The University of Queensland
School of Earth and Environmental Sciences

An Introduction to Finite Elements With Application To Gravity Fields

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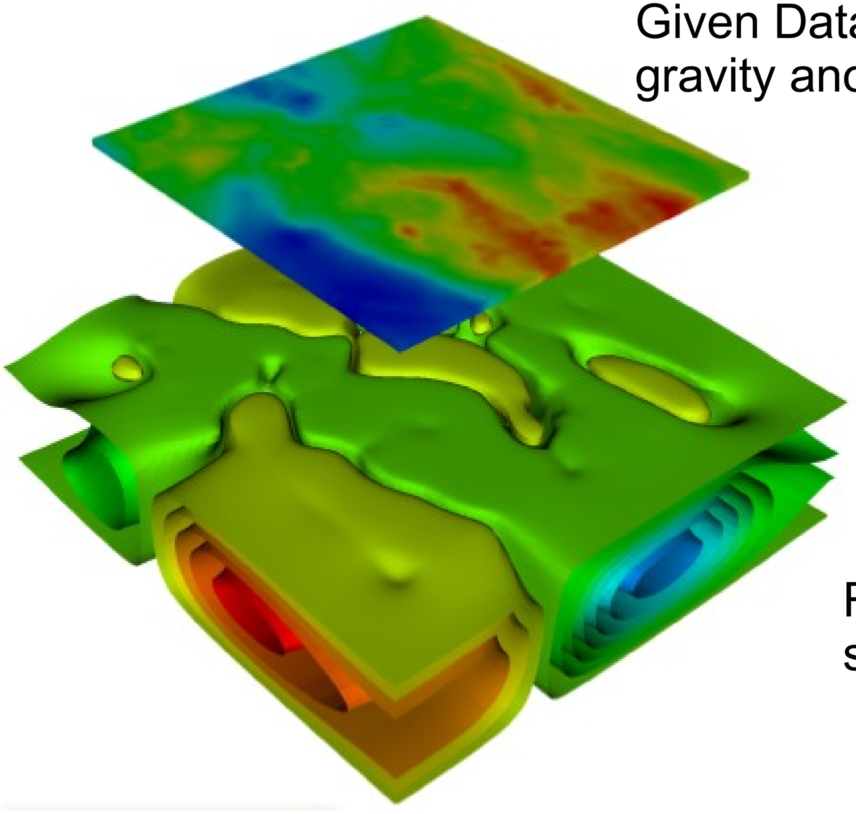
Objective: Geophysical Imaging

- constructing a 3D map of subsurface from from surface or near surface observation
  - For instance: density ρ from vertical gravity g_z
- This process is called inversion
  - Key step: forward model
    - calculate vertical gravity g_z at the surface from an estimated density distribution ρ

Geophyscial Imaging (cont.)

Example from Western Queensland



Given Data: vertical gravity anomalies g_z at surface

Recovered 3D map: surface density ρ

Gauss's law for gravity

- Gravity field $\boldsymbol{g}=(g_0,g_1,g_2)$ due to density ρ needs to fulfill:

$$\nabla^T \mathbf{g} = -4\pi G\rho$$

$$\text{universal gravitational constant } G = 6.67430 \cdot 10^{11} \frac{Nm^2}{kg^2}.$$

- Coordinate system $\boldsymbol{x}=(x_0,x_1,x_2)$:
  - x_0,x_1 horizontal
  - $x_2=z$ vertical

$$\nabla^T \mathbf{g} = \frac{\partial g_0}{\partial x_0} + \frac{\partial g_2}{\partial x_2} + \frac{\partial g_2}{\partial x_2}$$

Potential Field

- gravity field is a conservative field:

$$\nabla \times \mathbf{g} = \mathbf{0}$$

- Hence gravity field $\boldsymbol{g}$ the negative gradient of the so-called gravity potential u

$$\mathbf{g} = -\nabla u$$

PDE for the Potential

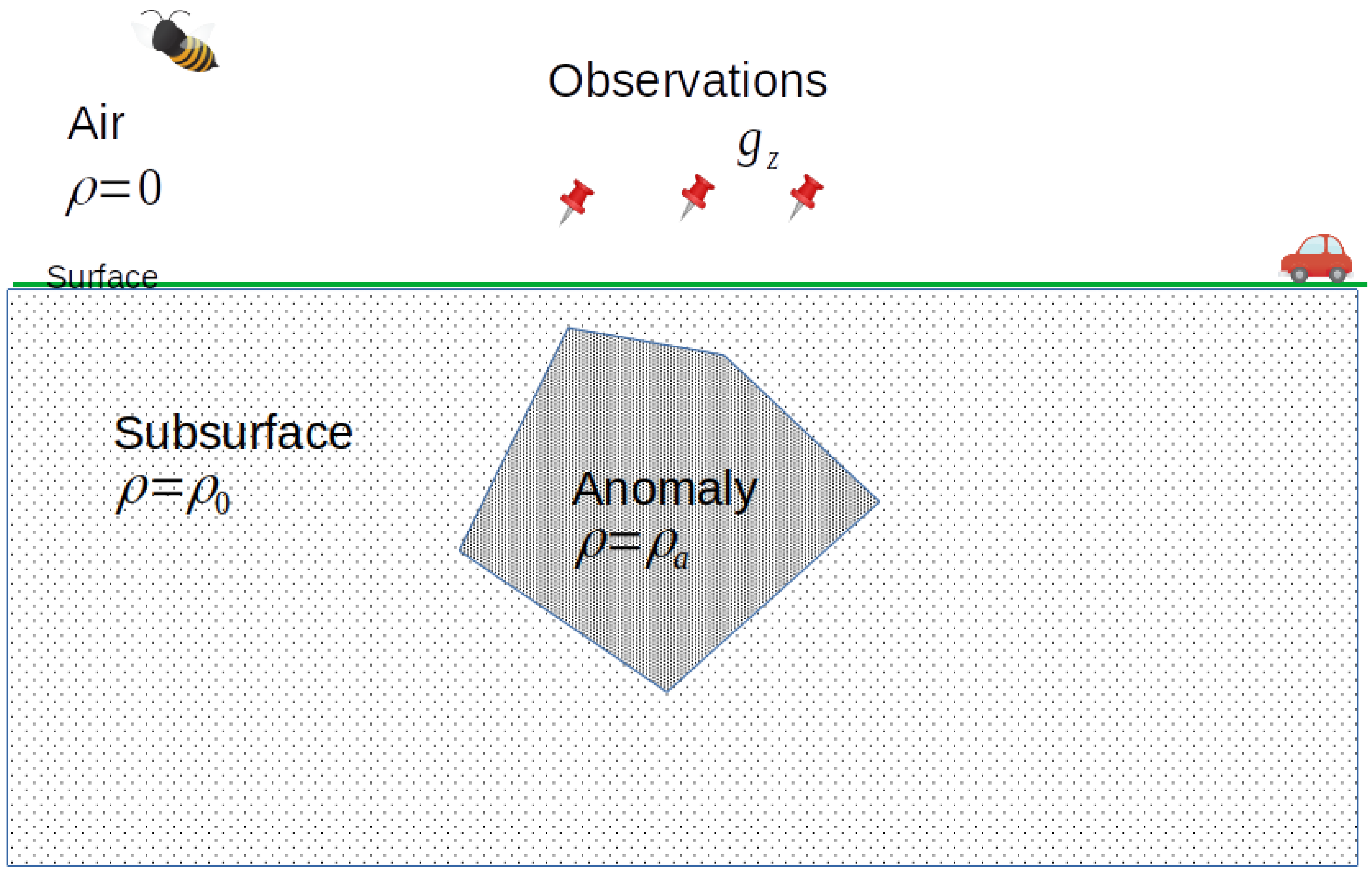
- Partial Differential Equation (PDE) for the potential *u*

