Object-oriented scientific computing

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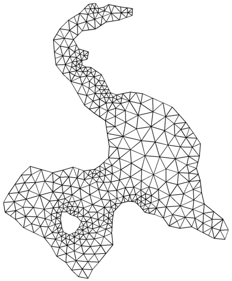
The finite element method

Advantages of the FE method over the FD method

Main advantages of FE over FD

1. Deal with Neumann boundary conditions in a natural (systematic) way
2. Deals with irregular geometries much more easily



FEM stages

Solve:

$$\nabla^2 u + f = 0$$

subject to boundary conditions

$$\begin{aligned} u &= u^* && \text{on } \Gamma_1 \\ (\boldsymbol{\nabla} u) \cdot \mathbf{n} &= g && \text{on } \Gamma_2 \end{aligned}$$

1. Set up the mesh and choose basis functions
2. Compute the matrix K and vector $\mathbf{b}$:

$$\begin{aligned} K_{jk} &= \int_\Omega \nabla \phi_j \cdot \nabla \phi_k \, \mathrm{d}V \\ b_j &= \int_\Omega f \phi_j \, \mathrm{d}V + \int_{\Gamma_2} g \phi_j \, \mathrm{d}S \end{aligned}$$

3. Alter linear system $KU = b$ to impose Dirichlet BCs
4. Solve linear system

This gives the solution $u_h(\mathbf{x}) = U_1 \phi_1(\mathbf{x}) + \ldots U_N \phi_N(\mathbf{x})$

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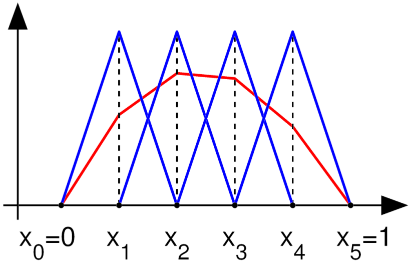
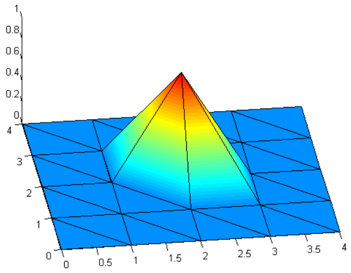
Basis functions





Implementing Dirichlet boundary conditions

In practice, rather using the basis functions in $\mathcal{V}_0^h$ (i.e. bases satisfying $\phi_i = 0$ on Γ_1), we use $\mathcal{V}^h$, i.e. all the basis functions corresponding to all nodes in the mesh.

We then impose (any) Dirichlet boundary conditions by altering the appropriate rows of the linear system, for example, for $K\mathbf{U} = b$, if we want to impose $U_1 = c$

$$\begin{bmatrix} K_{11} & K_{12} & \dots & K_{1N} \\ K_{21} & K_{22} & \dots & K_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ K_{N1} & K_{N2} & \dots & K_{NN} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_N \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{bmatrix}$$

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$$\begin{bmatrix} 1 & 0 & \dots & 0 \\ K_{21} & K_{22} & \dots & K_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ K_{N1} & K_{N2} & \dots & K_{NN} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_N \end{bmatrix} = \begin{bmatrix} c \\ b_2 \\ \vdots \\ b_N \end{bmatrix}$$

Solving linear systems

Consider the general problem of solving the linear system

$$A\mathbf{x} = \mathbf{b}$$

where A is an $n \times n$ matrix and $\mathbf{b}$ an n-vector.

Direct solvers

- One approach is to compute A^{-1} and calculate $\mathbf{x} = A^{-1}\mathbf{b}$
- **Gaussian elimination** is an algorithm that is often used and is essentially equivalent to computing A^{-1}
- These approaches get too costly (in time and memory) for large n
- For $n < 10000$ (maybe even 50000) this may be the best approach

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Iterative solvers

- Often A is **sparse**
- This means that computing $A\mathbf{y}$ for given $\mathbf{y}$ is cheap.
- Choose initial guess $\mathbf{x}_0$
- An iterative solver takes in a current guess $\mathbf{x}_n$ and provides an improved solution $\mathbf{x}_{n+1}$, just using matrix-vector products
- Common iterative solvers are *conjugate gradients* (for when A is symmetric and positive-definite) and *GMRES*.

