CS 294-73
Software Engineering for Scientific Computing

Lecture 8: Unstructured grids and sparse matrices

Back to Poisson's equation.

Some Vector Calculus

$$\text{Gradient operator: } \nabla\Psi = \left(\frac{\partial\Psi}{\partial x}, \frac{\partial\Psi}{\partial y}\right)$$

$$\text{Divergence operator: } \nabla \cdot (F_x, F_y) = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y}$$

$$\text{Laplacian: } \Delta\phi = \nabla \cdot (\nabla\phi) = \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}$$

- Green's theorem (aka integration by parts)

$$-\int_\Omega \Psi(\boldsymbol{x})(\nabla \cdot (\nabla\phi))(\boldsymbol{x})d\boldsymbol{x} = \int_\Omega \nabla\Psi \cdot \nabla\phi d\boldsymbol{x} + \int_{\partial\Omega} \Psi(\boldsymbol{x})(\nabla\phi)(\boldsymbol{x})dS$$

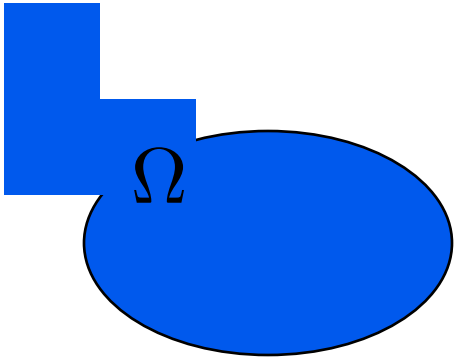
- If $\Psi \equiv 0$ on $\partial\Omega$, then

$$-\int_\Omega \Psi(\boldsymbol{x})(\nabla \cdot (\nabla\phi))(\boldsymbol{x})d\boldsymbol{x} = \int \nabla\Psi \cdot \nabla\phi d\boldsymbol{x}$$

Weak Form of Poisson's Equation

We want to solve Poisson's equation (note the sign convention)

$$-\Delta\phi = f \text{ on } \Omega$$
$$\phi = 0 \text{ on } \partial\Omega$$



We want find a weak solution, i.e.

$$\int_\Omega (-\Delta\phi)(\boldsymbol{x})\Psi(\boldsymbol{x})d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x})\Psi(\boldsymbol{x})d\boldsymbol{x} \text{ on } \Omega$$

For all continuous piecewise smooth test functions

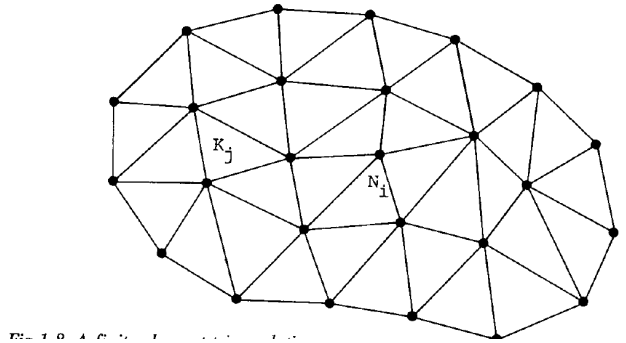
- $\Psi(\boldsymbol{x})$ with $\Psi = 0$ on $\partial\Omega$

Applying Green's Theorem, this is the same as

$$\int_\Omega \nabla\phi \cdot \nabla\Psi d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x})\Psi(\boldsymbol{x})d\boldsymbol{x} \ , \ \Psi \in V$$