$$-\nabla^T \nabla u = -4\pi G\rho \; .$$

- Spelled out in 2D: x_0 horizontal, x_1 vertical

$$-\left(\frac{\partial^2 u}{\partial x_0^2}+\frac{\partial^2 u}{\partial x_1^2}\right)=-4\,\pi G\,\rho$$

Anomalies


Air
$\rho=0$
Observations
g_z
Surface
Subsurface
$\rho=\rho_0$
Anomaly
$\rho=\rho_a$

Background gravity

- Common approach in geophysics:
  - Eliminate the background field and properties from the problem → looking at anomalies
  - Based on a 'homogeneous half-space' solution

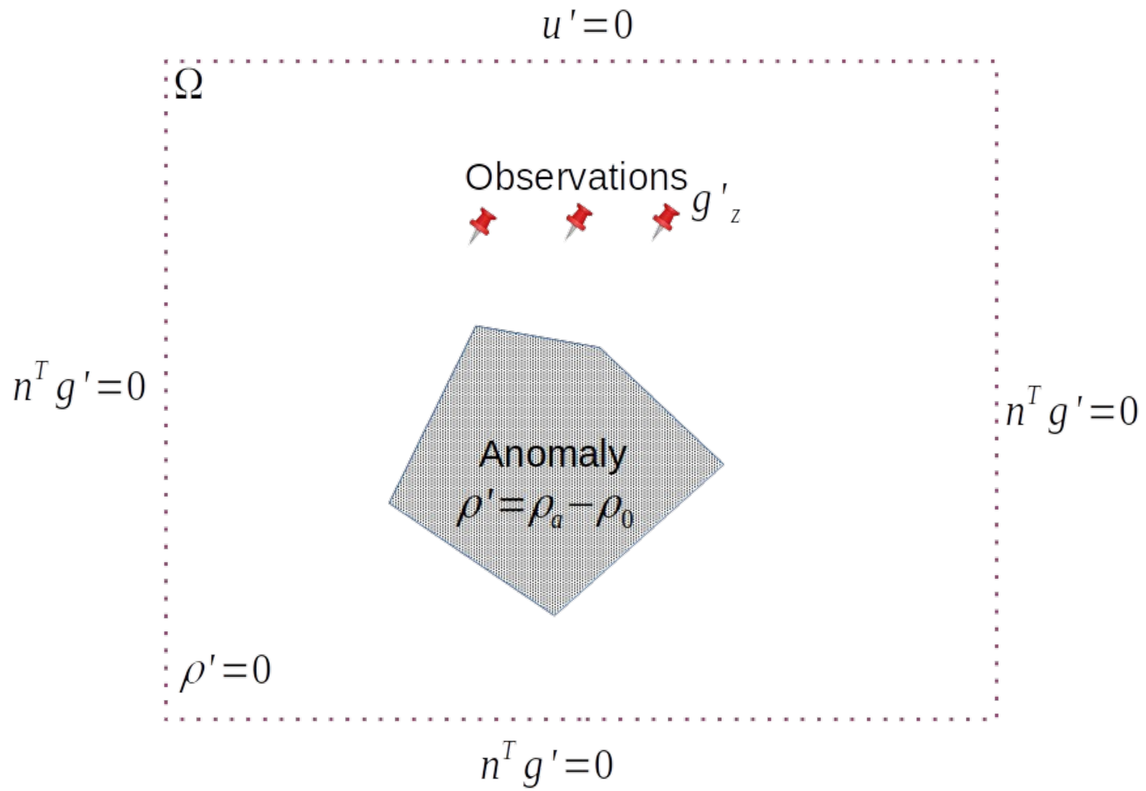
Background model constant density + air layer

$$\rho = \rho_{bg} + \rho' \qquad u = u_{bg} + u' \qquad \mathbf{g} = \mathbf{g}_{bg} + \mathbf{g}'$$

Residual model

Residual Model

- Assume bounded domain
- Homogeneous boundary conditions



Boundary conditions

- Dirichlet-type boundary conditions on Γ_D

$$u' = 0$$

  - Γ_D = top of the domain Ω
- Neumann-type boundary conditions on Γ_N

$$-\mathbf{n}^T \mathbf{g}' = \mathbf{n}^T \nabla u' = 0$$

  - Outer normal field $\boldsymbol{n}$
    - Set normal component of gravity field $\boldsymbol{g}$ to zero
  - Γ_N = all other faces of the domain Ω

PDE we need to solve

- Make life easy: drop the ‘
- PDE for gravity potential u on domain Ω:

$$-\nabla^T \nabla u = -4\pi G\rho \ .$$

- plus boundary conditions.

