

Lecture 12 - B

§5.4 Generalized Gaussian Quadrature

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We will answer these questions:

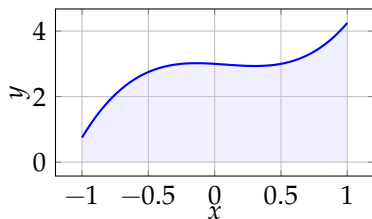
- What is **degree of precision**?
- In what way are **Newton-Cotes methods** restrictive?
- What is the main idea behind **Gaussian quadrature**?
- How does its **performance** compare?



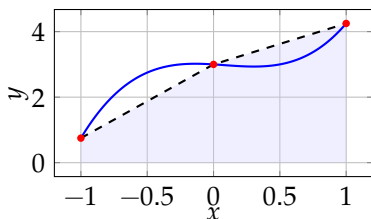
Composite Gauss



Using Trapezoid Twice



Exact integral over $[-1, 1]$



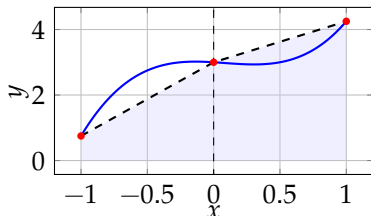
Composite Trapezoid

- **Composite Trapezoid** is approximating the integral with *multiple* trapezoids
- We can apply the same idea to Gaussian quadrature

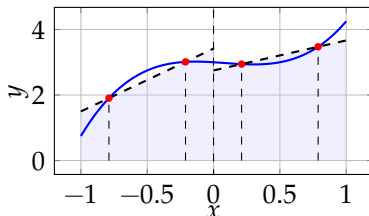


Using Gauss Quadrature Twice

- Apply Gauss quadrature on each subinterval separately
- Compare the composite Trapezoid vs. composite Gauss visually



Composite Trapezoid



Composite Gauss

No Formula

- Composite Trapezoid has a neat formula

$$\int_a^b f(x) dx \approx h \left(\frac{1}{2}f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{1}{2}f(x_n) \right)$$

- Composite Gauss does not have a formula

Question

How do you implement composite Gauss?



Implementation

- 1 Implement the Gauss with the interval change

$$\int_{x_i}^{x_{i+1}} f(x) dx \approx \frac{h}{2} \left[u \left(-\frac{\sqrt{3}}{3} \right) + u \left(\frac{\sqrt{3}}{3} \right) \right], u(t) = f \left(\frac{ht}{2} + \frac{x_i + x_{i+1}}{2} \right)$$

- 2 Divide the interval $[a, b]$ into n even subintervals

- 3 Apply Gauss to each subinterval $[x_i, x_{i+1}]$

- 4 Add up the result



Composite Two-Point Gauss

Method: Composite Two-Point Gauss

- **Given:** function $f(x)$, interval $[a, b]$, number of subintervals n
 - **Output:** Approximate integral $\int_a^b f(x) dx$
 - **Idea:** Create n even subintervals and add up two-point Gauss quadratures for each subinterval
-
- Unlike the Newton-Cotes, composite Gauss has no formulas
 - Composite Gauss is implemented *modularly*



Gauss Quadrature Theorem



Goal

- We have derived *two-point* Gauss

$$\int_{-1}^1 f(x) dx \approx f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right)$$

- Next, we learn the general $n + 1$ point Gauss

$$\int_a^b f(x) dx \approx \sum_{i=0}^n w_i f(x_i)$$

Goal

Learn the **Gaussian Quadrature Theorem**.



Inner Product

- We know the **inner product** of vectors u and v

$$u^T v = \sum_{i=1}^n u_i v_i$$

- Functions $f(x)$ and $g(x)$ are like “infinite dimensional vectors”

Definition: Inner Product

Let $f(x), g(x) \in C([a, b])$. The **inner product** of the functions is

$$\int_a^b f(x) g(x) dx$$



Orthogonal Functions

Definition: Orthogonal functions

Two functions $f(x)$ and $g(x)$ are orthogonal on $[a, b]$ if

$$\int_a^b f(x)g(x) dx = 0$$

- Example: $f(x) = x$, $g(x) = x^2 - 1$ on the interval $[-1, 1]$
- Inner product

$$\begin{aligned}\int_{-1}^1 f(x)g(x) dx &= \int_{-1}^1 x(x^2 - 1) dx \\ &= \int_{-1}^1 (x^3 - x) dx \\ &= \left. \frac{1}{4}x^4 - \frac{1}{2}x^2 \right|_{-1}^1 = 0\end{aligned}$$