Finite element discretization

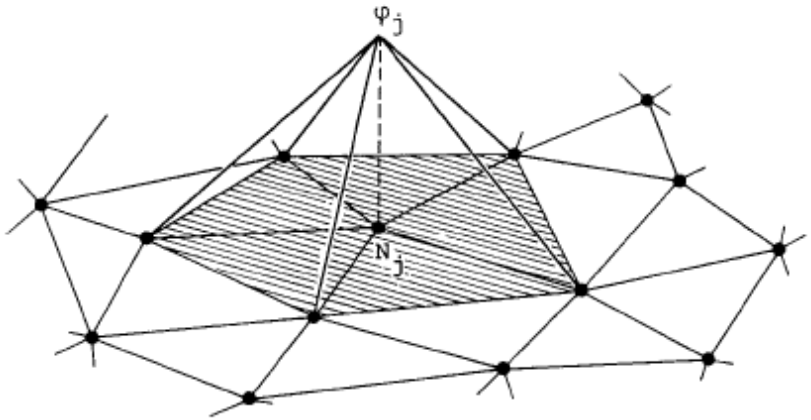
Step 1: we discretize our domain as a union of triangles.



Step 2: We replace V by V^h, a finite-dimensional space of test functions. For this exercise, we will use linear combinations of continuous, piecewise linear functions, indexed by interior nodes nodes, linear on each triangle containing the node. A basis for this space is given by $\{\Psi_n^h(\boldsymbol{x}) : n \in \mathcal{N}_I\}$.

$$\text{Interior Nodes} = \mathcal{N}_I$$

$$\text{Elements } e = 0, \ldots E-1$$



Step 3: We also approximate the solution as a linear combination of the the elements in V^h .

$$\Psi_n^h(\boldsymbol{x}_{n'}) = \delta_{nn'} \ , \ n' \in \mathcal{N}$$

Weak form -> matrix equation.

We apply the weak form of the equations to the finite-dimensional subspace V^h

$$\phi(\boldsymbol{x}) \approx \phi^h(\boldsymbol{x}) = \sum_{n \in \mathcal{N}_I} a_n \Psi_n^h(\boldsymbol{x})$$

$$\int_\Omega \nabla \phi^h \cdot \nabla \Psi_n^h d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) \Psi_n^h(\boldsymbol{x}) d\boldsymbol{x} \ , \ n \in \mathcal{N}_I$$

$$\sum_{n' \in \mathcal{N}_I} a_{n'} \int_\Omega \nabla \Psi_{n'}^h \cdot \nabla \Psi_n^h d\boldsymbol{x} = \int_\Omega f(\boldsymbol{x}) \Psi_n^h(\boldsymbol{x}) d\boldsymbol{x}$$

$$(La)_n = \sum_{n' \in \mathcal{N}_I} L_{n,n'} a_{n'} = b_n$$

$$L_{n,n'} = \int_\Omega \nabla \Psi_{n'}^h \cdot \nabla \Psi_n^h d\boldsymbol{x} \ , \ b_n = \int_\Omega f(\boldsymbol{x}) \Psi_n^h(\boldsymbol{x}) d\boldsymbol{x}$$

Elements

Two issues:

- Computing L.
- Quadrature for computing b.

$$L_{n,n'} = \int_\Omega \nabla \Psi^h_{n'} \cdot \nabla \Psi^h_n d\boldsymbol{x} \ , \ (n, n' \in \mathcal{N}_I)$$

$$= \sum_{e=0\ldots E-1} \int_{K_e} \nabla \Psi^h_{n'} \cdot \nabla \Psi^h_n d\boldsymbol{x}$$

$$= 0 \text{ unless } n, n' \in K_e$$

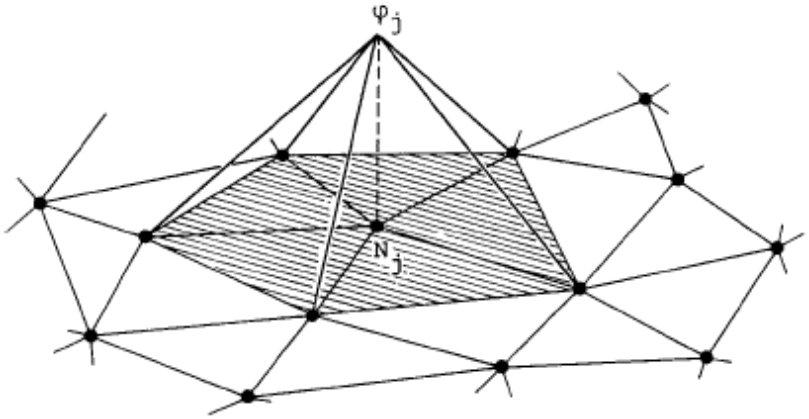


Fig 1.9 The basis function φ_j.

