جامعة الملك عبدالله للعلوم والتقنية
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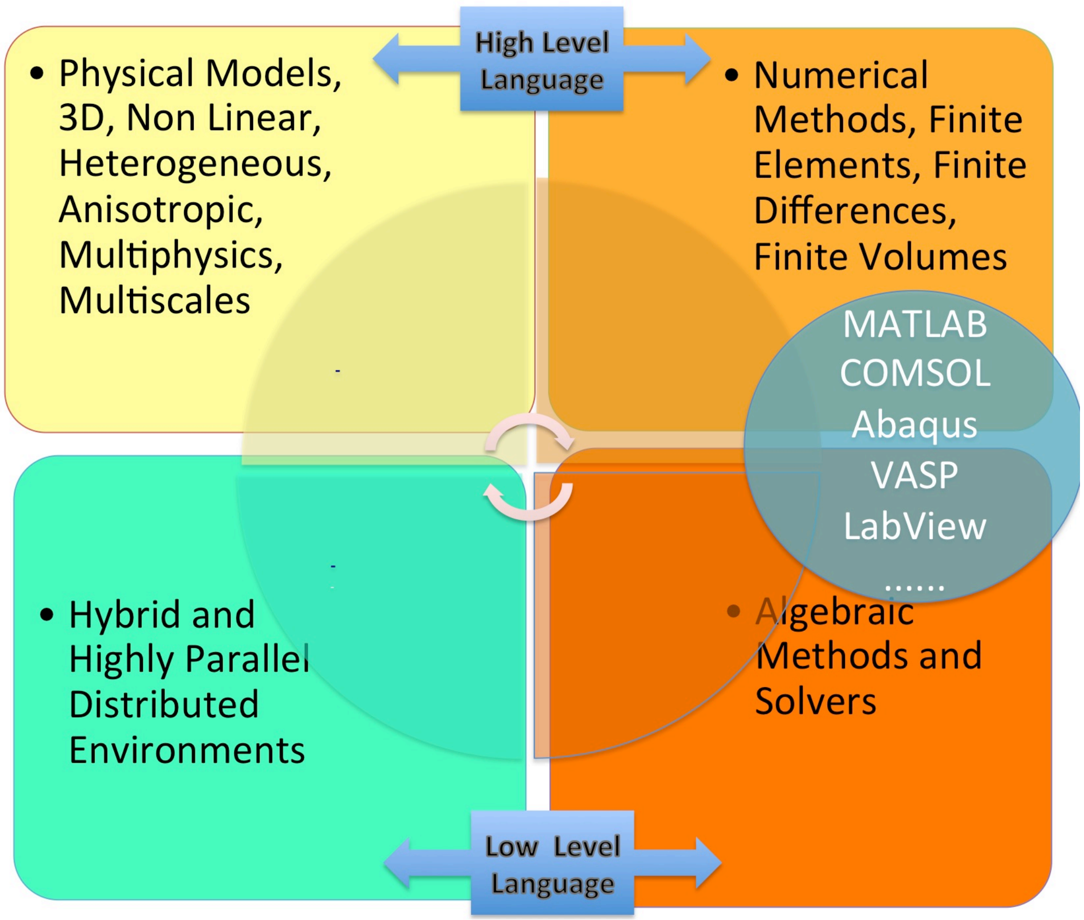
Information Technology
Research Computing

Numerical schemes
by Alain Clò

Numerical Schemes



Explicit and Implicit Methods

- Explicit scheme:

$$Y(t+\Delta t) = F(Y(t))$$

- Implicit scheme:

$$G(Y(t), Y(t+\Delta t)) = 0$$

Aim: Find $Y(t+\Delta t)$

More afford necessary for implicit scheme.

8

- Numerical Schemes
- Finite Difference
- Finite Elements
- Finite Volumes
- Integral Equations
- Spectral Methods

Numerical Schemes

- General comments
- Numerical Schemes
- Finite Difference
- Finite Elements

General comments

- From continuous space, functions, time to discrete, numeric world
- Well Posed Model
- Boundary Conditions (Dirichlet, Neumann, ...)
- Convergence
- Stability
- Consistency

Schemes of approximations in time

The equivalent ***approximations*** of the derivatives are:

$$\partial_t f^+ \approx \frac{f(x+dt) - f(x)}{dt}$$

forward difference => explicit

$$\partial_t f^- \approx \frac{f(x) - f(x-dt)}{dt}$$

backward difference => implicit

$$\partial_t f \approx \frac{f(x+dt) - f(x-dt)}{2dt}$$

centered difference => explicit or implicit

Explicit and Implicit schemes

- Discretisation in time
  - Centered difference - Explicit
  - Forward difference -Explicit
  - Backward difference - Implicit
- Finite Difference
  - Explicit scheme
  - Simple to implement and parallelize
  - Not always stable
- Finite Elements
  - Implicit scheme
  - Weak Formulation, Matrix inversion
  - Robust
- Finite Volumes
- Integral Equations

Acoustic 2D – Finite Differences

- The equation $$\frac{\partial^2 p}{\partial^2 t} = c^2\left(\frac{\partial^2 p}{\partial^2 x} + \frac{\partial^2 p}{\partial^2 y}\right) + s(x,y,t)$$
- The discretised domain is a 2D grid (x,y) where the Δx and Δy, are the steps in space. $\Delta x = \Delta y$
- Δt is the time step.
- The boundary condition :
  - at time t=0 $p=0$
  - on the borders of the grid : $p=0$ (full reflexion)