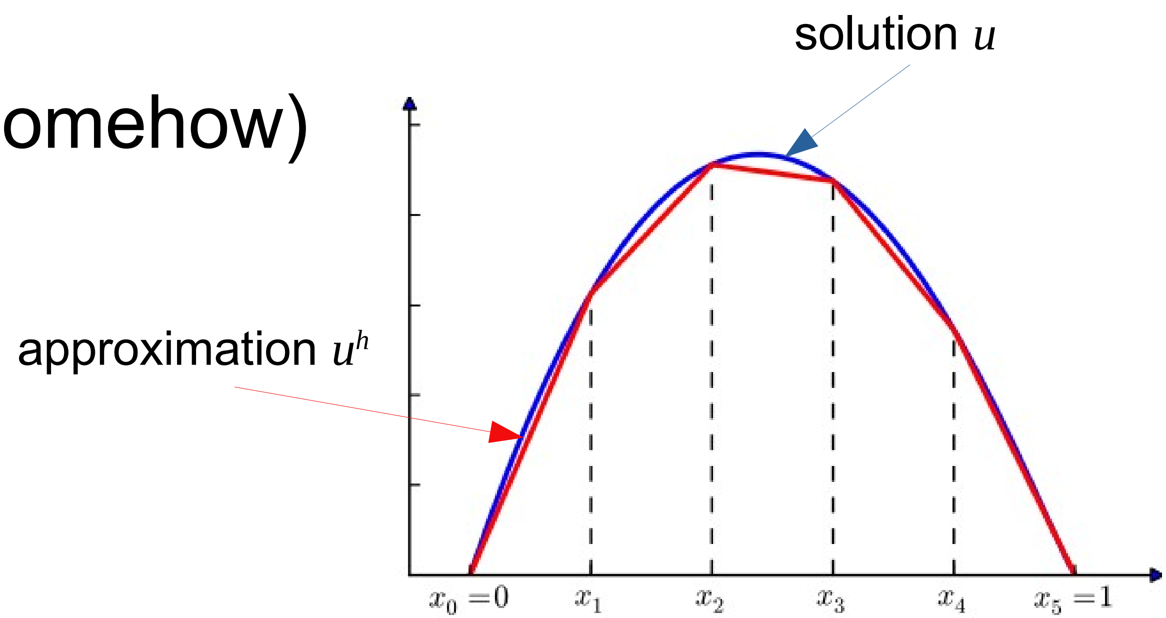
Finite Element Approximation

- Idea: approximate the solution u by function u^h that is

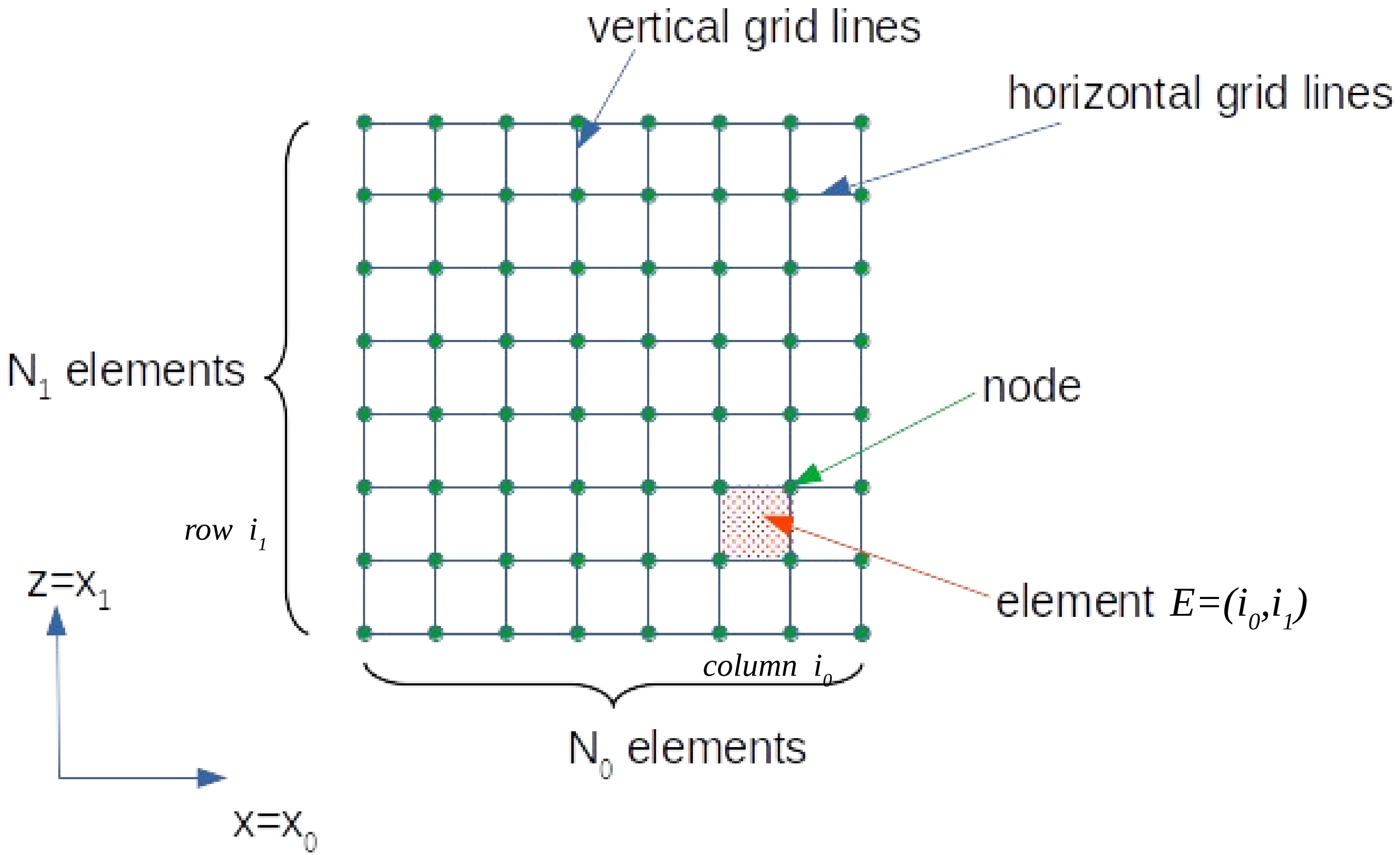
  1) continuous

  2) piecewise linear

  3) solves the PDE (somehow)



It all starts with a Grid



Grids

- Subdivide the domain into an array of elements arranged in N_1 rows and N_0 columns
  - A total of $N_1 N_0$ elements, and
  - A total $N=(N_1+1)(N_0+1)$ nodes
- The set of all these nodes:

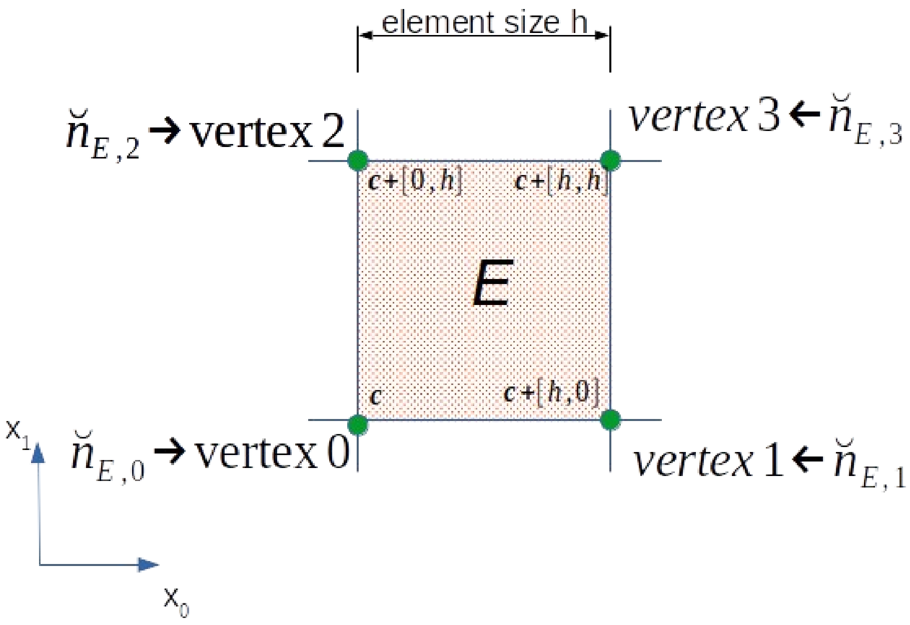
Elements

- The set of elements is an unordered list

$$\mathcal{E} = \{E = (i_0, i_1) | i_0 = 0, \ldots, N_0; i_1 = 0, \ldots, N_1\}$$

- An element is described by the node ids of its vertices:

$$\breve{n}_E = [\breve{n}_{E,0}, \breve{n}_{E,1}, \breve{n}_{E,2}, \breve{n}_{E,3}]$$