Matrix Assembly

Pseudocode: Interior Nodes $=\mathcal{N}_I$, Elements $e = 0, \ldots E-1$

```
Initialize L = 0
for e = 0 ... E - 1
  for (x_n, x_n') ∈ K_e : (n, n') ∈ N_I
    L_{n,n'} += ∫_{K_e} ∇Ψ^h_{n'} · ∇Ψ^h_n dx
  endfor
endfor
```

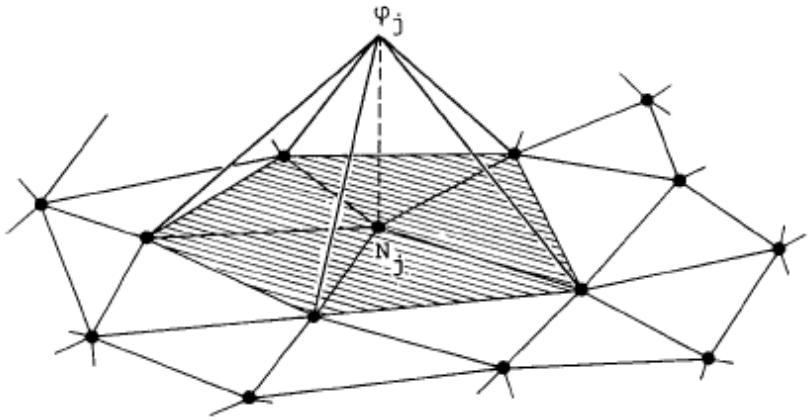


Fig 1.9 The basis function φ_j.

- L is a matrix with mostly zero entries. But it is nice: symmetric, positive-definite, M-matrix.
- $\nabla \Psi_n^h$ is a constant vector, easily computed.
- We're building a matrix dimensioned by nodes by iterating over elements and building it up incrementally.

Getting the right-hand side

Quadrature for b: midpoint rule on each element.

$$\int_\Omega \Psi_n^h f d\boldsymbol{x} = \sum_{K_e} \int_{K_e} \Psi_n^h f d\boldsymbol{x}$$

$$\int_{K_e} \Psi_n^h f d\boldsymbol{x} \approx Area(K_e) f(\boldsymbol{x}_e^{centroid}) \Psi_n^h(\boldsymbol{x}_e^{centroid})$$

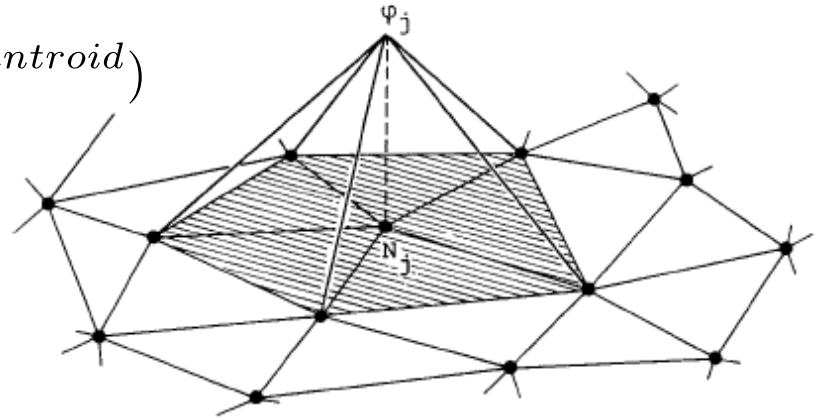


Fig 1.9 The basis function φ_j.

```
Initialize b = 0
for e = 0 ... E − 1
  for x_n ∈ K_e : n ∈ N_I
    b_n+ = Area(K_e) f(x_e^centroid) Ψ_n^h(x_e^centroid)
  endfor
endfor
```

$$\boldsymbol{x}_e^{centroid} = \frac{1}{Area(K_e)} \int_{K_e} \boldsymbol{x} d\boldsymbol{x}$$

More element magic.