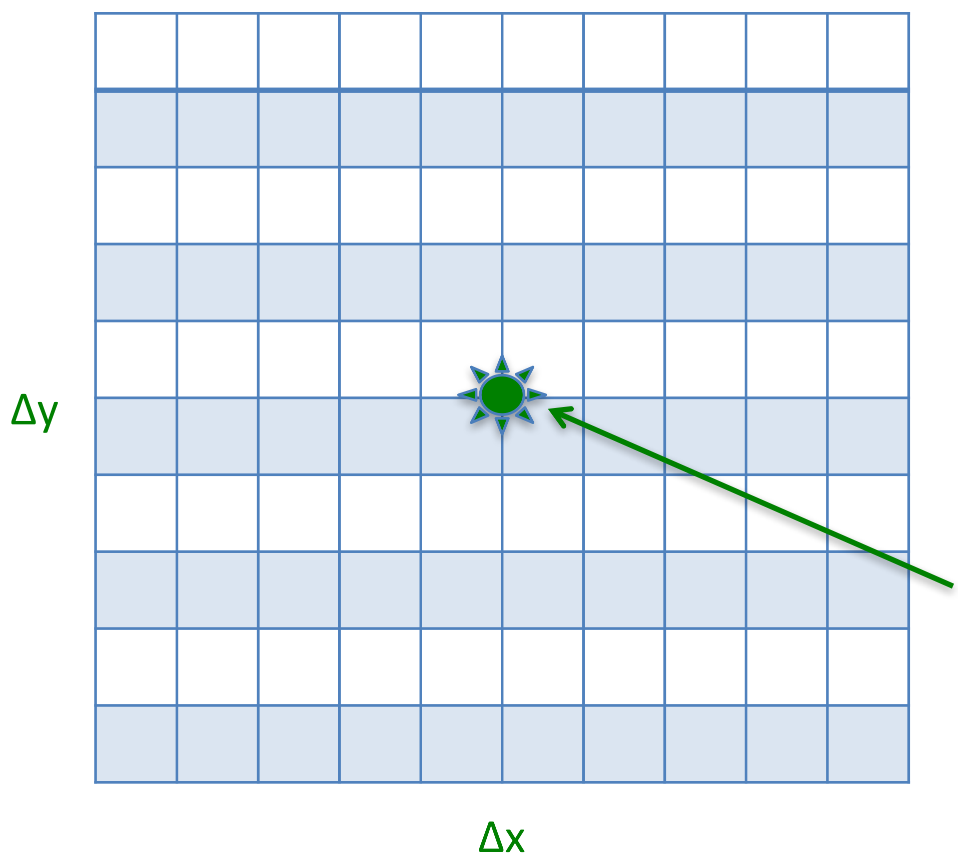
Finite Difference 2D Grid

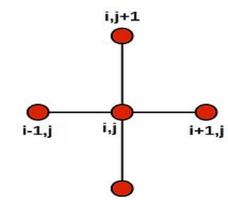
$$\frac{\partial^2 p}{\partial^2 t} = c^2\left(\frac{\partial^2 p}{\partial^2 x} + \frac{\partial^2 p}{\partial^2 y}\right) + s(x,y,t)$$

inside the domain Ω

outside Ω

p=0 on δΩ





stencil 2D in space

the source s(x,y,t)

Finite Difference

- The basic idea is to subdivide the domain into a regular grid where adjacent nodes are equidistant of each other of Δx or Δy.
- When of Δx or Δy are small enough, the differential equation can be approximated locally with finite difference equations.

Acoustic 2D – Discretisation

- Discretisation in time (Taylor Series)

$$\frac{\partial^2 p}{\partial^2 t} = \frac{p(t+\Delta t) - 2p(t) + p(t-\Delta t)}{\Delta t^2} + \mathrm{O}(\Delta t^2)$$

- Discretisation in space x:

$$\frac{\partial^2 p}{\partial^2 x} = \frac{p(x+\Delta x, y) - 2p(x,y) + p(x-\Delta x, y)}{\Delta x^2} + \mathrm{O}(\Delta x^2)$$

- Discretisation in space y:

$$\frac{\partial^2 p}{\partial^2 y} = \frac{p(x, y+\Delta y) - 2p(x,y) + p(x, y-\Delta y)}{\Delta y^2} + \mathrm{O}(\Delta y^2)$$

The Finite Element Method Defined

The Finite Element Method (FEM) is a weighted residual method that uses compactly-supported basis functions.

Brief Comparison with Other Methods

Finite Difference (FD) Method:

FD approximates an *operator* (e.g., the derivative) and solves a problem on a set of *points* (the grid)

Finite Element (FE) Method:

FE uses exact operators but approximates the *solution basis functions.* Also, FE solves a problem on the *interiors* of grid cells (and optionally on the grid points as well).

Brief Comparison with Other Methods

Spectral Methods:

Spectral methods use global basis functions to approximate a solution across the entire domain.

Finite Element (FE) Method:

FE methods use compact basis functions to approximate a solution on individual elements.