FEM Approximation

- FEM approximation is a linear combination of the FEM basis functions ϕ_p^h with p=0,…, N-1

$$u^h(\mathbf{x}) = \sum_{p=0}^{N-1} U_p^h \phi_p^h(\mathbf{x})$$

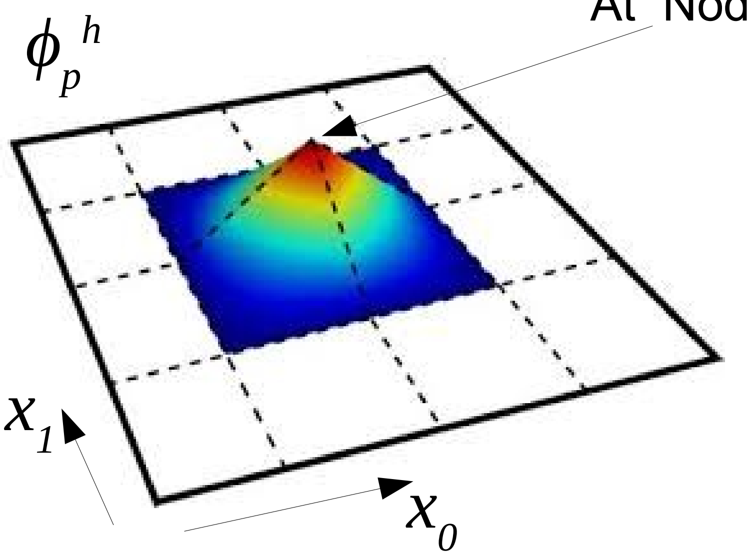
- Unknown coefficients U_p^h
- basis function ϕ_p^h is associated with node p

FEM Basis Function

Properties of basis function ϕ_p^h

- Continuous function
- Value one at node *p*
- Value zero at all other nodes $q \neq p$
- Linear function on each element

- Hence: it is identical zero on all elements that do not contain node *p* as vertex



Duality

- There is a duality of basis functions and nodes

$$\phi_p^h(\mathbf{x}_q) = \delta_{pq} \qquad \delta_{pq} = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{if } p \neq q \end{cases}$$