Point Jacobi Iteration

Motivation: to solve *La = b,* we compute it as a steady-state solution to an ODE.

$$\frac{da}{dt} = -La + b$$

If all of the eigenvalues of *L* are positive, then

$$La_\infty = b \ , \ a_\infty = \lim_{t \to \infty} a(t)$$

Point Jacobi: use forward Euler to solve ODE.

Stop when the *residual* has been reduced by a suitable amount.

$$a^{l+1} = a^l + \lambda(b - La^l) \ , \ l = 0, 1, \ldots \ ; \ a^0 = 0 \quad \lambda > 0$$

$$||b - La^l|| \leq \epsilon ||b||$$

Matrix Properties

Our matrix has the following properties:

- Symmetric, positive-definite: $L = L^T$, $v \cdot (Lv) > 0$ if $v \neq 0$
- Positive along diagonal.
- Rows sum to a non-negative number: $L_{k,k} \geq -\sum_{k'} L_{k,k'}$
- For triangles sufficiently close to equilateral, the nonzero off-diagonal elements are non-negative, i.e. $\nabla \Psi_n^h \cdot \Psi_{n'}^h \leq 0$ on K_e .

Choosing a Relaxation Parameter

This leads to the following choice for our relaxation parameter.

$$\lambda = \alpha \frac{1}{\max_k L_{k,k}} \ , \ \alpha < 1$$

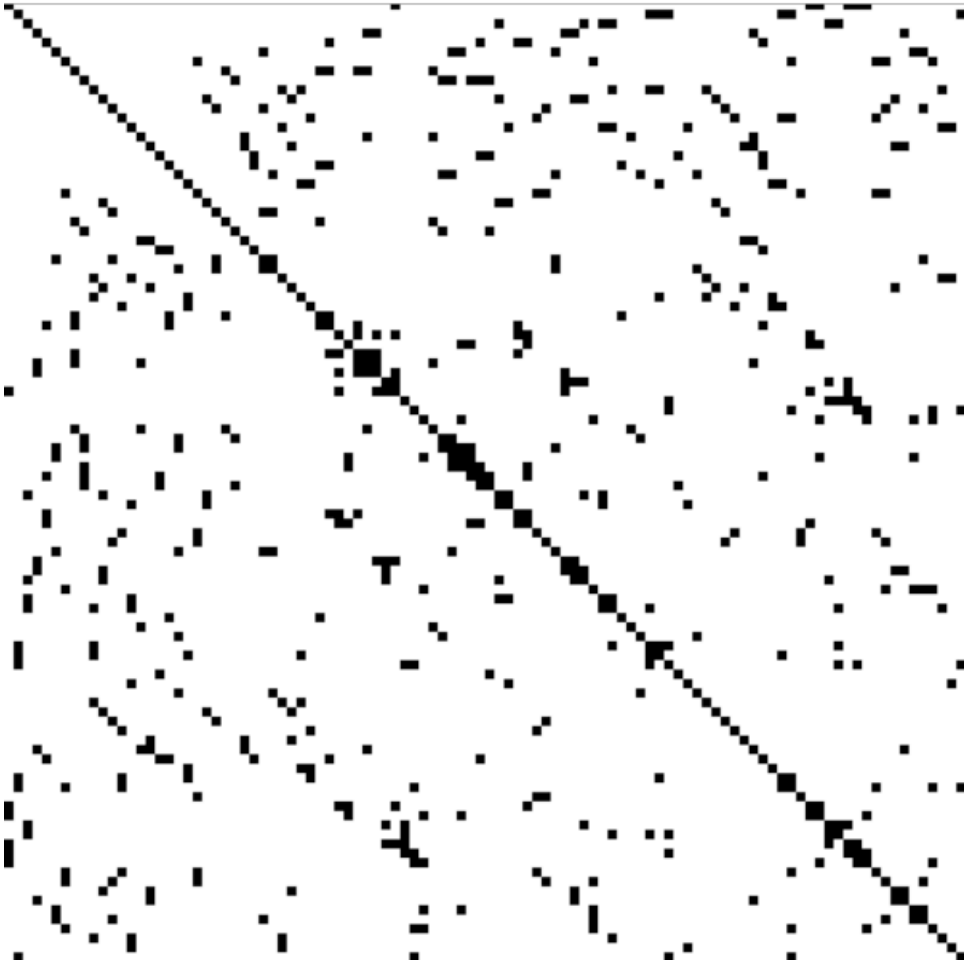
If your grid is strongly-varying, may want to use a local relaxation parameter (you will not be doing this in the present assignment).

