Numerical Analysis and Methods for PDE I

A. J. Meir

Department of Mathematics and Statistics
Auburn University

US-Africa Advanced Study Institute on Analysis, Dynamical Systems, and Mathematical Modeling of Biological Systems
Dec. 2–Dec. 12, 2011

This project is supported by a grant from the NSF

Outline

1. Introduction
2. Partial Differential Equations
3. Discretization
4. Model Problem
   - Finite Difference Discretization
   - Homogenization and Weak Formulation
   - Finite Element Discretization
   - Finite Volume Discretization

Modeling

Physical Problem

The actual problem we want to study

↓

Mathematical Model

Equations, usually o.d.e, or p.d.e., hence also continuous model, usually posed in an infinite dimensional space

↓

Approximate Model

Equations, usually algebraic equations, hence also discrete model, usually posed in a finite dimensional space

Modeling and Simulation

Physical Problem

↓

Mathematical Model

↓

Numerical Model

Direct Simulation	Finite Differences	Finite Volumes	Finite Elements	Spectral Methods	Particle Methods

↓

Algebraic Equations
(linear or nonlinear)

Motivation

- Many processes in natural sciences, engineering, and economics (social sciences) are governed by partial differential equations (p.d.e.)
- The efficient *numerical solution** of such equations plays an ever-increasing role in state-of-the-art technology
- The enormous computing power available allows us to simulate *real world problems*

---

*Numerical approximation of solutions

Partial Differential Equations (P.D.E.)

P.D.E. model many and various phenomena, but relatively few have closed form solutions

A p.d.e. is an equation that contains partial derivatives of an unknown function* $u : \Lambda \mapsto \mathbb{R}$

The domain $\Lambda \subset \mathbb{R}^d$ with $d \geq 2$ (if $d = 1$ it is an o.d.e.); $\Lambda = \Omega \times (0, T)$

- Poisson's equation $-\Delta u = f$
- Heat equation $u_t - \Delta u = f$
- Wave equation $u_{tt} - \Delta u = f$
- Biharmoninc equation $\Delta\Delta u = f$

---

*We can also consider systems of p.d.e.

** $-\Delta u = -\sum_{i=1}^{d} u_{x_i x_i}$

Partial Differential Equations

More generally for a domain $\Omega \subset \mathbb{R}^{d-1}$

$$Lu = -\sum_{i=1}^{d-1} a_{ij}(x) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{d-1} b_j(x) \frac{\partial u}{\partial x_i} + c(x)u$$

Assume $a_{ij} = a_{ji}$, the differential operator L is elliptic if there exists a $\lambda > 0$ such that for all $x \in \Omega$ and $\xi \in \mathbb{R}^{d-1}$

$$\sum_{i=1}^{d-1} a_{ij}(x)\xi_i \cdot \xi_j \geq \lambda \sum_{i=1}^{d-1} \xi_i^2$$

- Elliptic equation $\quad Lu = f$
- Parabolic equation $\quad u_t + Lu = f$
- Hyperbolic equation $\quad u_{tt} + Lu = f$

Partial Differential Equations

Classification of P.D.E.

- Poisson's equation $-\Delta u = f$
  elliptic - equilibrium $u : \Omega \mapsto \mathbb{R}$
- Heat equation $u_t - \Delta u = f$
  parabolic - diffusion, decay $u : \Lambda \mapsto \mathbb{R}$
- Wave equation $u_{tt} - \Delta u = f$
  hyperbolic - propagation $u : \Lambda \mapsto \mathbb{R}$

Note, here the domain $\Omega \subset \mathbb{R}^{d-1}$ and $\Lambda = \Omega \times (0, T)$, later we will denote the boundary of Ω by $\partial\Omega$

---

*This classification is not exhaustive and p.d.e. may change type

Remarks

- In order to obtain a well posed problem we may have to supplement the p.d.e. with initial conditions (i.c.), boundary conditions (b.c.), or both (as appropriate)
- In this talk I will introduce the finite element method.