- Hence: coefficient U_p^h is the value of the FEM approximation at node p:

$$u^h(\check{\mathbf{x}}_p) = \sum_{q=0}^{N-1} U_q^h \phi_q^h(\check{\mathbf{x}}_p) = \sum_{q=0}^{N-1} U_q^h \delta_{pq} = U_p^h$$

Some Notations

- Vector of node values $\boldsymbol{U}^h$:

$$\mathbf{U}^h = [u^h(\check{\mathbf{x}}_0), u^h(\check{\mathbf{x}}_1), \ldots, u^h(\check{\mathbf{x}}_{N-1})]^T = [U_0^h, U_1^h, \ldots, U_{N-1}^h]^T$$

  - Component of $\boldsymbol{U}^h$ called **degrees of freedom** (DOFs)
- arrange the basis function as a vector:

$$\boldsymbol{\Phi}^h = [\phi_0^h, \phi_1^h, \ldots, \phi_{N-1}^h]^T$$

- FEM approximation in a convenient way

$$u^h = \boldsymbol{\Phi}^{hT}\mathbf{U}^h$$

Basis Function on an Element

- On element E basis functions are bi-linear polynomial

$$\phi_p^h(x_0, x_1) = a + b \cdot x_0 + c \cdot x_1 + d \cdot x_0 x_1$$

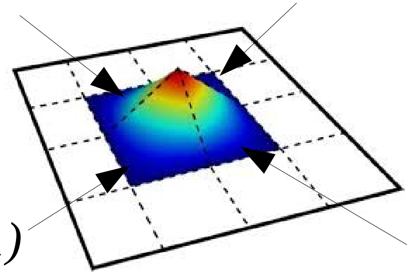
  – x_0,x_1 in element E,

- a,b,c and d are suitable factors depending on node p and element E
  - Determined by the duality condition!
- Note: $a=b=c=d=0$ if node p is not in element E

Local Basis Functions

- Local basis function = part of the global basis function on an element
  - Obviously: we are looking at non-zero part only
  - Here: four local basis functions N_0, N_1, N_2, N_3:

$$\phi_p^h = N_i \text{ for } p = \check{n}_{E,i} \quad (i = 0, 1, 2, 3)$$



Local Basis Functions

- For square element with edge length h and left-lower corner $c=(c_0,c_1)$

$$N_0(x_0,x_1) = \frac{1}{h^2}(c_0+h-x_0)\cdot(c_1+h-x_1)$$

$$N_2(x_0,x_1) = -\frac{1}{h^2}(c_0+h-x_0)\cdot(c_1-x_1)$$

$$N_1(x_0,x_1) = -\frac{1}{h^2}(c_0-x_0)\cdot(c_1+h-x_1)$$

$$N_3(x_0,x_1) = \frac{1}{h^2}(c_0-x_0)\cdot(c_1-x_1)$$

- Task: Check duality with the four vertices (c_0,c_1), (c_0+h,c_1), (c_0,c_1+h), (c_0+h,c_1+h)

The FEM Solution

- Motivation: get the FEM approximation u_h with the best gravity approximation:

$$\min_{u_h} \|\nabla u - \nabla u^h\|_2^2$$

- in the root means square (RMS) sense:

$$\|F\|_2 = \sqrt{\frac{1}{V}\int_\Omega |F(\mathbf{x})|^2 d\mathbf{x}}$$

Condition for FEM solution

- Apply ` virtual displacement`:

  Perturb solution u^h by small increment $v_h = \phi_p^h$ for any node *p:*

- Then we have for any α :

$$\|\nabla u - \nabla u^h\|_2^2 \leq \|\nabla u - \nabla(u^h + \alpha v_h)\|_2^2$$

A bit of calculus:

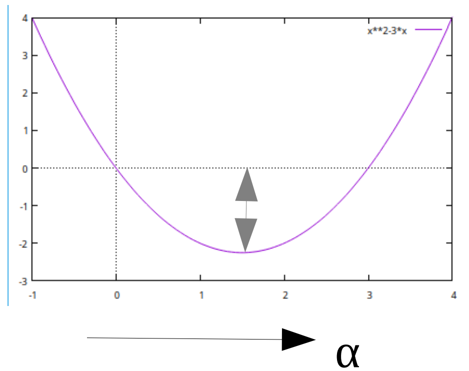
$$\begin{aligned}\|\nabla u - \nabla(u^h + \alpha v_h)\|_2^2 &= \frac{1}{V}\int_\Omega |\nabla u - \nabla u^h - \alpha \nabla v_h|^2 d\mathbf{x} \\ &= \frac{1}{V}\int_\Omega \left(|\nabla u - \nabla u^h|^2 - 2\alpha \nabla^T v^h \left(\nabla u - \nabla u^h\right) + \alpha^2 |\nabla v_h|^2\right) d\mathbf{x} \\ &= \|\nabla u - \nabla u^h\|_2^2 + \alpha^2 \|\nabla v^h\|_2^2 - 2\frac{\alpha}{V}\int_\Omega \nabla^T v^h \left(\nabla u - \nabla u^h\right) d\mathbf{x}\end{aligned}$$

We put this back into condition (1.26) and obtain

$$0 \le \alpha^2 \|\nabla v^h\|_2^2 - 2\frac{\alpha}{V}\int_\Omega \nabla^T v^h \left(\nabla u - \nabla u^h\right) d\mathbf{x}$$

which holds for any value of α. This can only be true if and only of

$$0 = \int_\Omega \nabla^T v^h \left(\nabla u - \nabla u^h\right) d\mathbf{x}$$



FEM Solution

- So FEM uh needs to fullfil this condition for all basis functions $v^h = \phi_p^{\ h}$

$$\int_\Omega \nabla^T v^h \, \nabla u^h \, d\mathbf{x} = \int_\Omega \nabla^T v^h \, \nabla u \, d\mathbf{x}$$

- But we don't know the solution u ?
  - Somehow we need to use:

$$-\nabla^T \nabla u = -4\pi G \rho \; .$$

FEM Solution (cont.)