Overview of the Finite Element Method

$$(S) \Leftrightarrow (W) \approx (G) \Leftrightarrow (M)$$

- Strong form

$$\frac{\partial^2 p}{\partial^2 t} - c^2 \left(\frac{\partial^2 p}{\partial^2 x} + \frac{\partial^2 p}{\partial^2 y}\right) - s(x,y,t) = 0$$

- Weak form

$$v(x,y) = \sum_{j=1}^{n} b_j(t)\varphi_j(x,y)$$

$$\int \varphi_j . \frac{\partial^2 p}{\partial^2 t} dxdy + c^2 \int \nabla\varphi_j . \nabla p . dxdy - \int \varphi_j s(x,y,t) . dxdy = 0$$

- Galerkin Approximation
  - Basis Function

$$p = \sum_{i=1}^{n} a_i(t)\varphi_i(x,y)$$

  - Galerkin Form

$$\sum_{i=1}^{n} \frac{\partial^2 a}{\partial^2 t} . \int \varphi_i . \varphi_j . dxdy + c^2 \sum_{i=1}^{n} a_i \int \nabla\varphi_i . \nabla\varphi_j \, dxdy - \int \varphi_j s(x,y,t) . dxdy = 0$$

- Matrix form

$$M^t . \frac{\partial^2 a}{\partial t^2} + c^2 . N^t . a = S$$

- Matrix form *K.a=f* after using the finite difference scheme in time for **a**

Strong formulation

$$\frac{\partial^2 p}{\partial^2 t} - c^2 \left(\frac{\partial^2 p}{\partial^2 x} + \frac{\partial^2 p}{\partial^2 y}\right) - s(x, y, t) = 0$$

Weak formulation

$$v(x,y)=\sum_{j=1}^{n} b_j(t)\varphi_j(x,y)$$

$$\int \varphi_j . \frac{\partial^2 p}{\partial^2 t} dxdy + c^2 \int \nabla \varphi_j . \nabla p . dxdy - \int \varphi_j s(x,y,t) . dxdy = 0$$

Galerkin Approximation

$$p = \sum_{i=1}^{n} a_i(t)\varphi_i(x,y)$$

$$\sum_{i=1}^{n} \frac{\partial^2 a}{\partial^2 t} . \int \varphi_i . \varphi_j . dxdy + c^2 \sum_{i=1}^{n} a_i \int \nabla \varphi_i . \nabla \varphi_j \, dxdy - \int \varphi_j \, s(x,y,t) . dxdy = 0$$

Matrix form

$$M^t.\frac{\partial^2 a}{\partial t^2}+c^2.N^t.a=S$$

$$K.a=f$$

Then the system has to be solved

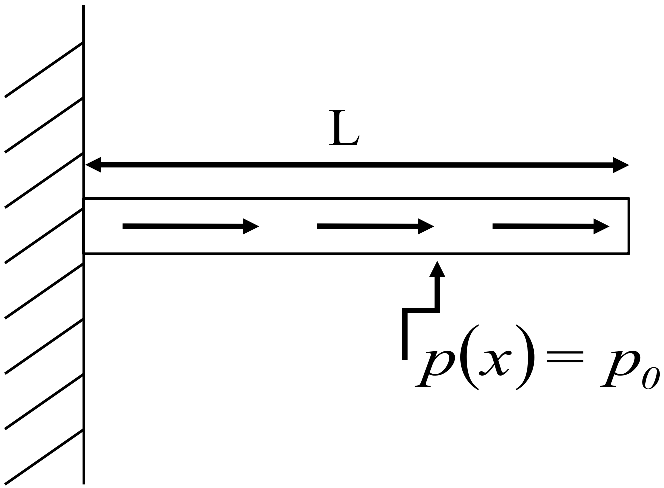
Solving the system

- Direct method
- Iterative method
- Using dense or sparse methods

Sample Problem

Axial deformation of a bar subjected to a uniform load

(1-D Poisson equation)



$$x = [0, L]$$

$$EA\frac{d^2u}{dx^2} = p_0$$

$$u(0) = 0$$

$$EA\left.\frac{du}{dx}\right|_{x=L} = 0$$

u = axial displacement

E=Young's modulus = 1

A=Cross-sectional area = 1

Strong Form

The set of governing PDE's, with boundary conditions, is called the "strong form" of the problem.

Hence, our strong form is (Poisson equation in 1-D):

$$\frac{d^2u}{dx^2} = p_0$$

$$u(0) = 0$$

$$\left.\frac{du}{dx}\right|_{x=L} = 0$$

Weak Form

We now reformulate the problem into the weak form.

The weak form is a *variational statement* of the problem in which we integrate against a *test function*. The choice of test function is up to us.

This has the effect of relaxing the problem; instead of finding an exact solution everywhere, we are finding a solution that satisfies the strong form on average over the domain.

Weak Form

$$\frac{d^2u}{dx^2} = p_0$$

Strong Form

$$\frac{d^2u}{dx^2} - p_0 = 0$$

Residual ***R****=0*

$$\int_0^L \left(\frac{d^2u}{dx^2} - p_0 \right) v dx = 0$$

Weak Form

v is our test function

We will choose the test function later.

Weak Form

Why is it "weak"?

It is a weaker statement of the problem.

A solution of the strong form will also satisfy the weak form, but not vice versa.

Analogous to "weak" and "strong" convergence:

$$\text{strong}: \lim_{n\to\infty} x_n = x$$

$$\text{weak}: \lim_{n\to\infty} \langle f \,|\, x_n \rangle = \langle f \,|\, x \rangle \;\; \forall f$$

Weak Form

Choosing the test function:

We can choose any *v* we want, so let's choose *v* such that it satisfies *homogeneous* boundary conditions wherever the actual solution satisfies *Dirichlet* boundary conditions. We'll see why this helps us, and later will do it with more mathematical rigor.

So in our example, $u(0)=0$ so let $v(0)=0$.