  Finite element methods may be used to solve* elliptic, parabolic, and hyperbolic equations, (as well as first order systems, and other types of equations) although they were originally developed to approximate solutions of elliptic p.d.e.**

---

*this is a misnomer it should be *approximate solutions of*

**We will initially look at the finite element method for elliptic p.d.e

Discretization

The basic idea behind any numerical method for approximating solutions of p.d.e. is to replace the *continuous* problem (p.d.e.) by a *discrete* problem

- Continuous problem (p.d.e.) - posed on an *infinite dimensional space**
- Discrete problem - posed on a *finite dimensional space***

*The solution lies in some infinite dimensional space
**The solution lies in some finite dimensional space

Common Discretizations

- Finite Difference Method - approximate the differential operator
- Finite Element Method - approximate the solution

- Finite Volume Method - write the equation in conservation form, approximate a conservation law
- Spectral Method - approximate the solution
- Spectral Element Method - approximate the solution
- Collocation Method - require that the equation hold at special points (collocation points)

Finite Elements

"The finite element method has been an astonishing success. It was created to solve the complicated equations of elasticity and structural mechanics, and for those problems it has essentially superseded the method of finite differences. Now other applications are rapidly developing. Whenever flexibility in geometry is important—and the power of the computer is needed not only to *solve* a system of equations, but also to *formulate* and *assemble* the discrete approximation in the first place—the finite element method has something to contribute."

Gilbert Strang and George J. Fix (1973)*

*Gilbert Strang, George Fix; An Analysis of the Finite Element Method, Second Edition, Wellesley-Cambridge Press (Distributed by SIAM) 2008.

Disclaimers

- I will try to illustrate the main ideas behind the finite element method (and maybe some other methods)
- All the statements I make can be made mathematically rigorous
- Can be extended to problems in d-dimensions
- Can be extended to more complex problems

History

- Finite difference methods
  - Ancient
- Finite element methods
  - Courant (1943)
  - Argyris (1954), Turner (1956)
  - Clough (1960)
  - Engineering literature 1960–1970 (early developments), and 1970–
  - Mathematics literature 1970–

Finite Elements vs. Finite Differences

Finite Elements - *approximate the solution*

Replace p.d.e. by a weak formulation (variational problem; optimization problem)

Approximate the solution by a function in a suitable finite dimensional function space

Finite Differences - *approximate the differential operator*

Replace p.d.e. by a difference equation

Solve the difference equation

Model Problem 1-d

Consider the model problem, $\Omega = (0, 1)$

$$-u''(x) + c(x)u(x) = f(x) \qquad x \in \Omega$$

with b.c.

$$u(0) = g_0 \qquad u(1) = g_1$$

Note, this is a t.p.b.v.p. (not an i.v.p.) this is the 1-d (d.e.) analog of the p.d.e. $-\Delta u + cu = f$ in Ω with (Dirichlet) b.c. $u|_{\partial\Omega} = g$

Finite Difference Approximation

$$u'(x) \approx \frac{u(x+h) - u(x)}{h} \qquad O(h)$$

$$u'(x) \approx \frac{u(x) - u(x-h)}{h} \qquad O(h)$$

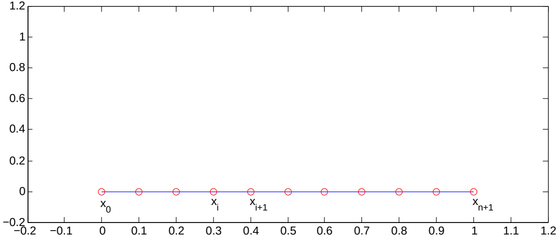
$$u'(x) \approx \frac{u(x+h) - u(x-h)}{2h} \qquad O(h^2)$$

$$u''(x) \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} \qquad O(h^2)$$

Finite Difference Mesh

Finite difference mesh, or grid

$$x_i = ih \qquad i = 0, 1, \ldots n+1 \qquad h = \frac{1}{n+1}$$



Finite Difference Discretization

Replace the equation for u

$$-u''(x) + c(x)u(x) = f(x) \qquad x \in \Omega$$

with b.c.