- Split integration over domain into integration over elements individual E:

$$\int_{\Omega} \nabla^T v^h \, \nabla u \; d\mathbf{x} = \sum_{E \in \mathcal{E}} \int_{E} \nabla^T v^h \, \nabla u \; d\mathbf{x}$$

- apply Green's first identity on each element

$$\int_{E} \nabla^T v^h \, \nabla u \; d\mathbf{x} = -\int_{E} v^h \, \nabla^T \nabla u \; d\mathbf{x} + \int_{\partial E} v^h \, \mathbf{n}^T \, \nabla u \; ds$$

FEM Solution (cont.)

- Insert PDE:

$$\int_E v^h \nabla^T \nabla u \, d\mathbf{x} = -\int_E (-4\pi G)\rho \, v^h \, d\mathbf{x}$$

- Two elements E_1 and E_2 with touching faces have normal n_1 and n_2 with opposite signs:

$$\mathbf{n}_1^T \nabla u = -\mathbf{n}_2^T \nabla u$$

- Hence: as v^h is continuous across element edges:

$$\sum_{E \in \mathcal{E}} \int_{\partial E} v^h \, \mathbf{n}^T \nabla u \, ds = \int_{\partial \Omega} v^h \, \mathbf{n}^T \nabla u \, ds$$

Boundary conditions:

- Neumann-type boundary conditions on Γ_N

$$\mathbf{n}^T \nabla u' = 0 \qquad \sum_{E \in \mathcal{E}} \int_{\partial E} v^h \, \mathbf{n}^T \nabla u \, ds = \int_{\boxed{\Gamma_D}} v^h \, \mathbf{n}^T \nabla u \, ds$$

- Dirichlet-type boundary condition on Γ_D

$$u = 0 \text{ on } \Gamma_D \rightarrow \text{only use } v^h \text{ with } v^h = 0 \text{ on } \Gamma_D$$

  - Only use $v^h = \phi_p^h$ with node p **not** in Γ_D

Condition for FEM Solution

- Putting it all together:
  - Find uh that fulfills the following conditions
    - Meets the Dirichlet boundary condition: $u^h=0$ on Γ_D
    - For all v^h with $v^h=0$ on Γ_D :

$$\int_\Omega \nabla^T v^h \, \nabla u^h \; d\mathbf{x} = \int_\Omega (-4\pi G)\rho \; v^h \; d\mathbf{x}$$

System of Linear Equations

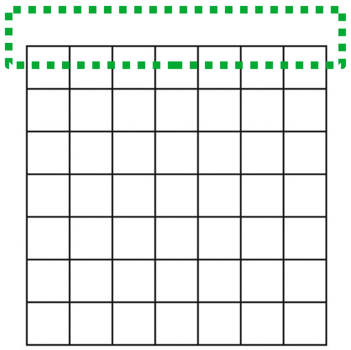
- Recall:

$$u^h(\mathbf{x}) = \sum_{p=0}^{N-1} U_p^h \phi_p^h(\mathbf{x})$$

- Dirichlet condition '$u^h=0$ on Γ_D ' translates:
  - If node *p* in Γ_D then

$$u^h(\check{\mathbf{x}}_p) = U_p^h = 0$$

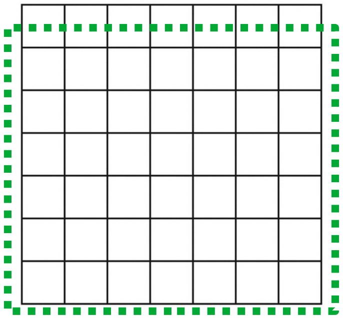
eg. all nodes localeted at the top face of the domain



System of Linear Equations (cont.)

- With $v^h = \phi_p^{\ h}$ for node p **not** in Γ_D

$$\sum_{q=0}^{N-1} U_q^h \int_\Omega \nabla^T \phi_p^h \, \nabla \phi_q^h \, d\mathbf{x} = \int_\Omega (-4\pi G)\rho \, \phi_p^h \, d\mathbf{x}$$



- This is a system of
  - N equations: one at each node
  - N unknowns = values of u^h at the nodes

Compact form

- In compact form this is

$$\mathbf{S}^h \mathbf{U}^h = \mathbf{b}^h$$

- With (ignoring Dirichlet Boundary conditions):

$$\mathbf{U}^h = [u^h(\check{\mathbf{x}}_0), u^h(\check{\mathbf{x}}_1), \ldots, u^h(\check{\mathbf{x}}_{N-1})]^T = [U_0^h, U_1^h, \ldots, U_{N-1}^h]^T$$

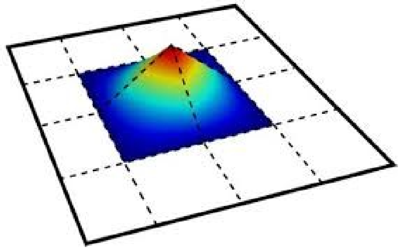
$$\mathbf{S}^h = [S_{pq}^h] \qquad S_{pq}^h = \int_\Omega \nabla^T \phi_p^h \, \nabla \phi_q^h \, d\mathbf{x}$$

$$\mathbf{b}^h = [b_p^h] \qquad b_p^h = \int_\Omega (-4\pi G)\rho \, \phi_p^h \, d\mathbf{x}$$