Weak Form

Returning to the weak form:

$$\int_0^L \left(\frac{d^2u}{dx^2} - p_0 \right) v dx = 0$$

$$\int_0^L \frac{d^2u}{dx^2} v dx = \int_0^L p_0 v dx$$

Integrate LHS by parts:

$$= -\int_0^L \frac{du}{dx} \frac{dv}{dx} dx + \left[v(x) \frac{du}{dx} \right]_{x=0}^{x=L}$$

$$= -\int_0^L \frac{du}{dx} \frac{dv}{dx} dx + v(L) \left. \frac{du}{dx} \right|_{x=L} - v(0) \left. \frac{du}{dx} \right|_{x=0}$$

Weak Form

Recall the boundary conditions on *u* and *v*:

$$u(0) = 0$$

$$\left.\frac{du}{dx}\right|_{x=L} = 0$$

$$v(0) = 0$$

Hence,

$$-\int_0^L \frac{du}{dx}\frac{dv}{dx}\,dx + v(L)\left.\frac{du}{dx}\right|_{x=L} - v(0)\left.\frac{du}{dx}\right|_{x=0}$$

$$\int_0^L \frac{du}{dx}\frac{dv}{dx}\,dx = \int_0^L p_0 v\,dx$$

The weak form satisfies Neumann conditions automatically!

Weak Form

Why is it "variational"?

$$\int_0^L \frac{du}{dx}\frac{dv}{dx}dx = \int_0^L p_0 v dx$$

Variational statement :

Find $u \in H^1$ such that $B(u,v) = F(v) \quad \forall v \in H_0^1$

B a bilinear functional, F a linear functional

u and *v* are functions from an infinite-dimensional function space *H*

Galerkin's Method

We still haven't done the "finite element method" yet, we have just restated the problem in the weak formulation.

So what makes it "finite elements"?

Solving the problem locally on elements

Finite-dimensional approximation to an infinite- dimensional space → **Galerkin's Method**

Galerkin's Method

Choose finite basis $\{\varphi_i\}_{i=i}^{N}$

Then,

$$u(x) = \sum_{j=1}^{N} c_j \varphi_j(x), \qquad c_j \text{ unkowns to solve for}$$

$$v(x) = \sum_{j=1}^{N} b_j \varphi_j(x), \qquad b_j \text{ arbitrarily chosen}$$

Insert these into our weak form :

$$\int_0^L \frac{du}{dx}\frac{dv}{dx}\,dx = \int_0^L p_0 v\,dx$$

$$\int_0^L \sum_{j=1}^{N} c_j \frac{d\varphi_j}{dx}(x) \sum_{i=1}^{N} b_i \frac{d\varphi_i}{dx}(x)\,dx = \int_0^L p_0 \sum_{j=1}^{N} b_j \varphi_j(x)\,dx$$

Galerkin's Method

$$\int_0^L \sum_{j=1}^{N} c_j \frac{d\varphi_j}{dx}(x) \sum_{i=1}^{N} b_i \frac{d\varphi_i}{dx}(x) dx = \int_0^L p_0 \sum_{j=1}^{N} b_j \varphi_j(x) dx$$

Rearranging :

$$\sum_{i=1}^{N} b_i \sum_{j=1}^{N} c_j \int_0^L \frac{d\varphi_j}{dx} \frac{d\varphi_i}{dx} dx = \sum_{i=1}^{N} b_i \int_0^L p_0 \varphi_i dx$$

Cancelling :

$$\sum_{j=1}^{N} c_j \int_0^L \frac{d\varphi_j}{dx} \frac{d\varphi_i}{dx} dx = \int_0^L p_0 \varphi_i dx$$

Galerkin's Method

$$\sum_{j=1}^{N} c_j \int_0^L \frac{d\varphi_j}{dx}\frac{d\varphi_i}{dx}\,dx = \int_0^L p_0 \varphi_i \, dx$$

We now have a matrix problem $\mathbf{Kc} = \mathbf{F}$, where c_j is a vector of unknowns,

$$K_{ij} = \int_0^L \frac{d\varphi_j}{dx}\frac{d\varphi_i}{dx}\,dx,$$

and $F_i = \int_0^L p_0 \varphi_i \, dx$

We can already see K_{ij} will be symmetric since we can interchange i, j without effect.

Galerkin's Method

So what have we done so far?

1) Reformulated the problem in the weak form.

2) Chosen a finite-dimensional approximation to the solution.

Recall weak form written in terms of residual:

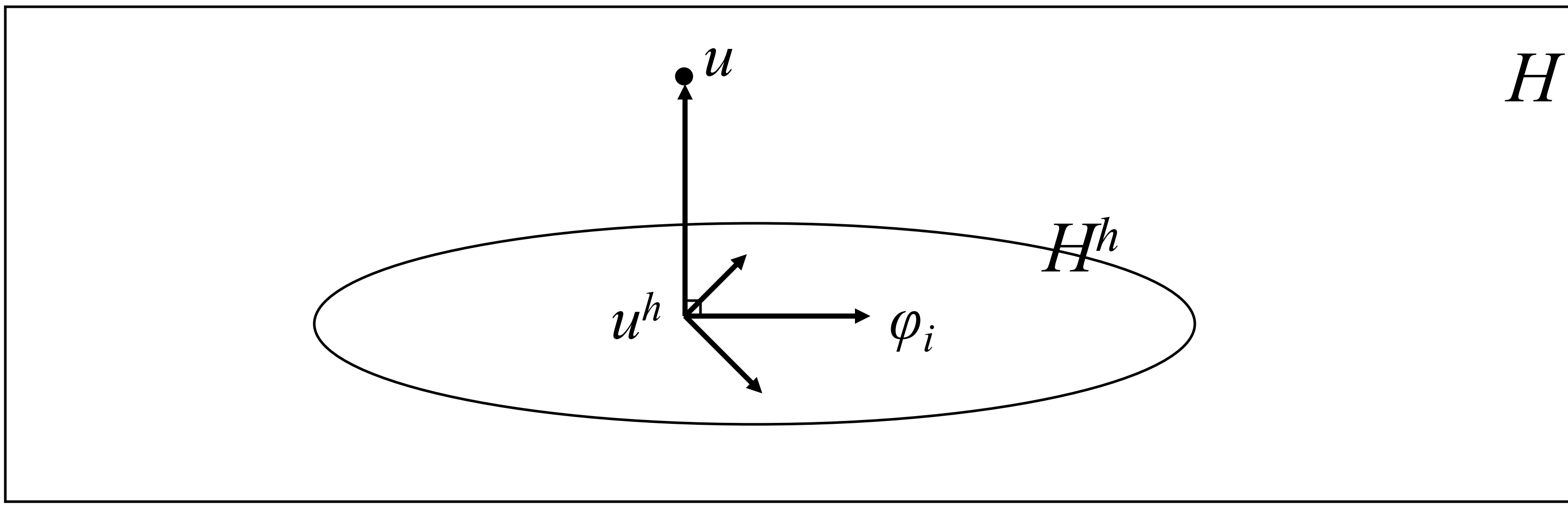
$$\int_0^L \left(\frac{d^2u}{dx^2} - p_0 \right) v\,dx = \int_0^L \mathbf{R} v\,dx = \sum_i b_i \int_0^L \mathbf{R} \varphi_i\,dx = 0$$