$$u(0) = g_0 \qquad u(1) = g_1$$

by algebraic equations for a grid function $u_i^h = u^h(x_i)$

$$\frac{-u_{i-1}^h + 2u_i^h - u_{i+1}^h}{h^2} + c(x_i)u_i^h = f(x_i) \qquad 1 \leq i \leq n$$

and

$$u_0^h = g_0 \qquad u_{n+1}^h = g_1$$

Finite Difference Approximation

This is the system of algebraic equations (for $c(x) = c$, a constant) we get

$$\frac{1}{h^2}\begin{bmatrix} 2+ch^2 & -1 & & & \\ -1 & 2+ch^2 & -1 & & \\ & -1 & 2+ch^2 & -1 & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 2+ch^2 \end{bmatrix}\begin{bmatrix} u_1^h \\ u_2^h \\ u_3^h \\ \vdots \\ u_n^h \end{bmatrix} = \begin{bmatrix} f_1 + \frac{g_0}{h^2} \\ f_2 \\ f_3 \\ \vdots \\ f_n + \frac{g_1}{h^2} \end{bmatrix}$$

This system matrix is symmetric, positive definite, hence the system has a unique solution and $u(x_i) \approx u_i^h$

Homogenization

Given

$$-u''(x) + c(x)u(x) = f(x) \qquad x \in \Omega$$

with b.c.

$$u(0) = g_0 \qquad u(1) = g_1$$

Find a function* g such that $g(0) = g_0$ and $g(1) = g_1$
Set $\hat{u} = u - g$

---

*The function g must belong to some space of admissible functions

Homogenization - Continued

Solve the homogeneous problem

$$-\hat{u}''(x) + c(x)\hat{u}(x) = \hat{f}(x) \qquad x \in \Omega$$

with b.c.

$$\hat{u}(0) = 0 \qquad \hat{u}(1) = 0$$

where

$$\hat{f}(x) = f(x) + g''(x) - c(x)g(x)$$

Then

$$u(x) = \hat{u}(x) + g(x)$$

Variational Lemma and Weak Derivative

Variational Lemma Let $v \in L^1(\Omega)_{\mathrm{loc}}$, $\Omega \subset \mathbb{R}^d$ nonempty, if

$$\int_\Omega v(x)\phi(x)\,dx = 0 \qquad \text{for all } \phi \in C_0^\infty(\Omega)$$

then $v = 0$ a.e. in Ω

Weak Derivative Let $\Omega \subset \mathbb{R}^d$ nonempty, $v, w \in L^1(\Omega)_{\mathrm{loc}}$, then w is the weak α^{th}derivative of v if

$$\int_\Omega v(x)D^\alpha\phi(x)\,dx = (-1)^{|\alpha|}\int_\Omega w(x)\phi(x)\,dx \qquad \text{for all } \phi \in C_0^\infty(\Omega)$$

$^*\alpha = (\alpha_1, \ldots \alpha_d)$ and $D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha 1} \ldots \partial x_d^{\alpha d}}$ where $|\alpha| = \sum_{i=1}^d \alpha_i$

Weak Form

Multiply the d.e. by a *test function* v and integrate over $\Omega = (0,1)$

$$\int_0^1 [-\hat{u}''(x) + c(x)\hat{u}(x)]v(x)\,dx = \int_0^1 \hat{f}(x)v(x)\,dx$$

v in some appropriate function space* V
Integrating by parts we get

$$\begin{aligned}\int_0^1 &(-\hat{u}''(x) + c(x)\hat{u}(x))v(x)\,dx \\ &= -\hat{u}'(1)v(1) + \hat{u}'(0)v(0) + \int_0^1 \hat{u}'(x)v'(x) + c(x)\hat{u}(x)v(x)\,dx\end{aligned}$$

*Here $V = H_0^1(0,1)$, those unfamiliar with Sobolev spaces can think $v \in C[0,1]$ such that v' is piecewise continuous and bounded on $[0,1]$ with $v(0) = v(1) = 0$

Weak and Variational Formulations

Define

$$(u, v) = \int_0^1 u(x)v(x)\,dx$$

and

$$F(v) = \frac{1}{2}[(v', v') + (cv, v)] - (\hat{f}, v)$$

Weak and Variational Formulations - Continued

The weak problem is find $\hat{u} \in V$ such that

$$(\hat{u}', v') + (c\hat{u}, v) = (\hat{f}, v) \quad \text{for all} \quad v \in V$$

The variational problem is find $\hat{u} \in V$ such that

$$F(\hat{u}) \leq F(v) \quad \text{for all} \quad v \in V$$

Then $u = \hat{u} + g$ is a weak (or variational) solution of the original problem

If u is sufficiently regular, it is a strong solution, or a classical solution of the p.d.e.