Matrix Structure

- S^h is called stiffness matrix
- Entries can be obtained element-by-element

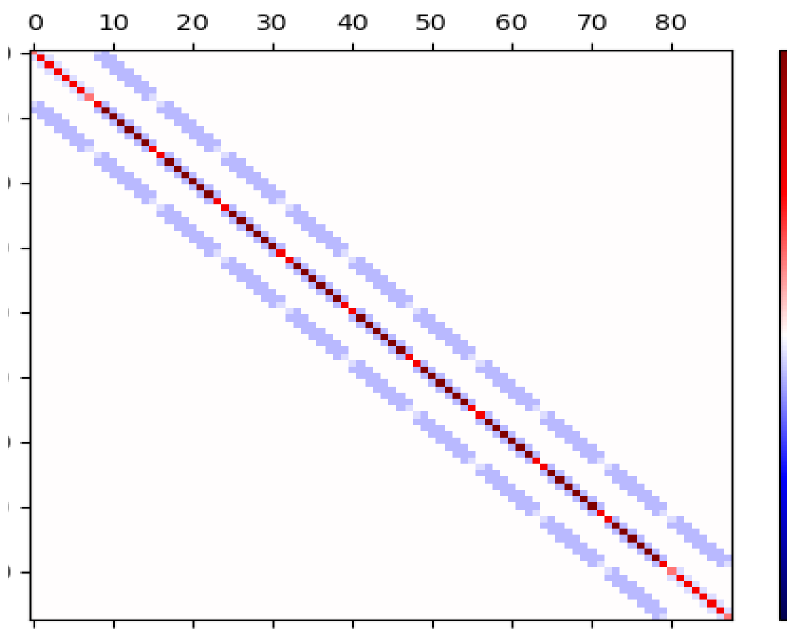
$$S^h_{pq} = \sum_{E \in \mathcal{E}} \int_E \nabla^T \phi^h_p \nabla \phi^h_q \, d\mathbf{x}$$



- Hence: S^h_{pq} is **zero** if there is **no** element E that has node p and q as a vertex.

Matrix Structure (cont.)

- The stiffness matrix is sparse
  - The number of non-zero entries is small compared to the size of the matrix



Sparsity

- Use special compressed formats such as
  - compressed sparse row (CSR): stores value + column index
  - dictionary of keys (DOK): stores value + (column, row) index
- For our case:
  - Size of full matrix N^2
  - Number of non-zeros: about 8 N
    - As each node has maximum of 8 neighboring nodes connected via an element.
  - For a 100x100 grid:
    - Sparsity < 0.08%
    - Savings of memory for CSR format: around a factor 600

Numerical Properties

- The stiffness matrix is
  - Symetric: $(\mathbf{S}^h)^T = \mathbf{S}^h$
  - Positive definite: $(\mathbf{U}^h)^T \mathbf{S}^h \mathbf{U}^h > 0$

  - See lecture nodes for details

- Solution methods for the linear system:
  - Direct method: Sparse LU factorization
  - Iterative method: Conjugate Gradient method

Matrix Assemblage

- The matrix and right-hand-side is build up on an element-by-element base.
  - This can be done in any order!
- We need an enumeration of the global nodes
  - Determines the sparsity pattern of non-zero entries in the stiffness matrix
    - Is impacting on computational performance and memory requirements

Node Enumeration

- Here we use a grid row-by-row scheme:
  - First count along the x_0 axis and secondly along the x1-axis:

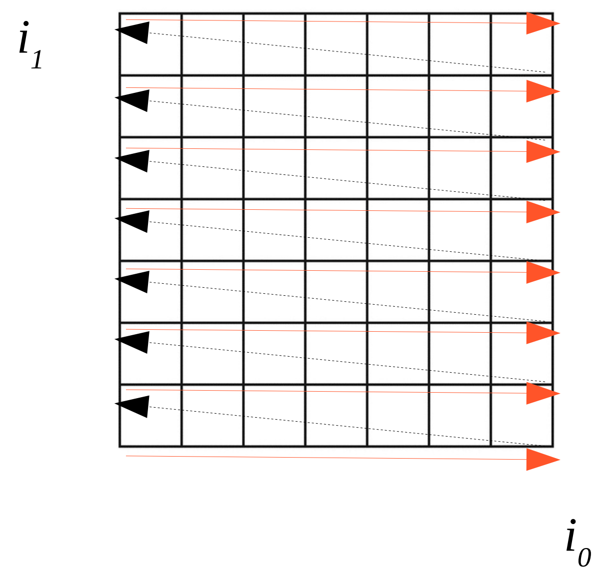
$$n = i_0 + (N_0 + 1) \cdot (i_1 + 1) \text{ for } i_0 = 0, \ldots, N_0; i_1 = 0, \ldots, N_1$$

- Lower, left corner:

  $(i_0,i_1)=(0,0)$: $n=0$

- Upper right corner:

  $(i_0,i_1)=(N_0,N_1)$: $n=N_0\, N_1\text{-}1$



Example

Element $E=(i_0,i_1)$

$$\check{n}_E = [\check{n}_{E,0}, \check{n}_{E,1}, \check{n}_{E,2}, \check{n}_{E,3}]$$

