Solve 2D Poisson Equation on 3D meshes

Mauricio Cele Lopez Belon

Abstract. Solve 2D Poisson's equation with Dirichlet boundary conditions on a 3D mesh using Finite Element Method (FEM).

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1. Introduction

This follows the method described in [3] and [1].

We aim to solve Poisson's equation

$$-\triangle U(x,y) = F(x,y) \tag{1.1}$$

where

$$\triangle U(x,y) = \nabla \cdot \nabla\, U(x,y) \tag{1.2}$$

with Dirichlet boundary conditions using Finite Element Method (FEM).

In 2D it can be written as:

$$\begin{aligned} -U(x,y)_{xx} - U(x,y)_{yy} &= F(x,y) \quad in\ \Omega \\ U(x,y) &= G(x,y) \quad in\ \partial\Omega \end{aligned}$$

The integral form (notice $\int_\Omega$ is a double integral):

$$-\int_\Omega \triangle U(x,y)\ dA = \int_\Omega F(x,y)\ dA \tag{1.3}$$

2. Weak Form

The weak form comes from the "variational method". Here one tries to get a solution to the PDE by translating it into a minimization problem. That's done by definig an energy function that is a linear functional on a function space Ω. The linear functional is artificial i.e., pure mathematical device to

enable optimization. In consequence, solving the variational problem may require less continuity than that of the actual solution (hence the name WEAK form).

Consider the weight function $\vartheta(x,y)$ (a.k.a. test function) with compact support defined on Ω. The "Galerkin" variational method states that the inner product of $\vartheta(x,y)$ with a residual function $R(x,y)$ should be zero.

$$\int_\Omega \vartheta(x,y)R(x,y)\ dA = 0$$

where $R(x,y)$ is the residual or error of the function i.e.,

$$R(x,y) = -\triangle U(x,y) - F(x,y)$$

The weak form of the PDE is:

$$\begin{aligned}\vartheta(x,y)R(x,y) &= 0\\ \vartheta(x,y)(-\triangle U(x,y) - F(x,y)) &= 0\\ -\vartheta(x,y)\triangle U(x,y) &= F(x,y)\vartheta(x,y)\end{aligned}$$

and the integral (variational) form of the PDE is

$$-\int_\Omega \vartheta(x,y)\triangle U(x,y)\ dA = \int_\Omega F(x,y)\vartheta(x,y)\ dA \tag{2.1}$$

NOTE on inner products: The integral form is more important since integral of the product of two functions $f(x,y)$ and $g(x,y)$ is the "inner product" $\int_\Omega f(x,y)g(x,y)\ dA$. If function $g(x,y)$ is a "test function" then the inner product is way to "measure" the function $f(x,y)$ on location where $g(x,y)$ is defined. Since $g(x,y)$ is not the Dirac Delta function then the measure is an averaged one.

Consider the vector field

$$E(\vec{X}) = \vartheta(\vec{X})\nabla U(\vec{X}) \tag{2.2}$$

Taking $\nabla \cdot E(\vec{X})$ by Green's first identity we get:

$$\begin{aligned}\nabla \cdot E &= \nabla \cdot (\vartheta\ \nabla U)\\ \nabla \cdot E &= \nabla\vartheta \cdot \nabla U + \vartheta \triangle U\end{aligned} \tag{2.3}$$

By applying the Divergence theorem:

$$\int_\Omega \nabla \cdot E\ dA = \int_{\partial\Omega} E \cdot n\ dS \tag{2.4}$$

where $n(\vec{X})$ is the normal to the boundary $\partial\Omega$

Replacing (2.3) on (2.4) we get:

$$\int_\Omega \nabla\vartheta \cdot \nabla U + \vartheta \triangle U\ dA = \int_{\partial\Omega} E \cdot n\ dS$$

By definition of $E(\vec{X}) = \vartheta(\vec{X})\nabla U(\vec{X})$ the RHS becomes:

$$\int_\Omega \nabla\vartheta \cdot \nabla U + \vartheta \triangle U \; dA = \int_{\partial\Omega} \vartheta \nabla U \cdot n \; dS$$
$$= \int_{\partial\Omega} \vartheta \left(\nabla U \cdot n\right) dS \tag{2.5}$$

since test function $\vartheta(\vec{X})$ can be considered "constant" at the boundary.

