MATH 676

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Finite element methods in scientific computing

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Lecture 33.5:

Which quadrature formula to use

The need for quadrature

Recall from lecture 4 and many example programs:

We compute

$$A_{ij} = (\nabla \phi_i, \nabla \phi_j) \qquad F_i = (\phi_i, f)$$

by mapping back to the reference cell...

$$\begin{aligned} A_{ij} &= (\nabla \phi_i, \nabla \phi_j) \\ &= \sum_K \int_K \nabla \phi_i(x) \cdot \nabla \phi_j(x) \\ &= \sum_K \int_{\hat{K}} J_K^{-1}(\hat{x}) \hat{\nabla} \hat{\phi}_i(\hat{x}) \cdot J_K^{-1}(\hat{x}) \hat{\nabla} \hat{\phi}_j(\hat{x}) \; |\det J_K(\hat{x})| \end{aligned}$$

...and quadrature:

$$A_{ij} \approx \sum_K \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q) \hat{\nabla} \hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q) \hat{\nabla} \hat{\phi}_j(\hat{x}_q) \; \underbrace{|\det J_K(\hat{x}_q)| \; w_q}_{=:\mathrm{JxW}}$$

Similarly for the right hand side *F*.

The need for quadrature

Question:

When approximating

$$A_{ij}=(\nabla\phi_i,\nabla\phi_j)$$

by

$$A_{ij} \approx \sum_K \sum_{q=1}^Q J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_j(\hat{x}_q) \; |\det J(\hat{x}_q)| \; w_q$$

how should we choose the points $\hat{x}_q$ and weights w_q?

In other words:

Which quadrature rule should we choose?

Considerations

Question: Which quadrature rule should we choose?

$$A_{ij} \approx \sum_K \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_j(\hat{x}_q) \; |\det J(\hat{x}_q)| \; w_q$$

Goals:

- Efficient: Make *Q* as small as possible
- Accurate: Do not introduce unnecessary errors

About accuracy:

In particular, do nothing that affects the convergence *order*!

1d: The matrix

Question: Which quadrature rule should we choose?

$$A_{ij} \approx \sum_K \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_j(\hat{x}_q) \; |\det J_K(\hat{x}_q)| \; w_q$$

Consider the 1d case:

- We use an element of polynomial degree *k*
- We use a linear mapping

Then:

- $J_K, J_K^{-1}, \det J_K$ are constant
- $\nabla\hat{\phi}_j(\hat{x}_q)$ is a polynomial of degree *k-1*
- The integrand has polynomial degree *2(k-1)*

1d: The matrix

Question: Which quadrature rule should we choose?

$$A_{ij} = (\nabla\phi_i, \nabla\phi_j)$$
$$\approx \sum_K \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_j(\hat{x}_q)\ |\det J_K(\hat{x}_q)|\ w_q$$

Consider the 1d case:

- The integrand has polynomial degree *2(k-1)*
- Gauss quadrature with *n* points is exact for polynomials up to degree *2n-1*

Consequence:

We can compute the integral $A_{ij}=(\nabla\phi_i, \nabla\phi_j)$ *exactly* via Gauss quadrature with *n=k* points!

1d: The right hand side

Question: How about the right hand side?

$$F_i = (\phi_i, f) \approx \sum_K \sum_{q=1}^{Q} \hat{\phi}_i(\hat{x}_q)\ f(x_q)\ |\det J_K(\hat{x}_q)|\ w_q$$

Consider the 1d case:

- We use an element of polynomial degree *k*
- We use a linear mapping

Then:

- $\det J_K$ is constant
- $\nabla \hat{\phi}_j(\hat{x}_q)$ is a polynomial of degree *k*
- $f(x)$ is not in general a polynomial
- The integrand is not polynomial

1d: The right hand side

Question: What to do here?

$$F_i = (\phi_i, f) \approx \sum_K \sum_{q=1}^{Q} \hat{\phi}_i(\hat{x}_q)\; f(x_q)\; |\det J_K(\hat{x}_q)|\; w_q$$

Consider Gauss integration with *n* points:

- Integrates polynomials of degree *2n-1* exactly
- For general *f(x)* essentially integrates

$$F_i = (\phi_i, f) \approx \sum_K \sum_{q=1}^{Q} \hat{\phi}_i(\hat{x}_q)\; f(x_q)\; |\det J_K(\hat{x}_q)|\; w_q \approx (\phi_i, I_{2n-k} f)$$

where $I_{2n-k} f = f$ at the n quadrature points + n-k others

1d: The right hand side

Consider Gauss integration with *n* points:

- Integrates polynomials of degree *2n-1* exactly
- For general *f(x)* essentially integrates

$$F_i = (\phi_i, f) \approx \sum_K \sum_{q=1}^{Q} \hat{\phi}_i(\hat{x}_q)\ f(x_q)\ |\det J_K(\hat{x}_q)|\ w_q$$
$$= \sum_K \int_K I_{2n}(\phi_i f) \approx (\phi_i, I_{2n-k} f)$$

where $I_{2n-k} f = f$ at the *n* quadrature points + *n-k* others on every cell

Consequence:

Inexact integration is equivalent to approximating the solution of a slightly perturbed problem!

1d: The right hand side

Consider the original and perturbed problems:

$$\begin{aligned} -\Delta u &= f \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned} \qquad\qquad \begin{aligned} -\Delta \tilde{u} &= \tilde{f} \quad \text{in } \Omega \\ u &= 0 \quad \text{on } \partial\Omega \end{aligned}$$

Consequence:

$$\|u-\tilde{u}_h\|_{H^1} \le \underbrace{\|u-\tilde{u}\|_{H^1}}_{\le C_1\|f-\tilde{f}\|_{H^{-1}} \le C_2 h^{2\mathrm{n}-k+1}\|f\|_{H^{2\mathrm{n}-k}}} + \underbrace{\|\tilde{u}-\tilde{u}_h\|_{H^1}}_{\le C_3 h^k \|\tilde{u}\|_{H^k}}$$

We want the first term to be at least as good as the second. We need to choose $n=k$.

Higher dimensions: The matrix

Question: Which quadrature rule should we choose?

$$A_{ij} \approx \sum_K \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_j(\hat{x}_q) \; |\det J_K(\hat{x}_q)| \; w_q$$

Consider the higher dimensional case:

- Use an element of polynomial degree *k* in each direction
- Use a *d*-linear mapping

Then:

- $J_K, \det J_K$ are polynomials of degree *k*, k^d
- J_K^{-1} is a rational function
- $\nabla\hat{\phi}_j(\hat{x}_q)$ is a polynomial of degree *dk-1*
- The integrand is rational
- For linear mappings, it is of degree *2(dk-1)*

Higher dimensions: The matrix

Question: Which quadrature rule should we choose?

$$A_{ij} \approx \sum_K \sum_{q=1}^{Q} J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_i(\hat{x}_q) \cdot J_K^{-1}(\hat{x}_q)\hat{\nabla}\hat{\phi}_j(\hat{x}_q) \; |\det J_K(\hat{x}_q)| \; w_q$$

Consider the higher dimensional case:

- The integrand is rational
- For linear mappings, it is of degree *2(dk-1)*
- Gauss quadrature with *n* points per direction is exact for degree *2n-1* in each variable

Nevertheless, using the tensor product structure:

We need to use Gauss quadrature with *n=k+1* points per direction.

Higher dimensions: The right hand side

Question: Which quadrature rule should we choose?

$$F_i = (\phi_i, f) \approx \sum_K \sum_{q=1}^{Q} \hat{\phi}_i(\hat{x}_q)\; f(x_q)\; |\det J_K(\hat{x}_q)|\; w_q$$

Similar considerations can be applied:

We need to use Gauss quadrature with *n=k+1* points per direction.

Summary

As a general rule of thumb:

- Gauss quadrature with *n=k+1* points per direction is sufficient
  - for the Laplace matrix $A_{ij} = (\nabla\phi_i, \nabla\phi_j)$
  - for the mass matrix $M_{ij} = (\phi_i, \phi_j)$
  - for the right hand side $F_i = (\phi_i, f)$

- It is generally also sufficient with variable coefficients:

$$A_{ij} = (a(x)\nabla\phi_i, \nabla\phi_j)$$

With *n=k+1*, the quadrature error does not dominate the overall error (if *a(x)* is smooth).

