonal. Notice that the factor $w_i l'_k(x_i)$ is the same for each block, and it can be written in matrix form as WL . With this notation W is the $n \times n$ diagonal matrix with the GLL-weights along the diagonal and L is the matrix containing the derivatives of the lagrange polynomials $(L)_{i,j} = l'_j(x_i)$. Since each block WL is multiplied with w_j the whole matrix can simply be written as the Kronecker tensor product $(W \otimes WL)$. Similar reasoning can be made with all the other block matrices $A_{m,n}$ and we end up with a matrix on the form

$$A^{LS} = \begin{bmatrix} W \otimes (L^T W L + W) & W L \otimes L^T W & W \otimes W L \\ L^T W \otimes W L & (L^T W L + W) \otimes W & W L \otimes W \\ W \otimes L^T W & L^T W \otimes W & L^T W L \otimes W + W \otimes L^T W L \end{bmatrix}$$

Note that without the reformulation of the PDE as a first order system and with regular Galerkin formulation the stiffness matrix will simply be $A_{3,3} = W \otimes L^T W L + L^T W L \otimes W$.

3.4 LS spectral method for Diffusion transport

The matrix corresponding to the discretized variational formulation can be divided into two parts where one depends on μ alone and the other one contains the contributions from the gradient term in the original equation.

$$A^{LS} = \begin{bmatrix} W \otimes (\mu L^T W L + W) & \mu W L \otimes L^T W & W \otimes W L \\ \mu L^T W \otimes W L & (\mu L^T W L + W) \otimes W & W L \otimes W \\ W \otimes L^T W & L^T W \otimes W & L^T W L \otimes W + W \otimes L^T W L \end{bmatrix}$$

In addition it will be added some extra terms dependent on \mathbf{b} to the upper left 2×2 block matrix. Let B_1 and B_2 be diagonal $n^2 \times n^2$ matrices with the values of the first and second component of \mathbf{b} evaluated in each spacial node along the diagonal.

$$G_{1,1} = -\mu B_1(W \otimes W L) - \mu(W \otimes L^T W)B_1 + B_1(W \otimes W)B_1 \quad (3.19)$$

$$G_{1,2} = -\mu B_2(W \otimes W L) - \mu(L^T W \otimes W)B_1 + B_1(W \otimes W)B_2 \quad (3.20)$$

$$G_{2,1} = -\mu B_1(W L \otimes W) - \mu(W \otimes L^T W)B_2 + B_2(W \otimes W)B_1 \quad (3.21)$$

$$G_{2,2} = -\mu B_2(W L \otimes W) - \mu(L^T W \otimes W)B_2 + B_2(W \otimes W)B_2. \quad (3.22)$$

Notice that $G_{2,1} = G_{1,2}^T$, the least-squares formulation always provide a symmetric system of equations. We can now define the total matrix for the diffusion transport problem K^{LS} as

$$K^{LS} = A^{LS} + G^{LS} \quad (3.23)$$

Where G^{LS} is the matrix given as $G^{LS} = \begin{bmatrix} G_{11} & G_{12} & 0 \\ G_{21} & G_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix}$.

Adding the gradient term in our equation also affects the loading function. In a compact notation the discretized loading vector from the variational formulation can be written

as $F^{LS} = \begin{bmatrix} \mu(W \otimes L^T W)F_m - (W \otimes W)B_1 F_m \\ \mu(L^T W \otimes W)F_m - (W \otimes W)B_2 F_m \\ 0 \end{bmatrix}$, where F_m is the vector with the loading function evaluated in each spacial node.

3.5 non-linear diffusion transport problem

The stepwise algorithm to solve the nonlinear equation is described in chapter 2. However there are several computational steps that needs to be taken care of, both with regular Galerkin and least squares. In both cases we obtain two matrices which we will name A and G and with superscript LS if they refer to the least squares formulation. In both cases only G will depend on the numerical solution u_h . An important difference however is that in the LS setting the F vector will depend on u_h while in the straight forward Galerkin setting it will not. For regular Galerkin spectral approach we obtain

$$A\tilde{u} + AR_g + G(\tilde{u} + R_g)(\tilde{u} + R_g) - F = 0 \quad (3.24)$$

Notice that for each iteration the matrix $G(\tilde{u} + R_g)$ needs to be evaluated, the homogeneous boundary conditions on \tilde{u} needs to be imposed and the Jacobian needs to be calculated. The Jacobian \mathcal{F} will for this setting be given as

$$\mathcal{J}_{i,j} = A_{i,j} + G(\tilde{u} + R_g)_{i,j} + (\tilde{u} + R_g)_i \frac{\partial}{\partial \tilde{u}_j} (G(\tilde{u} + R_g))_i. \quad (3.25)$$

With the LS formulation we obtain

$$A^{LS}\tilde{u} + A^{LS}R_g + G^{LS}(\tilde{u} + R_g)(\tilde{u} + R_g) - F^{LS}(\tilde{u} + R_g) = 0 \quad (3.26)$$

$$A^{LS}\tilde{u} + A^{LS}R_g + G^{LS}(\tilde{u} + R_g)\tilde{u} - F^{LS}(\tilde{u} + R_g) = 0 \quad (3.27)$$