$\check{n}_{(0,0)} = [0,1,5,6];$ $\check{n}_{(1,0)} = [1,2,6,7]$

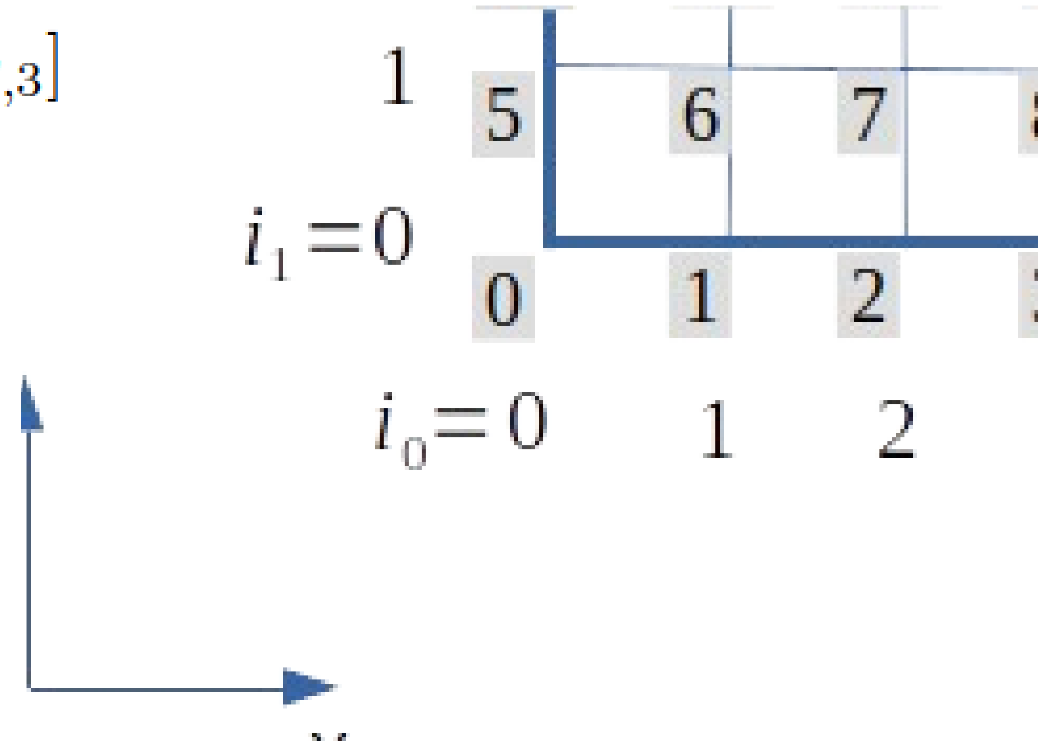
$\check{n}_{(2,0)} = [2,3,7,8];$ $\check{n}_{(3,0)} = [3,4,8,9]$

$\check{n}_{(0,1)} = [5,6,10,11];$ $\check{n}_{(1,1)} = [6,7,11,12]$

$\check{n}_{(2,1)} = [7,8,12,13];$ $\check{n}_{(3,1)} = [8,9,13,14]$

$\check{n}_{(0,2)} = [10,11,15,16];$ $\check{n}_{(1,2)} = [11,12,16,17]$

$\check{n}_{(2,2)} = [12,13,17,18];$ $\check{n}_{(3,2)} = [13,14,18,19]$



Local Element matrices

- Evaluate the local version of the PDE using the four local basis functions N_0, N_1, N_2, N_3:

$$S_{ij}^E = \int_E \nabla^T N_i \, \nabla N_j \; d\mathbf{x} \text{ for } i, j = 0, \ldots 3$$

$$b_i^E = \int_E (-4\pi G)\rho \; N_i \; d\mathbf{x} \text{ for } i = 0, \ldots 3$$

Add to Global Stiffness matrix

- Recall the connection between local and global basis functions:

$$\phi_p^h = N_i \text{ for } p = \check{n}_{E,i} \quad (i = 0, 1, 2, 3)$$

- This tells us where to **add** the local element matrices:

$$S^h_{\check{n}_{E,i}\check{n}_{E,j}} += S^E_{ij} \text{ and } b^h_{\check{n}_{E,i}} += b^E_i$$

Get the local element matrices ..

- Assume: density ρ is constant in each element
  - Density is given as an array: $[\rho_E]_{E \in \mathcal{E}}$
- We know the local basis functions so the integrals can be calculated analytically
  - They are scaled version of element matrix for edge length $h=1$.

Element Matrices for Gravity

For element E with edge length h

edge length h=1

$$\mathbf{S}^E = \hat{\mathbf{S}}$$

$$\hat{\mathbf{S}} = \begin{bmatrix} \frac{2}{3} & -\frac{1}{6} & -\frac{1}{6} & -\frac{1}{3} \\ -\frac{1}{6} & \frac{2}{3} & -\frac{1}{3} & -\frac{1}{6} \\ -\frac{1}{6} & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{6} \\ -\frac{1}{3} & -\frac{1}{6} & -\frac{1}{6} & \frac{2}{3} \end{bmatrix}$$

$$\mathbf{b}^E = \rho_E \cdot h^2 \cdot \hat{\mathbf{b}}^0$$

$$\hat{\mathbf{b}}^0 = \left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]^T$$

Dirichlet-Type Boundary condition

- Once the the stiffness matrix is assembled eliminate rows corresponding to nodes p with Dirichlet-Type boundary condition.
- Simplest way: overwrite row p with equation:

$$U_p^h = 0$$

- That is:

$$b_p^h = 0 \text{ and } S_{pq}^h = \delta_{pq} \text{ all } q = 0, \ldots N-1$$

Gradient Calculation

- Gradient of FEM solution is **not** continuous.
- calculated at element centers $\boldsymbol{m}^E$:

$$\nabla u^h(\mathbf{m}^E) = \sum_{i=0}^{3} U^h_{\check{n}_{E,i}} \nabla N_i(\mathbf{m}^E)$$

Collects values given at FEM nodes
at the element vertices

Gradient Calculation (cont.)

- Again this can be relayed back to local basis function on an element with edge length *h=1:*

$$\frac{\partial N_i}{\partial x_0}(\mathbf{m}) = \frac{1}{h} B_{i0} \text{ and } \frac{\partial N_i}{\partial x_1}(\mathbf{m}) = \frac{1}{h} B_{i1}$$

$$\hat{\mathbf{B}}^0 = \left[-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}\right]^T \text{ and } \hat{\mathbf{B}}^1 = \left[-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]^T$$

- And then:

$$\nabla u_E^h = \frac{1}{h} \sum_{p=0}^{3} U_{\check{n}_{E,i}}^h [\hat{\mathbf{B}}_i^0, \hat{\mathbf{B}}_i^1]^T$$

Pseudo program

1) Initial stiffness matrix **S** and right hand side **b**
2) for all element E
   (a) Calculate local element matrices $\mathbf{S}_E$, $\mathbf{b}_E$
   (b) Add $\mathbf{S}_E$, $\mathbf{b}_E$ onto **S** and **b**
3) Overwrite equations for Dirichlet conditions in **S** and **b**
4) Solve **AU=b**
5) Return FEM solution **U** at FEM nodes.