Preconditioning

- Question is then: (i) does $\mathbf{x}_n \to \mathbf{x}$ and (ii) how fast does $\mathbf{x}_n \to \mathbf{x}$?
- For any non-singular matrix P, the system

$$PA\mathbf{x} = P\mathbf{b}$$

  is equivalent to the original system $A\mathbf{x} = \mathbf{b}$.
- By choosing P appropriately, can obtain (massively) improved convergence—preconditioning

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The finite element method: assembly

Numerical quadrature

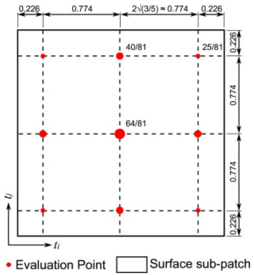
Suppose we want to compute

$$\int_{\text{unit square}} F(x, y)\,\mathrm{d}x\mathrm{d}y$$

We can use the approximation

$$\int_{\text{unit square}} F(x, y)\,\mathrm{d}x\mathrm{d}y \approx \sum_i w_i F(x_i, y_i)$$

where (x_i, y_i) are the *quadrature points*, and w_i the *weights*



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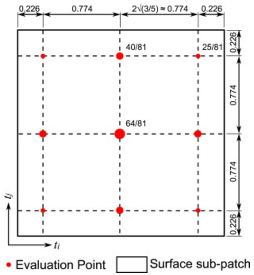

Computing a finite element matrix/vector by *assembly*

Consider computing the mass matrix $M_{jk} = \int_\Omega \phi_j \phi_k \, \mathrm{d}V$, an N by N matrix say, and let's suppose (for clarity only) that we are in 2D.

We **do not** write out the full basis functions explicitly in computing this integral. Instead: firstly, we break the integral down into an integral over elements:

$$M_{jk} = \sum_{\mathcal{K}} \int_{\mathcal{K}} \phi_j \phi_k \, \mathrm{d}V$$

Consider $\int_{\mathcal{K}} \phi_j \phi_k \, \mathrm{d}V$. **Key point**: The only basis functions with are non-zero in the triangle are the 3 basis functions corresponding to the 3 nodes of the element.

Therefore: compute the **elemental contribution to the mass matrix**, a 3 by 3 matrix of the form $\int_{\mathcal{K}} \phi_j \phi_k \, \mathrm{d}V$ for *3 choices of j and k only*.

Then **add** elemental contribution to full N by N mass matrix.

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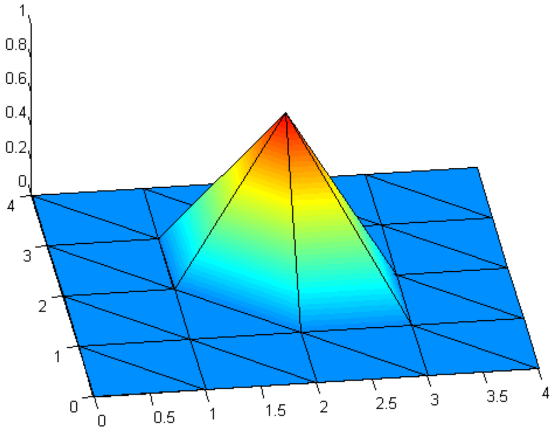

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We have reduced the problem to computing small matrices/vectors, for example the 3 by 3 matrix

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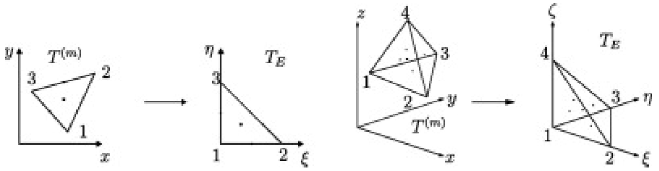

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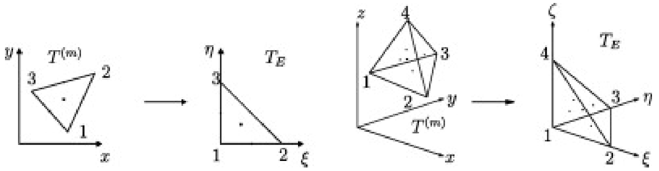

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Reference element (also called the canonical element)

We now need to be able to compute

$$\int_{\mathcal{K}} \phi_j \phi_k \, \mathrm{d}x\mathrm{d}y = \int_{\mathcal{K}_{\mathrm{ref}}} \phi_j \phi_k \, \det J \; \mathrm{d}\xi \mathrm{d}\eta$$

where J is the Jacobian of the mapping from the true element to the canonical element.

The basis functions on the reference triangle are easy to write down

$$\begin{aligned} \phi_1(\xi,\eta) &= 1 - \xi - \eta \\ \phi_2(\xi,\eta) &= \xi \\ \phi_3(\xi,\eta) &= \eta \end{aligned}$$

Computing an elemental contribution

J is also required if $\boldsymbol{\nabla}\phi_i$ is needed (for example, in computing the stiffness matrix), since $\boldsymbol{\nabla}\phi_i = J\boldsymbol{\nabla}_{\boldsymbol{\xi}} N_i$.