The Discrete Problem

Construct a finite dimensional space* $V^h \subset V$

Solve the discrete weak (or variational problem) find $\hat{u}^h \in V^h$ such that

$$(\hat{u}^{h\prime}, v^{h\prime}) + (c\hat{u}^h, v^h) = (\hat{f}, v^h) \quad \text{for all} \quad v^h \in V^h$$

or find $\hat{u}^h \in V^h$ such that

$$F(\hat{u}^h) \leq F(v^h) \quad \text{for all} \quad v^h \in V^h$$

Then $\hat{u}^h + g^h$ is an approximation to u the solution of the p.d.e. (where g^h is some approximation to g)

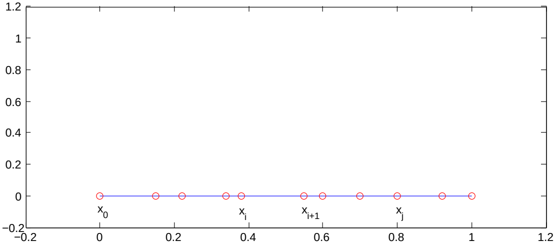
*This leads to, so called, conforming finite element methods, if this inclusion does not hold we have nonconforming finite elements

Finite Elements

Finite element mesh, or grid

$$0 = x_0 < x_1 < \ldots < x_n < x_{n+1} = 1$$

$$I_i = (x_{i-1}, x_i) \qquad h_i = |I_i| = x_i - x_{i-1}$$



Finite Elements

$$h = \max_{1 \le i \le n+1} \{h_i\}$$

h is a measure of the *size* of the grid (the smaller h the finer the grid, higher resolution, more accurate solution, higher dimensional space)

Linear Finite Element Space

The simplest finite element space is that of continuous piecewise linear functions (which are zero at 0 and 1)
A basis for V^h can be constructed as follows

$$\phi_j \in V^h \qquad 1 \leq j \leq n$$

$$\phi_j(x_i) = \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases}$$

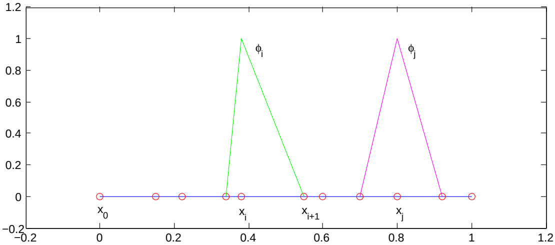
Obviously any $v^h \in V^h$ can be written as

$$v^h(x) = \sum_{i=1}^{n} v_i^h \phi_i(x) \qquad \text{for} \qquad x \in [0,1]$$

where $v_i^h = v^h(x_i)$

Linear Finite Elements

Piecewise linear basis functions



Weak Form - Revisited

$$(\hat{u}^{h'}, v^{h'}) + (c\hat{u}^h, v^h) = (\hat{f}, v^h) \quad \text{for all} \quad v^h \in V^h$$

is equivalent to

$$(\hat{u}^{h'}, \phi_j') + (c\hat{u}^h, \phi_j) = (\hat{f}, \phi_j) \quad \text{for} \quad 1 \le j \le n$$

and substituting $\hat{u}^h(x) = \sum_{i=1}^{n} \hat{u}_i^h \phi_i(x)$

$$\sum_{i=1}^{n} \hat{u}_i^h [(\phi_i', \phi_j') + (c\phi_i, \phi_j)] = (\hat{f}, \phi_j) \quad \text{for} \quad 1 \le j \le n$$

Algebraic System

This (for $c(x) = c$, a constant) is the algebraic system

$$\frac{1}{h}\begin{bmatrix} 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & & & \\ -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & & \\ & -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & \\ & \ddots & \ddots & \ddots & \\ & & & -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} \end{bmatrix}\begin{bmatrix} \hat{u}_1^h \\ \hat{u}_2^h \\ \hat{u}_3^h \\ \vdots \\ \hat{u}_n^h \end{bmatrix} = \begin{bmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \tilde{f}_3 \\ \vdots \\ \tilde{f}_n \end{bmatrix}$$