This is an L_2 inner-product. Therefore, the residual is orthogonal to our space of basis functions. "Orthogonality Condition"

Orthogonality Condition

$$\int_0^L \left(\frac{d^2 u}{dx^2} - p_0 \right) v\,dx = \int_0^L \mathbf{R} v\,dx = \sum_i b_i \int_0^L \mathbf{R} \varphi_i\,dx = 0$$

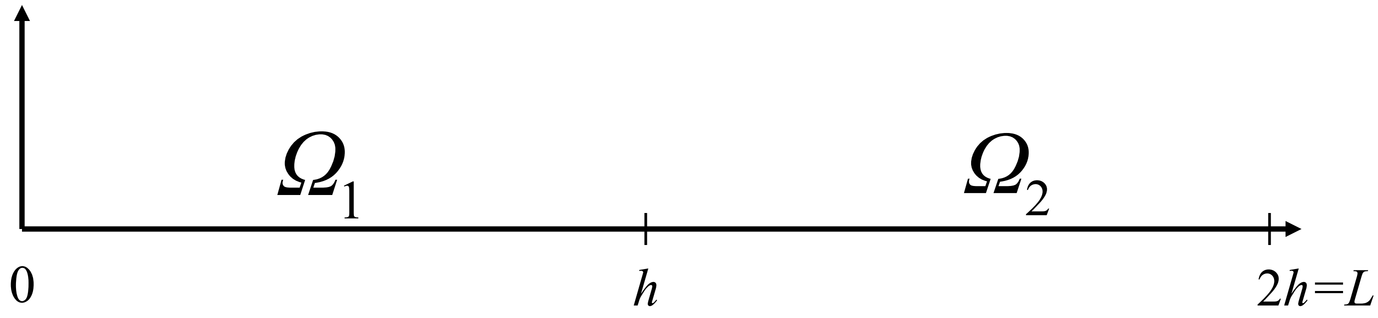
The residual is orthogonal to our space of basis functions:



Therefore, given some space of approximate functions H^h, we are finding u^h that is closest (as measured by the L_2 inner product) to the actual solution u.

Discretization and Basis Functions

Let's continue with our sample problem. Now we discretize our domain. For this example, we will discretize x=[0, L] into 2 "elements".