Non-smooth coefficients

What to with non-smooth terms?
For example

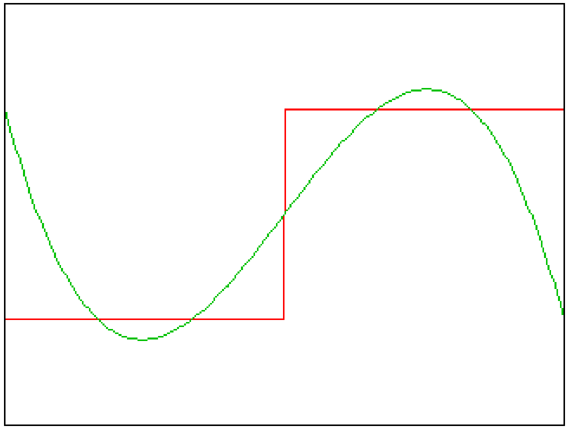
$$A_{ij} = \left(a(x)\nabla\phi_i, \nabla\phi_j\right)$$

$$F_i = \left(\phi_i, f\right)$$

where *a(x)* or *f(x)* are discontinuous.

Recall: Quadrature is equivalent to exact integration with an interpolated coefficient.

For discontinuous functions, interpolation does not help very much: Quadrature produces large errors.



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Before: $$\|u-\tilde{u}_h\|_{H^1} \le \underbrace{\|u-\tilde{u}\|_{H^1}}_{\le C_1\|f-\tilde{f}\|_{H^{-1}} \le C_2 h^{2\mathrm{n}-k+1}\|f\|_{H^{2\mathrm{n}-k}}} + \underbrace{\|\tilde{u}-\tilde{u}_h\|_{H^1}}_{\le C_3 h^k \|\tilde{u}\|_{H^k}}$$

Now: The interpolation step fails! We may only get

$$\|u-\tilde{u}_h\|_{H^1} \le \underbrace{\|u-\tilde{u}\|_{H^1}}_{\le C_1\|f-\tilde{f}\|_{H^{-1}} \le C_2 h^{s+1}\|f\|_{H^s}} + \underbrace{\|\tilde{u}-\tilde{u}_h\|_{H^1}}_{\le C_3 h^k \|\tilde{u}\|_{H^k}}$$

Non-smooth coefficients

What to with non-smooth terms?
For example

$$A_{ij} = (a(x)\nabla\phi_i, \nabla\phi_j)$$

$$F_i = (\phi_i, f)$$

where *a(x)* or *f(x)* are discontinuous.

Now: $$\|u-\tilde{u}_h\|_{H^1} \leq \underbrace{\|u-\tilde{u}\|_{H^1}}_{\leq C_1\|f-\tilde{f}\|_{H^{-1}} \leq C_2 h^{s+1}\|f\|_{H^s}} + \underbrace{\|\tilde{u}-\tilde{u}_h\|_{H^1}}_{\leq C_3 h^k \|\tilde{u}\|_{H^k}}$$

Solution: Subdivide the cell into *L* pieces so that

$$C_2\left(\frac{h}{L}\right)^{s+1}\|f\|_{H^s} \approx C_3 h^k \|\tilde{u}\|_{H^k}$$

This is what the *QIterated* class does.

Special purpose quadratures

There are situations where we want quadrature rules other than Gauss:

- To affect stability properties of a discretization
  - Underintegration for nearly incompressible elasticity
  - Special purpose quadrature for mixed problems

- To improve sparsity of matrices
  - Make some terms zero
  - Make a matrix diagonal

Sparsifying matrices

Using the trapezoidal rule for the Laplace matrix:
Assume:

- Uniform mesh with square cells
- Q_1 element with shape functions

$$\phi_1=(1-\hat{x})(1-\hat{y}), \quad \phi_2=\hat{x}(1-\hat{y}),$$
$$\phi_3=(1-\hat{x})\hat{y}, \quad \phi_4=\hat{x}\hat{y}$$

  and gradients

$$\hat{\nabla}\phi_1=\begin{pmatrix}-(1-\hat{y})\\-(1-\hat{x})\end{pmatrix}, \quad \hat{\nabla}\phi_2=\begin{pmatrix}(1-\hat{y})\\-\hat{x}\end{pmatrix}$$
$$\hat{\nabla}\phi_3=\begin{pmatrix}-\hat{y}\\1-\hat{x}\end{pmatrix}, \quad \hat{\nabla}\phi_4=\begin{pmatrix}\hat{y}\\\hat{x}\end{pmatrix}$$