Gauss Quadrature Theorem

Gauss proved the following result:

Theorem

Let $q(x)$ be a nontrivial polynomial of degree $n + 1$ such that

$$\int_a^b x^k q(x) dx = 0 \quad (0 \leq k \leq n)$$

and let $x_0, x_1, \dots, x_n$ be the zeros of $q(x)$. Then the quadrature

$$\int_a^b f(x) dx \approx \sum_{i=0}^n A_i f(x_i), \text{ where } A_i = \int_a^b \ell_i(x) dx$$

is exact for all polynomials of degree at most $2n + 1$.

Recall $\ell_i(x)$ is the i th **Lagrange basis function**. Here, $\ell_i(x)$ is defined with respect to the $x_0, x_1, \dots, x_n$ zeros of $q(x)$.



Variables and Assumptions in Gauss Quadrature

Variable	Definition / Assumptions
$q(x)$	$n + 1$ degree polynomial that is orthogonal to all monomials $\int_a^b x^k q(x) dx = 0$ for $k = 0, 1, \dots, n$
$\{x_0, x_1, \dots, x_n\}$	Roots (zeros) of $q(x)$ within the interval $[a, b]$
$\ell_i(x)$	The i -th Lagrange basis polynomial, defined as $\ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j}$
$f(x)$	Continuous function being integrated over $[a, b]$



Result of Theorem

Variable	Result
A_i	Quadrature weights, calculated by $A_i = \int_a^b \ell_i(x) dx$
$\sum_{i=0}^n A_i f(x_i)$	Approximation to $\int_a^b f(x) dx$
$f(x)$	If $f(x)$ is a polynomial of degree at most $2n + 1$ then there is no error in the quadrature

Significance:

- This theorem tells us that a quadrature

$$\int_a^b f(x) dx \approx \sum_{i=0}^n A_i f(x_i)$$

with D.O.P. $2n + 1$ exists.

- A formula for A_i is given



Begin the Proof

Goal

Show that if $f(x)$ is a polynomial of degree $2n + 1$ then the approximation

$$\int_a^b f(x)dx \approx \sum_{i=0}^n A_i f(x_i)$$

has **no error!**

- We assume $f(x)$ is degree $2n + 1$
- We assume $q(x)$ is degree $n + 1$
- We can do polynomial division

$$\frac{f(x)}{q(x)} = \underbrace{p(x)}_{\text{degree } n} + \underbrace{R(x)}_{\text{remainder}}$$



Sketch of Proof

Part 1

1 Polynomial Division:

- ▶ Let $f(x)$ be

$$f(x) = p(x)q(x) + r(x),$$

where:

- ▶ $p(x)$ is a polynomial of degree at most n , and
- ▶ $r(x) = R(x)q(x)$ must be degree $\leq n$.

2 Orthogonality Property:

- ▶ Since $q(x)$ is orthogonal to monomials:

$$\int_a^b x^k q(x) dx = 0, \quad \text{for } 0 \leq k \leq n,$$

and $\deg p(x) \leq n$, it follows q is orthogonal to p :

$$\int_a^b p(x)q(x) dx = 0.$$



Sketch of Proof

Part 2

3 Simplifying the Integral:

- ▶ Therefore:

$$\int_a^b f(x) dx = \int_a^b \left(\overset{0}{\cancel{p(x)q(x)}} + r(x) \right) dx = \int_a^b r(x) dx.$$

4 Interpolating $r(x)$:

- ▶ Since $\deg r(x) \leq n$, we can interpolate $r(x)$ using the Lagrange basis polynomials $\ell_i(x)$ with *zero error*

$$r(x) = \sum_{i=0}^n r(x_i) \ell_i(x).$$

- ▶ The nodes x_i are chosen to be the roots of $q(x)$.