It is clear from this equation that the term surging from the loading function also needs to be handled when calculating the Jacobian. The lifting function R_g does only have nonzero values in the third "block", hence it belongs to the kernel of the G -matrix.

$$\mathcal{J}_{i,j} = A_{i,j} + G(\tilde{u} + R_g)_{i,j} + [\frac{\partial}{\partial \tilde{u}_j}(G(\tilde{u} + R_g))_{i,:}] \tilde{u} - \frac{\partial}{\partial \tilde{u}_j} F(\tilde{u} + R_g)_i. \quad (3.28)$$

Let us first consider the F -vector. The terms are given in equation (3.4) and it is clear that only the last terms in each block depends on u , notice that it does not depend on the components of the gradient $[w_1 \ w_2]$. Hence the contribution to the total Jacobi matrix will only be in block $(1, 3)$ and $(2, 3)$. Further since B_1 and B_2 are both diagonal matrices where $B_{i,i}(u) = B_{i,i}(u_i)$ the Jacobian can be calculated efficiently by creating the matrices dB_1 and dB_2 which has the partial derivative of B_1, B_2 wrt. u evaluated in each node.

Chapter 4

Results

4.1 The main differences

Using least squares will always give you a SPD system of equations which can be advantageous. However for second order equations this system is three times as big as if we were to solve it using more standard methods. Comparing the correctness of the solution as done in figure [4.1](#) shows that the convergence rate is the same as for standard methods, but the the value of the residual is slightly higher for the least squares method. This can be explained by the functional that is minimized. Notice that in the least squares methods you minimize the square of the residual. since the correctness of both methods are restricted by the smoothness of the solution and the number of discrete points LS-methods will minimize the residual squared down to a given precision and hence the residual itself to a slightly higher value.

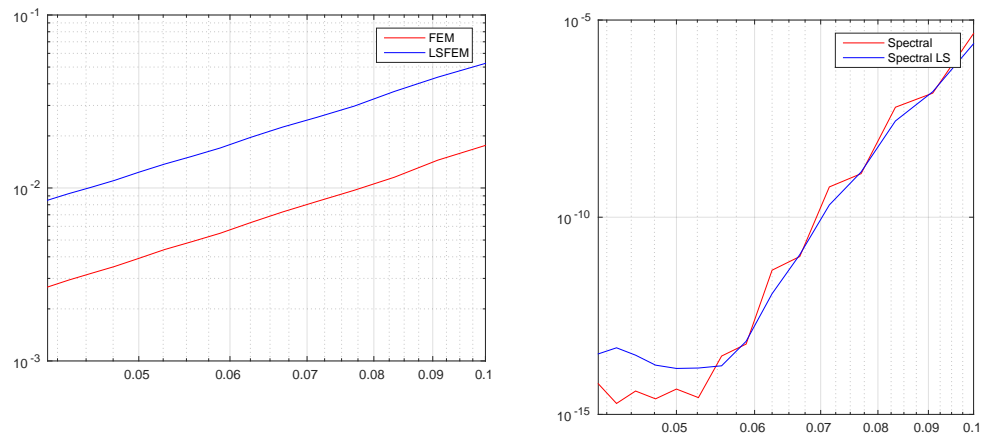


FIGURE 4.1: Convergence of Galerkin and corresponding least-squares formulation on the Poisson problem.

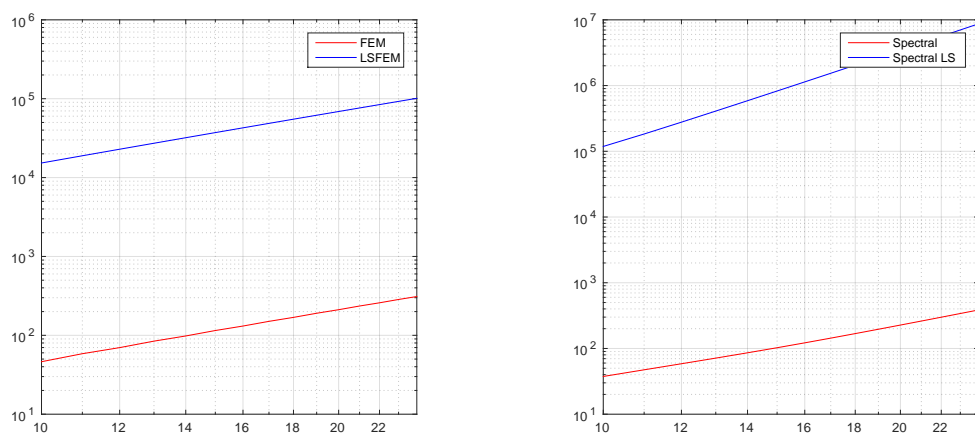


FIGURE 4.2: Condition number of Galerkin and corresponding least-squares formulation on the Poisson problem.

Appendix A

Appendix Title Here

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