$$a_k^{l+1} = a_k^l + \lambda_k (b - La^l)_k$$

$$\lambda_k = \alpha \frac{1}{L_{k,k}}$$

Sparse Matrices.

- Compact basis function space results in a linear operator (Matrix) that has mostly zero entries.



Typical non-zero entries in A matrix from a finite element problem

RectMDArray can hold this matrix, but wasteful

- Wasteful in several ways
  - You waste memory storing the number 0 in a lot of places
  - You was floating point instructions performing multiplication with 0
  - You waste processor bandwidth to memory
  - You waste hits in your cache

Sparse Matrix representation using vectors

$$\mathbf{A} = \begin{pmatrix} 1.5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.3 & 0 & 1.4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3.7 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1.6 & 0 & 2.3 & 9.9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5.8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 7.4 & 0 & 0 \\ 0 & 0 & 1.9 & 0 & 0 & 0 & 4.9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.6 \end{pmatrix}$$

1		
2	4	
3		
2	4	5
5		
6		
7	3	
8		

1.5		
2.3	1.4	
3.7		
-1.6	2.3	9.9
5.8		
7.4		
4.9	1.9	
3.6		

We represent a sparse matrix as two vectors of vectors:
`vector<vector<double> >` to hold the matrix elements,
`vector<vector<int> >` to hold the column indices.

Compressed-sparse-row (CSR) representation.

SparseMatrix Class

```
class SparseMatrix
{
public:
  /// set up an M rows and N columns sparse matrix
  SparseMatrix(int a_M, int a_N);
  /// Matrix Vector multiply.  a_v.size()==a_N, returns vector of size a_M
  vector<double> operator*(const vector<double>& a_v) const;
  ///accessor functions for get and set operations of matrix elements
  double& operator[](const array<int,2>&);
private:
  int m_m, m_n;
  float m_zero;
  vector<vector<double> > m_data;
  vector<vector<int> >   m_colIndex;
};
```

If necessary, sparse matrix automatically adds a new matrix element when you reference that location, and initializes it to zero.

For each non-zero entry in 'A' we keep one float, and one int indicating which column it is in

Part of your homework 2 will be to implement this class, with a few more functions

Setup for Homework 2

- Build an operator corresponding to a triangular element discretization of the Poisson equation.
- Use an iterative solver to solve the equation.
- What we will provide:
  - Triangular grids, stored in files.
  - Classes for reading those files, and storing and manipulating computing geometric information.
  - A class for writing out the solution in a form that can be viewed by VisIt.
- You will write:
  - A class `FEPoissonOperator` that generates and stores the sparse matrix, and applies the operator to the right-hand side.
  - The `SparseMatrix` class.
  - An implementation of point Jacobi iteration to solve the resulting linear system.