Sketch of Proof

Part 3

5 Evaluating the Integral:

- Substituting into the integral:

$$\int_a^b f(x) dx = \int_a^b \sum_{i=0}^n r(x_i) \ell_i(x) dx = \sum_{i=0}^n r(x_i) \int_a^b \ell_i(x) dx.$$

6 Final Quadrature Formula:

- Since x_i are the roots of $q(x)$ we get

$$f(x_i) = p(x_i)q(x_i) + r(x_i) = r(x_i)$$

- Therefore:

$$\int_a^b f(x) dx = \sum_{i=0}^n f(x_i) A_i, \quad \text{where } A_i = \int_a^b \ell_i(x) dx.$$

Key Idea

We have shown that it is possible to derive a quadrature with a degree of precision of $2n + 1$ using only $n + 1$ points!

Degree of Precision

# Points	Newton-Cotes D.O.P.	Gauss D.O.P.
1	1	1
2	1	3
3	3	5
4	3	7
5	5	9

Key Idea

Gaussian Quadrature uses degrees of freedom more efficiently to achieve higher accuracy



Legendre Polynomials



From Theorem to Formula

Result of the Gauss Quadrature Theorem

The quadrature with $n + 1$ nodes

$$\int_a^b f(x) \approx \sum_{i=0}^n A_i f(x_i)$$

has a theoretical limit on the degree of precision $r = 2n + 1$.

Question

So how do get the formula for x_i and A_i ?



Orthogonal Polynomials

- Imagine a family of polynomials:

$$\mathcal{F} = \{\phi_0(x), \phi_1(x), \phi_2(x), \dots\}$$

where each member $\phi_i(x)$ is a polynomial of degree i .

- These polynomials are orthogonal to one another on the interval $[-1, 1]$, meaning that for $i \neq j$:

$$\int_{-1}^1 \phi_i(x) \phi_j(x) dx = 0.$$

- This family of orthogonal polynomials is called the **Legendre polynomials**. They are important for Gaussian quadrature and approximation theory.



Legendre Polynomials

Definition: Legendre Polynomials

The **Legendre Polynomials** are a family of polynomials

$$\mathcal{F} = \{\phi_0(x), \phi_1(x), \phi_2(x), \dots\}$$

such that $\phi_n(x)$ is a polynomial of degree n and they are all orthogonal to each other, i.e. for $i \neq j$:

$$\int_{-1}^1 \phi_i(x) \phi_j(x) dx = 0.$$

- By convention, we let the first polynomial be $\phi_0(x) = 1$.
- The orthogonality condition requires the 2nd polynomial to be $\phi_1(x) = x$

$\vdots$



Legendre Polynomials

First few examples

$$\phi_0 = 1$$

$$\phi_1 = x$$

$$\phi_2 = \frac{3x^2 - 1}{2}$$

$$\phi_3 = \frac{5x^3 - 3x}{2}$$

$\vdots$

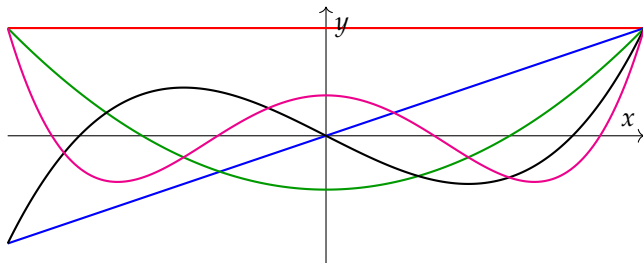
In general, you have the recurrence relation

$$\phi_n(x) = \frac{(2n-1)x}{n} \phi_{n-1}(x) - \frac{n-1}{n} \phi_{n-2}(x)$$



Legendre Polynomials

First few examples



— $P_0(x)$ — $P_1(x)$ — $P_2(x)$ — $P_3(x)$ — $P_4(x)$

Key Idea

We can construct Legendre polynomials of *any* order.



Revisit Gauss' Theorem

Let $a = -1$ and $b = 1$.

Theorem

Let $q(x)$ be a nontrivial polynomial of degree $n + 1$ such that

$$\int_{-1}^1 x^k q(x) dx = 0 \quad (0 \leq k \leq n) \quad (*)$$

and let $x_0, x_1, \dots, x_n$ be the zeros of $q(x)$. Then the quadrature

$$\int_{-1}^1 f(x) dx \approx \sum_{i=0}^n A_i f(x_i), \text{ where } A_i = \int_{-1}^1 \ell_i(x) dx$$

is exact for all polynomials of degree at most $2n + 1$.