- Trapezoidal rule with integration points at the vertices

Sparsifying matrices

Using the trapezoidal rule for the Laplace matrix:

- Q_1 element with shape gradients

$$\hat\nabla\phi_1=\begin{pmatrix}-(1-\hat y)\\-(1-\hat x)\end{pmatrix},\quad \hat\nabla\phi_2=\begin{pmatrix}(1-\hat y)\\-\hat x\end{pmatrix}$$
$$\hat\nabla\phi_3=\begin{pmatrix}-\hat y\\1-\hat x\end{pmatrix},\qquad \hat\nabla\phi_4=\begin{pmatrix}\hat y\\\hat x\end{pmatrix}$$

- Trapezoidal rule with integration points at the vertices:

$$A_{ij}\approx\sum_K\sum_{q=1}^Q J_K^{-1}(\hat x_q)\hat\nabla\hat\phi_i(\hat x_q)\cdot J_K^{-1}(\hat x_q)\hat\nabla\hat\phi_j(\hat x_q)\ |\det J_K(\hat x_q)|\ w_q$$

- At all *vertices*, we have

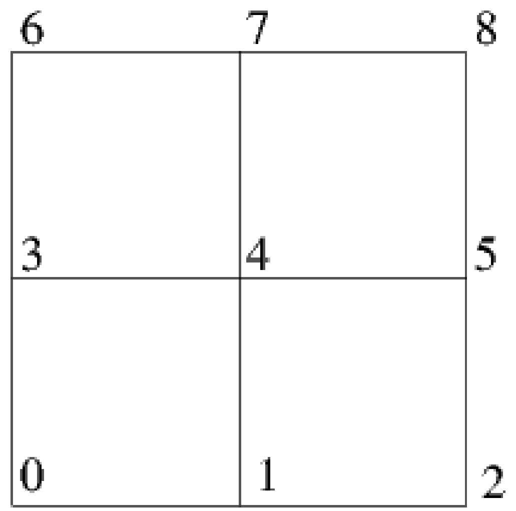
$$\nabla\phi_1\cdot\nabla\phi_3=0,\qquad \nabla\phi_2\cdot\nabla\phi_4=0,$$

- Degrees of freedom diagonal across cells do not couple

Sparsifying matrices

Using the trapezoidal rule for the Laplace matrix:

- Degrees of freedom diagonal across cells do not couple:



- $A_{40}=A_{42}=A_{46}=A_{48}=0$
- We can also show: $A_{41}=A_{43}=A_{45}=A_{47}= -A_{44}/4$
- This is exactly the 5-point stencil (→ finite differences)!
- In 3d, this leads to the usual 7-point stencil
- This matrix is sparser than normal

Diagonal mass matrices

Using the trapezoidal rule for the mass matrix:

- Q_1 element with shape values

$$\phi_1=(1-\hat{x})(1-\hat{y}), \quad \phi_2=\hat{x}(1-\hat{y}),$$
$$\phi_3=(1-\hat{x})\hat{y}, \quad \phi_4=\hat{x}\,\hat{y}$$

- Trapezoidal rule with integration points at the vertices:

$$M_{ij} \approx \sum_K \sum_{q=1}^{Q} \hat{\phi}_i(\hat{x}_q)\ \hat{\phi}_j(\hat{x}_q)\ |\det J_K(\hat{x}_q)|\ w_q$$

- At all *vertices*, we have $\hat{\phi}_i(\hat{x}_q)\hat{\phi}_j(\hat{x}_q)=\delta_{ij}\delta_{iq}$ and thus

$$M_{ij} \approx \sum_K \left(\sum_{q=1}^{Q} |\det J_K(\hat{x}_q)|\ w_q\right)\delta_{ij} = \sum_K |K \cap \operatorname{supp} \phi_i|\delta_{ij}$$

- This mass matrix is diagonal!

Diagonal mass matrices

Using the trapezoidal rule for the mass matrix:

- This results in a diagonal mass matrix
- This is useful in explicit time stepping schemes

- Generalized to arbitrary elements by choosing quadrature points at nodal interpolation points

Summary

General rule:

- Use Gaussian quadrature with $n=k+1$ per coordinate direction where k is the highest polynomial degree in your finite element
- Think about the implications if you have non-smooth coefficients
- Only use quadrature rules other than Gaussian if you know why.

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