We will discuss the details of these in the next few slides.

Node , Element, and FEGrid

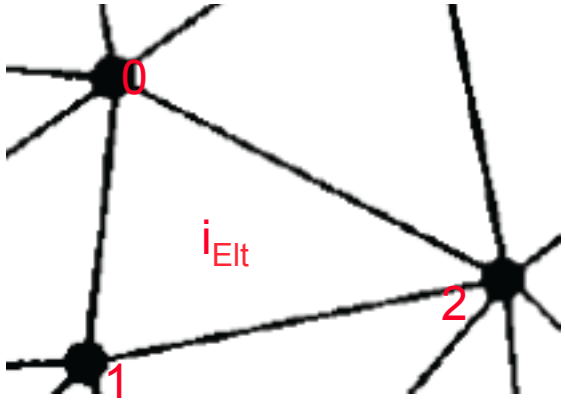
```
class Node
{
 public:
  Node();
  Node(array<double,DIM> a_position,
       const int&  a_interiorNodeID,
       const bool& a_isInterior);
  /// Constant access to node Location in space.
  const array<double,DIM>& getPosition() const;
  const int& getInteriorNodeID() const;
  const bool& isInterior() const;
 private:
  array<double,DIM>  m_position;
  bool  m_isInterior;
  int m_interiorNodeID;
};
```

Three different integer ID's for nodes:

- Where they are in the vector of all nodes making up the triangular grid;
- Where they are in the vector making up the interior nodes;
- Where they are in the vector making up the nodes on an element (`localNodeNumber`)

Node , Element, and FEGrid

```
#define VERTICES 3
class Element
{
public:
  Element();
  /// Constructor.
  Element(array<int,VERTICES>& a_tr);
  /// Destructor.
  ~Element();
  /// local indexing to get nodeNumber.
  const int& operator[](const int& a_localNodeNumber) const;
private:
  array<int,VERTICES> m_vertices;
};
```



Local node numbers for element i_{Elt}.

Node , Element, and FEGrid

```
class FEGrid
{
public:
  FEGrid();
  /// Constructor by reading from file.
  FEGrid(char* a_nodeFileName,char* a_elementFileName);
  ///Destructor.
  ~FEGrid();
/// Get number of elements, nodes, interior nodes.
  int getNumElts() const;
  int getNumNodes() const;
  int getNumInteriorNodes() const;
```

We're implementing this one (along with `Node and Element`) for you – you just have to use them correctly.

Read in the file names from argv.

Node , Element, and FEGrid

Element-centered calculus.

```
...
 /// Compute gradient of basis function at node
 /// a_localNodeNumber = 0,..,VERTICES-1, on element
  a_eltNumber.
  array<double,DIM> gradient(const int& a_eltNumber,
                             const int& a_localNodeNumber) const;
  /// Compute centroid of element.
  array<double,DIM> centroid(const int& a_eltNumber) const;
  /// Compute area of element.
  float elementArea(const int& a_eltNumber) const;
  /// Compute value of basis function.
  float elementValue(const array<double,DIM>& a_xVal,
                     const array<double,DIM>& a_gradient,
                     const int& a_eltNumber,
                     const int& a_localNodeNumber) const;
```

Node , Element, and FEGrid

```
...
  /// get reference to node on an element.
  const Node& getNode(const int& a_eltNumber,
                      const int& a_localNodeNumber) const;
  /// Get reference to a Node given its global index.
  const& Node& getNode(const int& a_nodeNumber) const;

private:
  vector<Node > m_nodes;
  vector<Element > m_elements;
  int m_numInteriorNodes;
};
```

Notice what we *don't* have: neither an explicit mapping that gives all of the elements touching a given node, nor one that maps interiorNodes into nodes. The first one we don't need, and the second is encoded implicitly in `Node`.