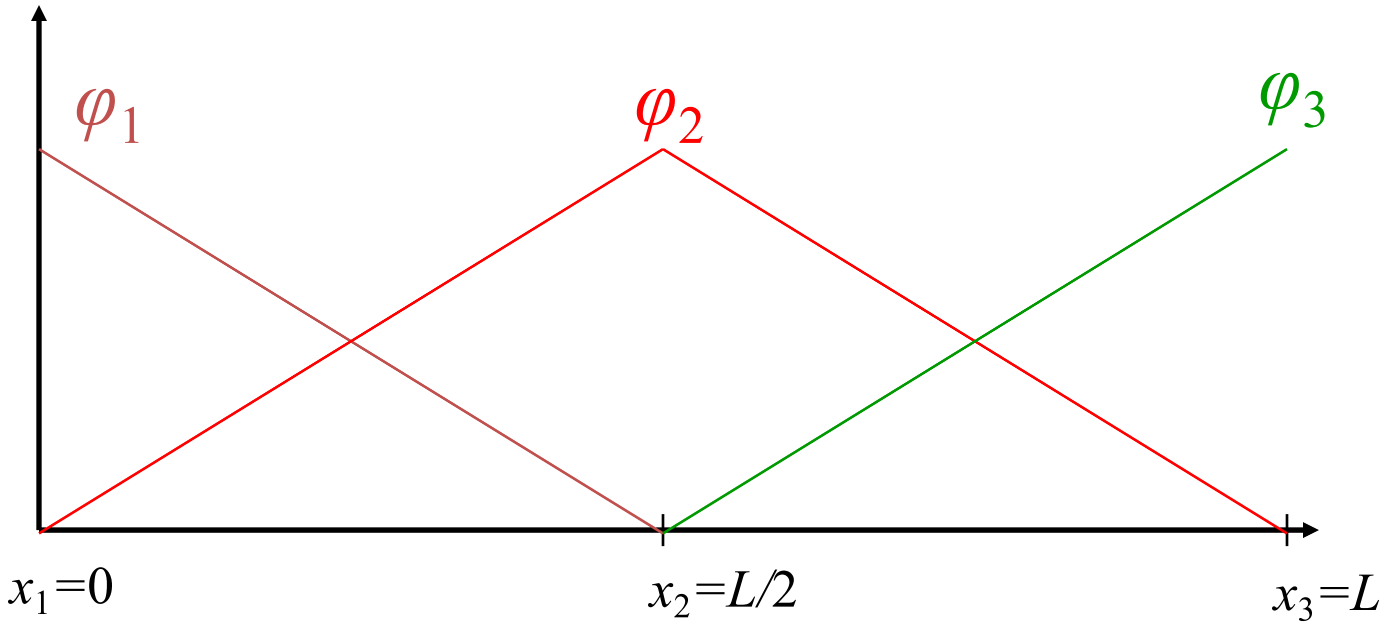


In 1-D, elements are segments. In 2-D, they are triangles, tetrads, etc. In 3-D, they are solids, such as tetrahedra. We will solve the Galerkin problem on each element.

Discretization and Basis Functions

For a set of basis functions, we can choose anything. For simplicity here, we choose piecewise linear "hat functions".

Our solution will be a linear combination of these functions.



Basis functions satisfy: $\varphi_i(x_j) = \delta_j^i \Rightarrow$ Our solution will be interpolatory. Also, they satisfy the partition of unity.

Matrix Formulation

Given our matrix problem $\mathbf{Kc} = \mathbf{F}$:

$$\sum_{j=1}^{N} \underbrace{c_j}_{\mathbf{c}} \underbrace{\int_0^L \frac{d\varphi_j}{dx}\frac{d\varphi_i}{dx}\,dx}_{\mathbf{K}} = \underbrace{\int_0^L p_0\varphi_i dx}_{\mathbf{F}} \Rightarrow \mathbf{Kc} = \mathbf{F}$$

We can insert the φ_i chosen on the previous slide and arrive at a linear algebra problem. Differentiating the basis functions, then evaluating the integrals, we have :

$$\mathbf{K} = \frac{1}{L}\begin{bmatrix} 4 & -2 \\ -2 & 2 \end{bmatrix}, \quad \mathbf{F} = \frac{p_0}{L}\begin{bmatrix} \frac{1}{2} \\ \frac{1}{4} \end{bmatrix}$$

In a computer code, differentiating the basis functions can be done in advance, since the basis functions are known, and integration would be performed numerically by quadrature. It is standard in FEM to use Gaussian quadrature, since it is exact for polynomials.

Notice $\mathbf{K}$ is symmetric as expected.

Solution

Solving the Gaussian elimination problem on the previous slide, we obtain our coefficients c_i :

$$\mathbf{c} = \begin{bmatrix} \frac{3 p_0 L^2}{8} \\ \frac{p_0 L^2}{2} \end{bmatrix},$$ which when multiplied by basis functions φ_i gives our final numerical solution :

$$\varphi(x) = \begin{cases} \frac{3}{4} p_0 L x & \text{when } x \in \left[0, \frac{L}{2}\right] \\ \frac{1}{4} p_0 (L^2 + Lx) & \text{when } x \in \left[\frac{L}{2}, L\right] \end{cases}$$

The exact analytical solution for this problem is :

$$u(x) = p_0 L x - \frac{p_0 x^2}{2}$$

Thank You

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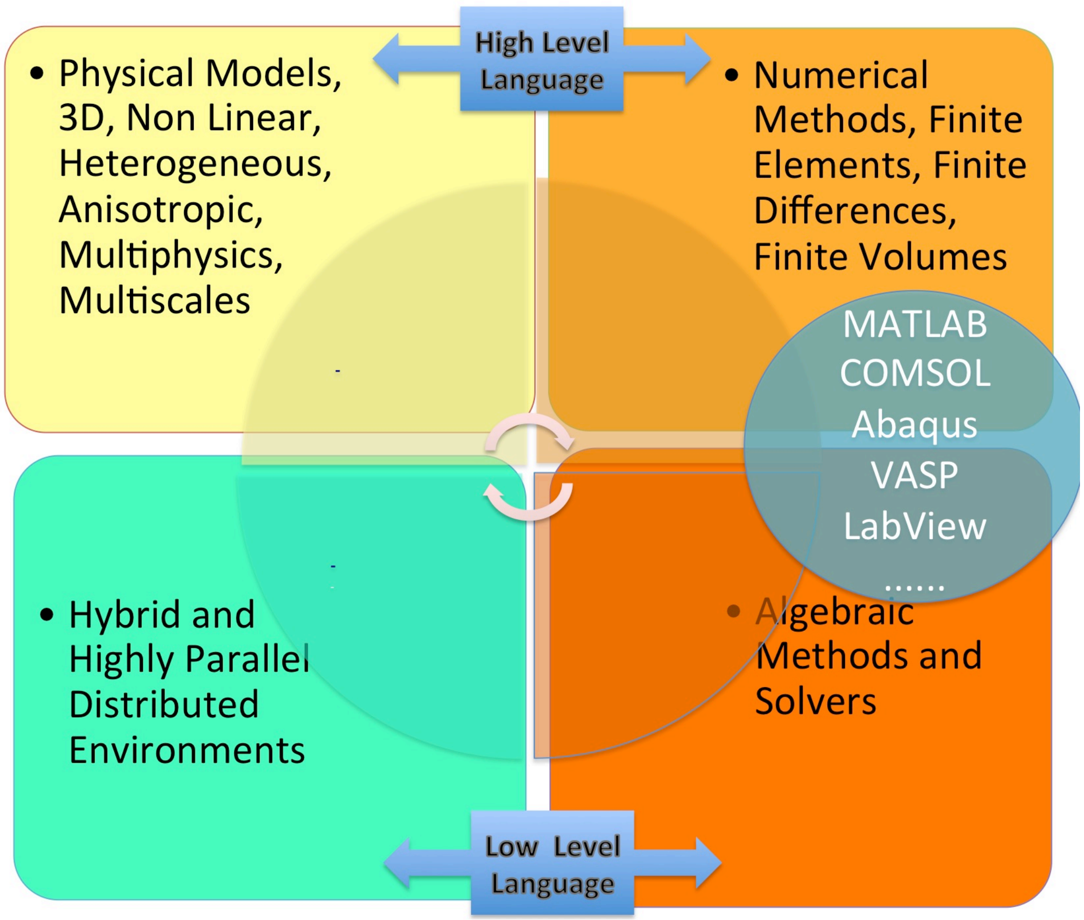
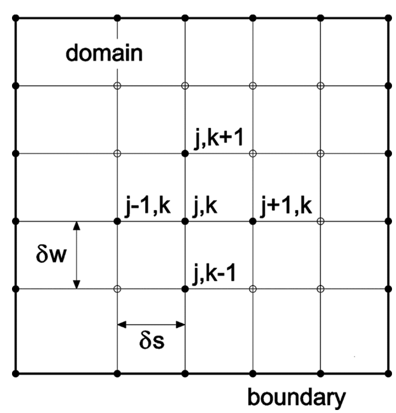
Discretisation