This system matrix is symmetric, positive definite, hence the system has a unique solution and

$$u(x) \approx u^h(x) = \hat{u}^h(x) + g^h(x) = \sum_{i=1}^{n} \hat{u}_i^h \phi_i(x) + g^h(x)$$

Finite Elements vs. Finite Difference

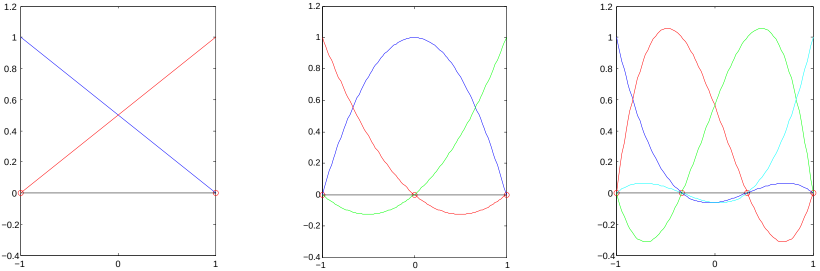
$$\frac{1}{h^2}\begin{bmatrix} 2+ch^2 & -1 & & \\ -1 & 2+ch^2 & -1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2+ch^2 \end{bmatrix}\begin{bmatrix} u_1^h \\ u_2^h \\ u_3^h \\ \vdots \\ u_n^h \end{bmatrix} = \begin{bmatrix} f_1 + \frac{g_0}{h^2} \\ f_2 \\ f_3 \\ \vdots \\ f_n + \frac{g_1}{h^2} \end{bmatrix}$$

$$u(x_i) \approx u_i^h$$

$$\frac{1}{h}\begin{bmatrix} 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & & \\ -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & \\ & \ddots & \ddots & \ddots \\ & & -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} \end{bmatrix}\begin{bmatrix} \hat{u}_1^h \\ \hat{u}_2^h \\ \hat{u}_3^h \\ \vdots \\ \hat{u}_n^h \end{bmatrix} = \begin{bmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \tilde{f}_3 \\ \vdots \\ \tilde{f}_n \end{bmatrix}$$

$$u(x) \approx u^h(x) = \sum_{i=1}^{n} \hat{u}_i^h \phi_i(x) + g^h(x)$$

Higher Order Elements



Finite Elements vs. Finite Differences - Revisited

Finite Elements - *approximate the solution*

- Replace p.d.e. by a weak formulation (variational problem; optimization problem)
- Approximate the solution by a function in a suitable finite dimensional function space

Finite Differences - *approximate the differential operator*

- Replace p.d.e. by a difference equation
- Solve the difference equation

Finite Elements vs. Finite Differences - Continued

Finite Elements

- Complicated domains
- Variable material properties
- Nonlinear equations
- Rigorous theoretical foundations

Finite Differences

- Simple (easy to program)
- Lower complexity (memory footprint)
- Easier to parallelize

Finite Volumes

Recall the homogeneous model problem

$$-\hat{u}''(x) + c(x)\hat{u}(x) = \hat{f}(x) \qquad x \in \Omega$$

with b.c.

$$\hat{u}(0) = 0 \qquad \hat{u}(1) = 0$$

where

$$\hat{f}(x) = f(x) + g''(x) - c(x)g(x)$$

Then

$$u(x) = \hat{u}(x) + g(x)$$

Finite Volumes

The main idea behind the finite volume method is the introduction of a *flux* for some quantity and writing conservation equation for that quantity. First consider the simpler problem

$$-\hat{u}''(x) = \hat{f}(x) \qquad x \in \Omega$$

with b.c.