So we can re-arrange the left-hand-side to get:

$$\int_\Omega \vartheta \triangle U \; dA = \int_{\partial\Omega} \vartheta \left(\nabla U \cdot n\right) \; dS - \int_\Omega \nabla\vartheta \cdot \nabla U \; dA \tag{2.6}$$

Replacing the left-hand-side of our variational form of PDE (2.1) with the above we get:

$$-\int_{\partial\Omega} \vartheta \left(\nabla U \cdot n\right) \; dS + \int_\Omega \nabla\vartheta \cdot \nabla U \; dA = \int_\Omega F \; \vartheta \; dA \tag{2.7}$$

giving the standard weak form:

$$\int_\Omega \nabla\vartheta \cdot \nabla U \; dA = \int_\Omega F \cdot \vartheta \; dA + \int_{\partial\Omega} \vartheta \left(\nabla U \cdot n\right) \; dS \tag{2.8}$$

We now define that all $\vartheta(\vec{X})$ at the boundary $\partial\Omega$ has zero value, which is a necessary condition for the variational problem to converge e.g., test function must have compact support.

$$\vartheta(\vec{X}) = 0 \quad \forall \vec{X} \in \partial\Omega \tag{2.9}$$

So the weak form is now:

$$\int_\Omega \nabla\vartheta \cdot \nabla U \; dA = \int_\Omega F \; \vartheta \; dA \tag{2.10}$$

3. Discretization

The domain Ω has to be meshed in N nodes and T triangles. For linear elements the nodes coincides with mesh vertices (but for quadratic elements there will be nodes defined on the triangle's edge mid-points, so there can be more nodes than vertices).

The first discretisation is easy. We discretize the test functions

$$\vartheta(\vec{X}) = \sum_i \varphi_i(\vec{X}) \tag{3.1}$$

as a linear combination of $\varphi_i(\vec{X})$ over the entire domain Ω. $\varphi_i(\vec{X})$ is a function with compact support defined at every node of Ω to be equal to 1 at center node $\vec{N}_i$, equal to 0 at sorrounding nodes N_j and linear everywhere else inside triangles in triangle-set Ω_i a.k.a., a tent function:

$$\varphi_j(\vec{N}_j) = 1 \quad \forall j = i$$
$$\varphi_j(\vec{N}_j) = 0 \quad \forall j \neq i$$
$$\varphi_j(\vec{X}) = linear \; in \; \Omega_i$$

when restricted to individual triangle, test functions defined at nodes are also known as barycentric coordinates of triangles.

Plugging (3.1) into (2.10) we get a system of integral equations, one equation per triangle-set Ω_i corresponding to the compact support of test function $\varphi_i(\vec{X})$:

$$\int_\Omega \nabla \sum_i \varphi_i \cdot \nabla U \; dA = \int_\Omega F \sum_i \varphi_i \; dA$$
$$\int_\Omega \sum_i \nabla \varphi_i \cdot \nabla U \; dA = \int_\Omega \sum_i F \; \varphi_i \; dA$$
$$\sum_i \int_\Omega \nabla \varphi_i \cdot \nabla U \; dA = \sum_i \int_\Omega F \; \varphi_i \; dA$$

where the integrals are now much smaller i.e., per triangle-set Ω_i around nodes $\vec{N}_i$ or tent function $\varphi_i(\vec{X})$

The second discretization is of solution $U(\vec{X})$. We define the global solution $U(\vec{X})$ to be a finite sum:

$$U(\vec{X}) = \sum_j^N U_j \psi_j(\vec{X}) \tag{3.2}$$

where U_j are coefficients to be determined at each node on entire domain Ω and $\psi_j(\vec{X})$ are the so-called "shape functions" (i.e., interpolation functions) also defined with compact support of triangle-sets Ω_i.

Functions defined on triangle-set Ω_i around node $\vec{N}_i$ to be equal to 1 at center node $\vec{N}_i$, equal to 0 at sorrounding nodes N_j and linear everywhere else at triangles in Ω_i a.k.a., a tent function also known as P1 linear functions.

$$\psi_j(\vec{N}_j) = 1 \quad \forall j = i$$
$$\psi_j(\vec{N}_j) = 0 \quad \forall i \neq j$$
$$\psi_j(\vec{X}) = linear \; in \; \Omega_i$$

when restricted to individual triangles, shape functions are also known as barycentric coordinates of triangles.

At this point we can see $\varphi_i(\vec{X})$ and $\psi_i(\vec{X})$ are the same, but they don't have to be the same. When those that the same the FEM is so-called "Galerkin FEM".