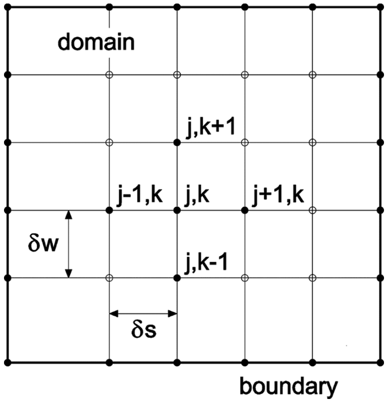
$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$



Discretisation

- Taylor Series
- Finite Differences
- Let's try to discretise with the wave equation
- Other Numerical Methods
  - finite elements
  - finite volumes
  - pseudospectral

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$



Approximations of the derivatives

Common definitions of the derivative of f(x):

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x) - f(x-dx)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x-dx)}{2dx}$$

These are all correct definitions in the limit dx->0.

But we want dx to remain <u>FINITE</u>

Schemes of approximations in space

The equivalent ***approximations*** of the derivatives are:

$$\partial_x f^+ \approx \frac{f(x+dx)-f(x)}{dx}$$

forward difference

$$\partial_x f^- \approx \frac{f(x)-f(x-dx)}{dx}$$

backward difference

$$\partial_x f \approx \frac{f(x+dx)-f(x-dx)}{2dx}$$

centered difference

Schemes of approximations in time

The equivalent ***approximations*** of the derivatives are:

$$\partial_t f^+ \approx \frac{f(x+dt)-f(x)}{dt}$$

forward difference => explicit

$$\partial_t f^- \approx \frac{f(x)-f(x-dt)}{dt}$$

backward difference => implicit

$$\partial_t f \approx \frac{f(x+dt)-f(x-dt)}{2dt}$$

centered difference => explicit or implicit

Taylor Series

Taylor series are expansions of a function f(x) for some finite distance dx to f(x+dx)

$$f(x \pm dx) = f(x) \pm \mathrm{dx} f^{'}(x) + \frac{dx^2}{2!} f^{''}(x) \pm \frac{dx^3}{3!} f^{'''}(x) + \frac{dx^4}{4!} f^{''''}(x) \pm \ldots$$

What happens, if we use this expression for

$$\partial_x f^+ \approx \frac{f(x+dx) - f(x)}{dx}$$

?

Taylor Series

... that leads to :

$$\frac{f(x+dx)-f(x)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^{2}}{2!}f^{''}(x)+\frac{dx^{3}}{3!}f^{'''}(x)+\ldots\right]$$

$$=f^{'}(x)+O(dx)$$

The error of the first derivative using the *forward* formulation is ***of order dx***.

Is this the case for other formulations of the derivative?
Let's check!

Taylor Series

... with the *centered* formulation we get:

$$\frac{f(x+dx/2)-f(x-dx/2)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^{3}}{3!}f^{'''}(x)+\ldots\right]$$

$$=f^{'}(x)+O(dx^{2})$$

The error of the first derivative using the centered approximation is ***of order dx^2***.

This is an **important** result: it DOES matter which formulation we use. The **centered scheme** is more accurate!

Let‘s try the wave equation

- Simple geophysical partial differential equations
- Finite differences – definitions
- Finite Difference Approximations to PDEs
  – Acoustic wave equation in 2D
- Finite differences and Taylor Expansion
- Stability -> The CFL Criterion
- Numerical dispersion
- Other Numerical Methods

$$\partial_x f \approx \frac{f(x+dx)-f(x)}{dx}$$

Acoustic 2D – Finite Differences

- The equation $$\frac{\partial^2 p}{\partial^2 t} = c^2\left(\frac{\partial^2 p}{\partial^2 x} + \frac{\partial^2 p}{\partial^2 y}\right) + s(x,y,t)$$
- The discretised domain is a 2D grid (x,y) where the Δx and Δy, are the steps in space. Δx = Δy
- Δt is the time step.
- The boundary condition :
  - at time t=0 *p*=0
  - on the borders of the grid : *p*=0 (full reflexion)