Consider the mapping from an element with nodes $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, to the canonical element. The inverse mapping can in fact be easily written down using the basis functions.

$$\mathbf{x}(\xi,\eta) = \sum_{j=1}^{3} \mathbf{x}_j N_j(\xi,\eta)$$

from which it is easy to show that J is the following function of nodal positions

$$J = \mathrm{inv}\begin{bmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{bmatrix}$$

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$$\begin{aligned} K_{jk} &= \int_\Omega \nabla\phi_j \cdot \nabla\phi_k \, \mathrm{d}V \\ b_j &= \int_\Omega f\phi_j \, \mathrm{d}V + \int_{\Gamma_2} g\phi_j \, \mathrm{d}S \end{aligned}$$

3. Alter linear system $K\mathbf{U} = \mathbf{b}$ to impose Dirichlet BCs
4. Solve linear system

This gives the solution $u_h(\mathbf{x}) = U_1\phi_1(\mathbf{x}) + \ldots U_N\phi_N(\mathbf{x})$

FEM stages - full algorithm

Write

$$b_j = \int_\Omega f \phi_j \, \mathrm{d}V + \int_{\Gamma_2} g \phi_j \, \mathrm{d}S$$

as $\mathbf{b} = \mathbf{b}^{\text{vol}} + \mathbf{b}^{\text{surf}}$

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FEM for simple PDEs: Object-oriented implementation (general ideas)

Note that in the following:

- We consider *one possible* approach - the appropriate design will depend fundamentally on the precise nature of the solver required (eg, a solver for a particular equation versus a general solver of several)
- `Purple` represents an abstract class/method, `red` represents a concrete class or implemented method, `blue` represents a self-contained class (no inheritance).
- Important members or methods of the classes will be given, but obvious extra methods will be omitted, such as Get/Set methods

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Object-oriented design

What are the self-contained ‘concepts’ (objects) that form the overall simulation code, and what functionality should each of these objects have?

Geometry

`Node`

Member var: `mLocation`

- ▷ *a vector*

Member var: `mIsBoundaryNode`

- ▷ *a boolean (true/false)*

`Element`

Member var: `mNodes`

- ▷ *(Pointers to) the 3 nodes (assuming a 2d simulation) of this element*

Method: `ComputeJacobian()`

Method: `ComputeJacobianDeterminant()`

`SurfaceElement`

Member var: `mNodes`

- ▷ *(Pointers to) the 2 nodes of this element*
- ▷ *Also has corresponding methods to the Jacobian methods above*

Geometry

Mesh

- `mNodes`
  - ▷ *a list of `Node` objects*
- `mElements`
  - ▷ *a list of `Element` objects*
- `mBoundaryElements`
  - ▷ *a list of surface elements (`SurfaceElement`) on the boundary*
- *Method:* `ReadFromFile(filename)`
- *Method:* `GenerateRegularMesh(width,height,stepsize)`
- *Method:* `Refine()`

Note

- Here, boundary nodes/elements represent the *entire* boundary—'mesh' concept is self-contained and **not** dependent on PDE problem being solved.

Boundary conditions

- There are various ways this could be implemented
- **Key point**: the implementation requires that
  - Dirichlet BCs be defined at boundary *nodes*
  - Neumann BCs be defined on boundary *elements* (ie element interiors)

```
BoundaryConditions<DIM>

    mDirichletBoundaryNodes
    mDirichletValues
    mNeumannBoundaryElements
    mNeumannValues

    AddDirichletBoundaryCondition(node,dirichletBcValue)
    AddNeumannBoundaryCondition(boundaryElement,neumannBcValue)
```

A simple solver

Suppose we want to write a solver for Poisson's equation $\nabla^2 u = f$ for general forcing terms $f(\mathbf{x})$ and general boundary conditions. The solver class could be self-contained, and look like:

```
PoissonEquationSolver:
    Solve(mesh,abstractForce,boundaryConditions)
```

A simple solver

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The `Solve` method needs to:

1. Initialise a matrix K and vector $\mathbf{b}$
2. Set up stiffness matrix $K_{ij} = \int_\Omega \phi_i \phi_j \,\mathrm{d}V$
    - Loop over elements of mesh (“`mesh.GetNumElements()`”, “`mesh.GetElement(i)`”)
    - For each element set-up the elemental stiffness matrix – loop over quadrature points, call `element.GetJacobian()` etc
    - Add elemental contribution to K
3. Similarly, loop over elements and assemble $b_i^{\mathsf{vol}} = \int_\Omega f \phi_i \,\mathrm{d}V$
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A (possible) more complete interface

```
PoissonEquationSolver:
    PoissonEquationSolver(mesh,abstractForce,boundaryConditions)
    Solve()
    PlotSolution()
    PlotForce()
    ComputeQOI()
    WriteSolutionToFile(filename)
```