FEPoissonOperator

```
class FEPoissonOperator
{
 public:
  FEPoissonOperator();
  FEPoissonOperator(const FEGrid& a_grid);
  void applyOperator(vector<float> & a_LOfPhi, const
  vector<double> & a_phi) const;
  void makeRHS(vector<double> & a_rhsAtNodes, const
  vector<float> & a_rhsAtCentroids) const;
  const FEGrid& getFEGrid() const;
   const SparseMatrix& getSparseMatrix() const;
  ~FEPoissonOperator();
 private:
  SparseMatrix m_matrix;
  FEGrid m_grid;
};
```

Note that `a_phi` is defined only on the interior nodes, as is `a_LOfPhi, a_rhsAtNodes` .

Building the Sparse Matrix (`FEPoisson::FEPoisson( ... )`

- Our sparse matrix has dimensions $\mathcal{N}_I \times \mathcal{N}_I$ (`getNumInteriorNodes()`)
- To compute the inner product on each element, you need `gradient, elementArea.`
- Fill in $L_{n,n'}$ incrementally, by incrementing matrix elements corresponding to pairs of interior nodes in each element, then iterating over elements (`getNode(...),Node::InteriorNodeID()`).

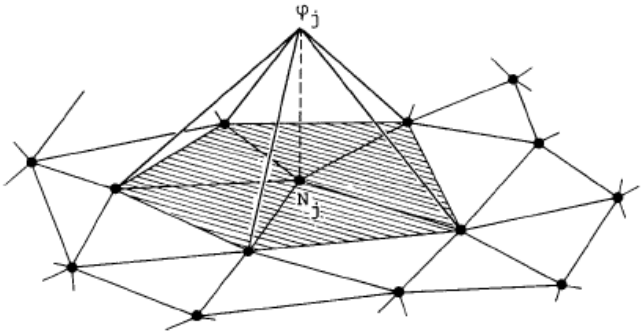


Fig 1.9 The basis function φ_j.

$$L_{n,n'} = \int_\Omega \nabla\Psi^h_{n'} \cdot \nabla\Psi^h_n d\boldsymbol{x} \ , \ (n, n' \in \mathcal{N}_I)$$
$$= \sum_{e=0\ldots E-1} \int_{K_e} \nabla\Psi^h_{n'} \cdot \nabla\Psi^h_n d\boldsymbol{x}$$
$$= 0 \text{ unless } n, n' \in K_e$$

```
Initialize L = 0
for e = 0 ... E - 1
  for (x_n, x_n') ∈ K_e : (n, n') ∈ N_I
    L_{n,n'} += ∫_{K_e} ∇Ψ^h_{n'} · ∇Ψ^h_n dx
  endfor
endfor
```

Sparse matrix automatically adds new matrix element when you index that location, and initializes it to zero.

Building the Right-hand Side (`makeRHS`)

- Our right-hand side is an $\mathcal{N}_I$ -dimensional vector (`getNumInteriorNodes()`), while our input f a vector of values evaluated at the centroids of elements (`getNumElements()`, `centroid(...)`).
- Fill in *b* incrementally, by iterating over elements , then computing interior nodes in each element (`getNode(...)`, `Node::InteriorNodeID()`).
- Use `elementValue(...)`, `elementArea(...)` to compute contribution from each node in an element.

$$\int_\Omega \Psi_n^h f d\boldsymbol{x} = \sum_{K_e} \int_{K_e} \Psi_n^h f d\boldsymbol{x}$$

$$\int_{K_e} \Psi_n^h f d\boldsymbol{x} \approx Area(K_e) f(\boldsymbol{x}_e^{centroid}) \Psi_n^h(\boldsymbol{x}_e^{centroid})$$

Initialize $b = 0$

for $e = 0 \ldots E-1$

  for $\boldsymbol{x}_n \in K_e : n \in \mathcal{N}_I$

    $b_n += Area(K_e) f(\boldsymbol{x}_e^{centroid}) \Psi_n^h(\boldsymbol{x}_e^{centroid})$

  endfor

endfor