The third discretization is of the gradients $\nabla U(\vec{X})$ and $\nabla \vartheta(\vec{X})$ using (3.2) and (3.1). The grandient of $U(\vec{X})$ is just the linear combination of gradients at the triangle nodes:

$$\nabla U(\vec{X}) = \nabla \left(\sum_i U_i \psi_i(\vec{X}) \right)$$
$$\nabla U(\vec{X}) = \sum_i U_i \nabla \psi_i(\vec{X}) \tag{3.3}$$

where the las equality holds by product rule. The gradient is defined in terms of $\nabla\psi_i(\vec{X})$ and U_i can be treated as a "constant" coefficient that need to be determined at every node. Note that triangles sharing vertices also shares the same U_i coefficient. $\nabla U(\vec{X})$ is a smooth function inside triangles so it gives us a "continuous" gradient at the whole Ω.

The gradient of test functions, is defined in the same manner:

$$\nabla\vartheta(\vec{X}) = \sum_i \nabla\varphi_i(\vec{X}) \tag{3.4}$$

Now we can discretize the inner product $\langle\nabla\vartheta(\vec{X}), \nabla U(\vec{X})\rangle$ which is characteristic of the Laplacian:

$$\begin{aligned}\nabla\vartheta \cdot \nabla U &= \sum_i \nabla\varphi_i \cdot \sum_j U_j \nabla\psi_j \\ &= \sum_{i,j} \nabla\varphi_i \cdot U_j \nabla\psi_j \\ &= \sum_{ij} U_j \left(\nabla\varphi_i \cdot \nabla\psi_j\right)\end{aligned} \tag{3.5}$$

summation inidices run for all connected nodes i and j.

Plugging (3.5) into (2.10) we get a system of linear equations

$$\begin{aligned}\int_\Omega \nabla\vartheta \cdot \nabla U \; dA &= \int_\Omega \sum_{ij} U_j \left(\nabla\varphi_i \cdot \nabla\psi_j\right) \; dA \\ &= \sum_{ij} U_j \int_\Omega \nabla\varphi_i \cdot \nabla\psi_j \; dA\end{aligned}$$

So we get the following system of linear equations:

$$\sum_{ij} U_j \int_\Omega \nabla\varphi_i \cdot \nabla\psi_j \; dA = \sum_i \int_\Omega F \; \varphi_i \; dA \tag{3.6}$$

Which can be written in matrix form as follows. First define a set of "stiffness" matrices M_T^i per triangle of size $N \times N$ defined as:

$$M_T^k(i,j) = \int_T \nabla\varphi_i \cdot \nabla\psi_j \; dA$$

inidices (i,j) run for all nodes of triangle T.

Then the $N \times 1$ boundary conditions vector F_i:

$$F_i = \int_\Omega F \; \varphi_i \; dA$$

The $N \times N$ stiffness matrix M can be assembled as $M = \sum_k M_T^k$ and boundary conditions can be assembled as $F = \sum_i F_i$ to form a global $N \times N$ matrix system (we choose to have shape functions ψ_i equal to test functions φ_i so we have same number of equations than unknowns)

$$MU = F \tag{3.7}$$

4. Assembly

The process of creating the stiffness matrix M is called assembly. It consist of creating the matrix M_k for each triangle T_k and then add it to the global M matrix.

The global matrix M is $N \times N$ where N is number of mesh nodes. In previous section 3 the matrix M_k is a $N \times N$ super-sparse matrix just with a few non-zero entries which corresponds to a single triangle contribution.

$$M = \sum_k M_k \tag{4.1}$$

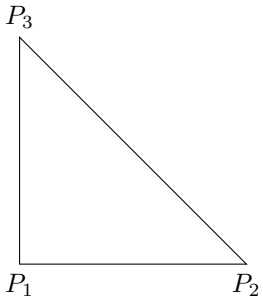
In practice the M_k matrix is not $N \times N$ super-sparse, but a 3×3 matrix (in case of linear triangle elements). There is a map from indices of the 3×3 matrix to the $N \times N$ matrix as follows.

Each triangle's nodes has a global index assigned in the mesh, we also establish a local indexing of triangle like 1, 2 and 3. We define a trivial bijective map between global and local indices.

5. Reference Elements

One of the novelties of FEM is to be able to compute the integrals per individual elements on an easy and generic way by using so called Reference Elements.

For triangle elements we just need a single reference triangle



$$P_1 = (0, 0)$$
$$P_2 = (1, 0)$$
$$P_3 = (0, 1)$$

The P1 (linear) 2D Lagrange shape functions $\psi(u, v)$ has the form

$$\psi(u, v) = Au + Bu + C$$

For the reference trignale defined above the $\psi(u, v)$ takes the simple form:

$$\begin{aligned}\psi_1(u, v) &= 1 - u - v \\ \psi_2(u, v) &= u \\ \psi_3(u, v) &= v\end{aligned}$$

We can check that $\psi_i \cdot \psi_j = \delta_{ij}$

$$\begin{aligned}&\psi_1(P_1) = 1 \quad \psi_1(P_2) = 0 \quad \psi_1(P_3) = 0 \\ &\psi_2(P_1) = 0 \quad \psi_2(P_2) = 1 \quad \psi_2(P_3) = 0 \\ &\psi_3(P_1) = 0 \quad \psi_3(P_2) = 0 \quad \psi_3(P_3) = 1\end{aligned}$$

We define a function $F(\vec{U})$, a.k.a., *pushforward*, that maps reference 2D triangle to "physical" 2D triangle on the mesh (the inverse $F^{-1}(\vec{X})$, a.k.a., *pullback*, maps triangle from physical to reference frame).