$$\hat{u}(0) = 0 \qquad \hat{u}(1) = 0$$

Introduce the flux $F(x) = -\hat{u}'$ and write the eq. in conservation form

$$\nabla \cdot F = \hat{f}(x) \qquad x \in \Omega$$

$$F'(x) = \hat{f}(x) \qquad x \in \Omega$$

Finite Volumes

Introduce a mesh, or grid

$$0 = x_0 = x_{1/2} < x_1 < x_{3/2} < \ldots < x_n < x_{n+1/2} = x_{n+1} = 1$$

$$I_i = (x_{i-1/2}, x_{i+1/2}) \qquad h_i = |I_i| = x_{i+1/2} - x_{i-1/2}$$

Finite Volumes

Conservation of F on each volume

$$\int_{I_i} F'(x)dx = \int_{I_i} \hat{f}(x)dx$$

$$F(x_{i+1/2}) - F(x_{i-1/2}) = \int_{I_i} \hat{f}(x)dx$$

$$-u'(x_{i+1/2}) + u'(x_{i-1/2}) = \int_{I_i} \hat{f}(x)dx$$

Finite Volumes

We still need to approximate the fluxes

$$F(x_{i+1/2}) \approx -\frac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i}$$

and the integral

$$\int_{I_i} \hat{f}(x)dx \approx h_i \hat{f}(x_i)$$

Finite Volumes

Putting it all together

$$F(x_{i+1/2}) - F(x_{i-1/2}) = h_i \hat{f}(x_i) \qquad i = 1, \ldots, N$$

$$F(x_{i+1/2}) \approx -\frac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i} \qquad i = 0, \ldots, N$$

where

$$u(x_0) = 0 \qquad u(x_{N+1}) = 0$$

Finite Volumes

Back to our model problem we get

$$F(x_{i+1/2}) - F(x_{i-1/2}) + \int_{I_i} cu(x)dx = \int_{I_i} \hat{f}(x)dx$$

approximating the integrals

$$F(x_{i+1/2}) - F(x_{i-1/2}) + h_i \hat{u}(x_i) = h_i \hat{f}(x_i)$$

Finite Volumes

Ending up with

$$F(x_{i+1/2}) - F(x_{i-1/2}) + h_i c u^h(x_i) = h_i \hat{f}(x_i) \qquad i = 1, \ldots, N$$

$$F(x_{i+1/2}) = -\frac{u^h(x_{i+1}) - u^h(x_i)}{x_{i+1} - x_i} \qquad i = 0, \ldots, N$$

where

$$u^h(x_0) = 0 \qquad u^h(x_{N+1}) = 0$$

Finite Volumes

Finite Differences vs. Finite Elements vs. Finite Volumes

$$\frac{1}{h}\begin{bmatrix} 2+ch^2 & -1 & & \\ -1 & 2+ch^2 & -1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2+ch^2 \end{bmatrix}\begin{bmatrix} u_1^h \\ u_2^h \\ u_3^h \\ \vdots \\ u_n^h \end{bmatrix} = h\begin{bmatrix} f_1 + \frac{g_0}{h^2} \\ f_2 \\ f_3 \\ \vdots \\ f_n + \frac{g_1}{h^2} \end{bmatrix}$$

$$u(x_i) \approx u_i^h$$

$$\frac{1}{h^2}\begin{bmatrix} 2+ch^2 & -1 & & \\ -1 & 2+ch^2 & -1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2+ch^2 \end{bmatrix}\begin{bmatrix} u_1^h \\ u_2^h \\ u_3^h \\ \vdots \\ u_n^h \end{bmatrix} = \begin{bmatrix} f_1 + \frac{g_0}{h^2} \\ f_2 \\ f_3 \\ \vdots \\ f_n + \frac{g_1}{h^2} \end{bmatrix}$$

$$u(x_i) \approx u_i^h$$

Finite Volumes

Finite Differences vs. Finite Elements vs. Finite Volumes

$$\frac{1}{h}\begin{bmatrix} 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & & \\ -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} & -1+\frac{ch^2}{6} & \\ & \ddots & \ddots & \ddots \\ & & -1+\frac{ch^2}{6} & 2+\frac{2ch^2}{3} \end{bmatrix}\begin{bmatrix} \hat{u}_1^h \\ \hat{u}_2^h \\ \hat{u}_3^h \\ \vdots \\ \hat{u}_n^h \end{bmatrix} = \begin{bmatrix} \tilde{f}_1 \\ \tilde{f}_2 \\ \tilde{f}_3 \\ \vdots \\ \tilde{f}_n \end{bmatrix}$$

$$u(x) \approx u^h(x) = \sum_{i=1}^{n} \hat{u}_i^h \phi_i(x) + g^h(x)$$