Finite Difference 2D Grid

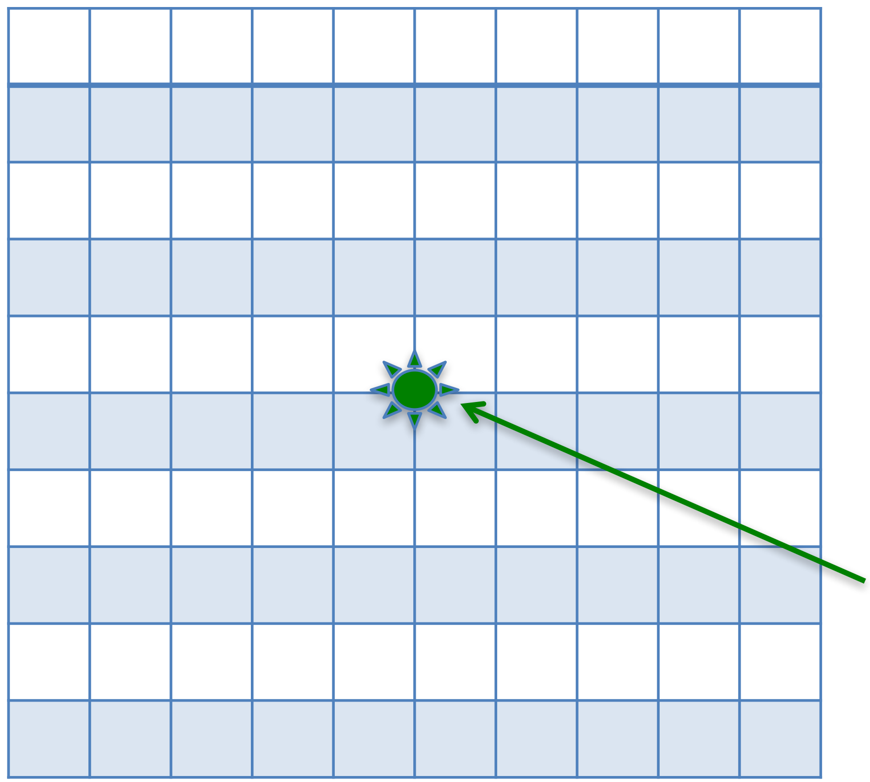
$$\frac{\partial^2 p}{\partial^2 t} = c^2\left(\frac{\partial^2 p}{\partial^2 x} + \frac{\partial^2 p}{\partial^2 y}\right) + s(x,y,t)$$

inside the domain Ω

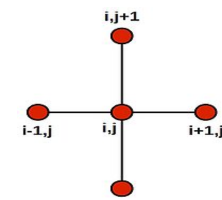
outside Ω

p=0 on δΩ

Δy



Δx



stencil 2D in space

the source s(x,y,t)

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- The basic idea is to subdivide the domain into a regular grid where adjacent nodes are equidistant of each other of Δx or Δy.
- When of Δx or Δy are small enough, the differential equation can be approximated locally with finite difference equations.

Acoustic 2D – Discretisation

- Discretisation in time (Taylor Series)

$$\frac{\partial^2 p}{\partial^2 t} = \frac{p(t+\Delta t) - 2p(t) + p(t-\Delta t)}{\Delta t^2} + \mathrm{O}(\Delta t^2)$$

- Discretisation in space x:

$$\frac{\partial^2 p}{\partial^2 x} = \frac{p(x+\Delta x, y) - 2p(x,y) + p(x-\Delta x, y)}{\Delta x^2} + \mathrm{O}(\Delta x^2)$$

- Discretisation in space y:

$$\frac{\partial^2 p}{\partial^2 y} = \frac{p(x, y+\Delta y) - 2p(x,y) + p(x, y-\Delta y)}{\Delta y^2} + \mathrm{O}(\Delta y^2)$$

Acoustic 2D – Discretisation

- Total Discretisation with central difference, 2nd order, explicit scheme

$$
\boxed{
\begin{aligned}
&p(t+\Delta t) = 2p(t) - p(t-\Delta t) + \\
&\Delta t^2 * c^2 * (\\
&\frac{p(x+\Delta x, y) - 2p(x,y) + p(x-\Delta x, y)}{\Delta x^2} + \\
&\frac{p(x, y+\Delta y) - 2p(x,y) + p(x, y-\Delta y)}{\Delta y^2} \\
&+ s(x,y,t))
\end{aligned}
}
$$

- Conversion, Stability, Dispersion CFL

$$\boxed{c\frac{\Delta t}{\Delta x} \leq 1}$$

Numerical methods: Finite Difference

Finite Differences - Summary

- Conceptually the most simple of the numerical methods and can be learned quite quickly
- Depending on the physical problem FD methods are conditionally stable (relation between time and space increment)
- FD methods have difficulties concerning the accurate implementation of boundary conditions (e.g. free surfaces, absorbing boundaries)
- FD methods are usually explicit and therefore very easy to implement and efficient on parallel computers
- FD methods work best on regular, rectangular grids

Numerical methods: properties

Finite differences →

- time-dependent PDEs
- seismic wave propagation
- geophysical fluid dynamics
- Maxwell's equations
- Ground penetrating radar

-> robust, simple concept, easy to parallelize, regular grids, explicit method

Finite elements →

- static and time-dependent PDEs
- seismic wave propagation
- geophysical fluid dynamics
- all problems

-> implicit approach, matrix inversion, well founded, <u>irregular grids</u>, more complex algorithms, engineering problems

Finite volumes →

- time-dependent PDEs
- seismic wave propagation
- mainly fluid dynamics

-> robust, simple concept, <u>irregular grids</u>, explicit method

Thank You

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