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}$$

Which cab be expressed in vector form

$$\begin{aligned}F(\vec{U}) &= B\vec{U} + \vec{X}_1 \\ F^{-1}(\vec{X}) &= B^{-1}(\vec{X} - \vec{X}_1)\end{aligned}$$

We denote ψ_i^k the function ψ_i defined on physical triangle K.

$$\begin{aligned}\psi_i^k(\vec{X}) &= \psi_i \circ F^{-1}(\vec{X}) \\ \psi_i^k(\vec{X}) &= \psi_i(F^{-1}(\vec{X}))\end{aligned}$$

The gradient of $\psi_i^k(\vec{X})$ in physical triangle is:

$$\begin{aligned}\nabla_{\vec{X}} \psi_i^k(\vec{X}) &= \nabla_{\vec{X}} \psi_i(F^{-1}(\vec{X})) \\ &= \nabla_{\vec{U}} \psi_i(\vec{U}) \cdot \nabla_{\vec{X}} F^{-1}(\vec{X}) \\ &= B^{-T} \nabla_{\vec{U}} \psi_i(\vec{U})\end{aligned}$$

where we used $\vec{U} = F^{-1}(\vec{X})$ and $\nabla_{\vec{X}} F^{-1}(\vec{X}) = B^{-T}$.

The gradient of $\psi_i(\vec{U})$ in reference triangle is:

$$\begin{aligned}\nabla\psi_1 &= (-1, -1) \\ \nabla\psi_2 &= (1, 0) \\ \nabla\psi_3 &= (0, 1)\end{aligned}$$

So the gradient of $\psi_i^k(\vec{X})$ in physical triangle is "constant":

$$\nabla\psi_1^k = B^{-T}(-1,-1)$$
$$\nabla\psi_2^k = B^{-T}(1,0)$$
$$\nabla\psi_3^k = B^{-T}(0,1)$$

5.1. For 3D Triangles

For 3D triangles the map function F changes as follows:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \\ z_2 - z_1 & z_3 - z_1 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} x_1 \\ y_1 \\ z_1 \end{bmatrix}$$

In matrix algebra it can be expressed as:

$$F(\vec{U}) = B\vec{U} + \vec{X}_1$$
$$F^{-1}(\vec{X}) = (B^T B)^{-1} B^T (\vec{X} - \vec{X}_1)$$

or

$$F^{-1}(\vec{X}) = B^{-*}(\vec{X} - \vec{X}_1)$$

where $B^{-*} = (B^T B)^{-1} B^T$ is the Moore-Penrose pseudo-inverse of B.

The same analysis as before holds so:

$$\nabla\psi_1^k = B^{-*T}(-1,-1)$$
$$\nabla\psi_2^k = B^{-*T}(1,0)$$
$$\nabla\psi_3^k = B^{-*T}(0,1)$$

6. Numerical Quadrature

The entries of the matrix M_T^k are the following double integrals:

$$M_T^k(i,j) = \int_{T^k} \nabla\psi_i^k(\vec{X}) \cdot \nabla\psi_j^k(\vec{X})\, dA$$

inidices (i,j) run for all nodes of triangle T.

Let define the inner product of basis functions as

$$I_{ij}^k(\vec{X}) = \nabla\psi_i^k(\vec{X}) \cdot \nabla\psi_j^k(\vec{X})$$

The 3-point Gauss quadrature rule for the linear triangle is:

$$M_T^k(i,j) = \frac{area(T^k)}{3}(I_{ij}^k(P_1) + I_{ij}^k(P_2) + I_{ij}^k(P_3)) \tag{6.1}$$

evaluated at the vertices of the triangle P_1, P_2 and P_3. Which is an exact quadrature formula for linear function on a triangle. However since $\nabla\psi_i^k(\vec{X})$ does not depends on $\vec{X}$ the quadrature expression reduces to:

$$M_T^k(i,j) = area(T^k)\nabla\psi_i^k(\vec{X}) \cdot \nabla\psi_j^k(\vec{X})$$

7. Implementation

Implementation can be found in [2]

8. Appendix - Differential Forms

d	exterior derivative
$\star$	Hodge dual
$f(x,y)$	scalar valued function (scalar-field) : 0-form
$g(x,y)$	vector valued function (vector-field): 1-form
$df(x,y)$	gradient vector field : 1-form
$\star d\star g(x,y)$	divergence of g(x,y): 0-form
$\star df(x,y)$	dual of the 1-form in R^2: 1-form (in dual space)
$d\star df(x,y)$	curl of the 1-form in the cotangent space: 2-form
$\star d\star df(x,y)$	divergence of gradient: 0-form
$U(x,y)$	twice differentiable scalar-valued function (scalar field) : 0-form
$d\star d + dd\star$	Laplace-Beltrami operator
$d\star dU(x,y) = \star f(x,y)$	Laplacian-Beltrami equation, since $dd\star U(X) = 0$

Laplacian-Beltrami equation:

$$d\star dU(x,y) = \star f(x,y)$$

the $d\star dU(x,y)$ and $\star f(x,y)$ are 2-forms (pseudo-scalar fields). The residual $R(X)$ is

$$R(X) = d\star dU(X) - \star f(X)$$

So we want to minimize $\int V(X)R(X)$ using Galerkin method we get the optimality condition for the variational form:

$$\int V(X)R(X) = 0$$

$$\int V(X)\ d\star dU(X) = \int V(X)\ \star f(X)$$

Recall product rule:

$$d\left(V(X)dU(X)\right) = dV(X) \wedge dU(X) + V(X)\ ddU(X)$$

Consider the vector field $E(X) = V(X)\star dU(X)$ where $V(X)$ and $\star dU(X)$ are 0-forms. Taking $dE(X)$ we get:

$$dE(X) = d\left(V(X)\ \star dU(X)\right)$$

$$dE(X) = dV(X) \wedge \star dU(X) + V(X)\ d\star dU(X)$$

Since wedge product of a k-form with a (N-k)-form is same as inner product:

$$V(X) \wedge \star U(X) = V(X) \cdot U(X)$$
$$V(X) \wedge \star U(X) = V(X)U(X)$$

The last equality holds when $V(X)$ and $U(X)$ are 0-forms. Then we can re-write $dE(X)$ as:

$$dE(X) = dV(X) \cdot dU(X) + V(X)\ d\star d\ U(X)$$

By applying the Stokes theorem to $\int_\Omega dE(X)$:

$$\int_\Omega dE(X)\ dA = \int_{\partial\Omega} E(X)\ dS$$
$$\int_\Omega dE(X)\ dA = \int_{\partial\Omega} V(X) \wedge *dU(X)\ dS$$
$$\int_\Omega dE(X)\ dA = \int_{\partial\Omega} V(X)dU(X) \cdot dS$$

the last equality holds since $V(X) \cdot dU(X) = V(X)dU(X)$ since $V(X)$ is 0-form and $dU(X)$ is a 1-form. Also since dS is a 1-form the product of $dU(X)dS$ is actually $dU(X) \cdot dS$.

Replacing left hand side:

$$\int_\Omega dV(X) \cdot dU(X) + V(X)\ d\star d\ U(X)\ dA = \int_{\partial\Omega} V(X)dU(X) \cdot dS \quad (8.1)$$

So we can re-arrange as:

$$\int_\Omega V(X)\ d\star d\ U(X)\ dA = \int_{\partial\Omega} V(X)dU(X) \cdot dS - \int_\Omega dV(X) \cdot dU(X)\ dA (8.2)$$

We have performed essentially Integration By Parts. Replacing into the left-hand-side of the variational form we get:

$$\int_\Omega V(X)\ d\star dU(X)\ dA = \int_\Omega V(X)\star f(X)\ dA$$
$$\int_{\partial\Omega} V(X)dU(X) \cdot dS - \int_\Omega dV(X) \cdot dU(X)\ dA = \int_\Omega V(X)\star f(X)\ dA$$

Since $V(X) = 0$ on the boundary of the domain $\partial\Omega$ then we get:

$$-\int_\Omega dV(X) \cdot dU(X)\ dA = \int_\Omega V(X)\star f(X)\ dA$$

References

[1] H. P. Langtangen. Introduction to finite element methods. 2014.

[2] M. C. Lopez Belon. Project on github. Available at https://github.com/mauriciocele/basic-fem-2d, 2024.

[3] F.-J. Sayas. A gentle introduction to the finite element method. 2015.

Mauricio Cele Lopez Belon
Madrid, Spain
e-mail: mclopez@outlook.com