- Let q be the Legendre polynomial $q(x) = \phi_{n+1}(x) \in \mathcal{F}$
- Then equation $(*)$ will always be satisfied



Connection between the Theorem and Legendre

- Gauss' Theorem gave us a powerful quadrature

$$\int_{-1}^1 f(x) dx \approx \sum_{i=0}^n A_i f(x_i)$$

with weights

$$A_i = \int_{-1}^1 \ell_i(x) dx$$

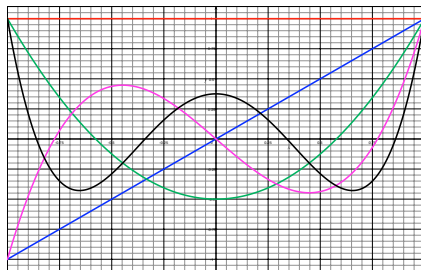
- But, the nodes were never specified because we did not know $q(x)$

Key Idea

We let $q(x)$ be the Legendre polynomial to get the Gaussian quadrature formula of any order.



Properties of Legendre Polynomials

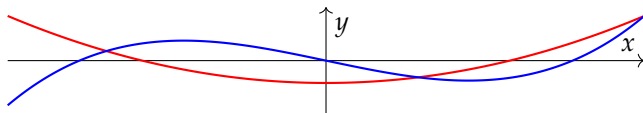


Properties:

- ϕ_n is a degree n polynomial
- ϕ_i is orthogonal to ϕ_j if $i \neq j$
- Don't suffer from poor conditioning (unlike monomials)
- Recursion equation can be used to find $\phi_n(x)$, for $n > 1$
- The roots of $\phi_n(x)$ are the nodes for Gaussian quadrature
- The roots of $\phi_n(x)$ are distributed symmetrically



Roots



$$\text{— red — } \phi_2(x) = \frac{1}{2}(3x^2 - 1) \quad \text{— blue — } \phi_3(x) = \frac{1}{2}(5x^2 - 3x)$$

- The roots of $\phi_2(x)$ are

$$x_0 = -\frac{1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}}$$

- The roots of $\phi_3(x)$ are

$$x_0 = -\sqrt{\frac{3}{5}}, \quad x_1 = 0, \quad x_2 = \sqrt{\frac{3}{5}}$$



Question

How do you find the Gauss weights?

- We want to know the weights and nodes for the approximation

$$\int_{-1}^1 f(x) dx \approx w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2)$$

- The third Legendre polynomial is

$$\phi_3(x) = \frac{5x^3 - 3x}{2}$$

which has roots at $x = 0, \pm \sqrt{\frac{3}{5}}$ so

$$x_0 = -\sqrt{\frac{3}{5}}, \quad x_1 = 0, \quad x_2 = \sqrt{\frac{3}{5}}$$



- The weights w_i can be found by integrating the Lagrange basis functions

$$w_0 = \int_{-1}^1 \ell_0(x) dx = \int_{-1}^1 \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} dx = \frac{5}{9}$$

$$w_1 = \int_{-1}^1 \ell_1(x) dx = \frac{8}{9}$$

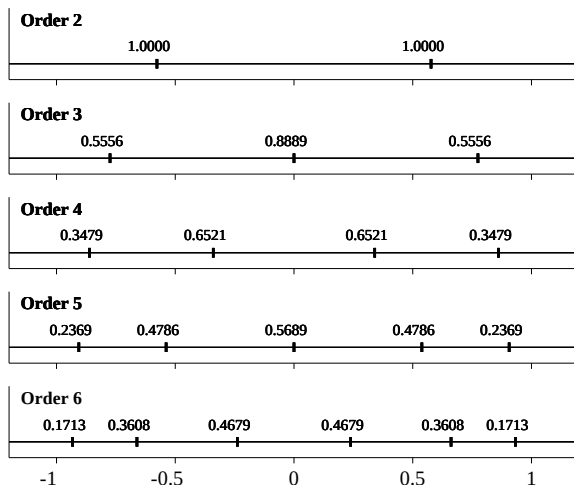
$$w_2 = \int_{-1}^1 \ell_2(x) dx = \frac{5}{9}$$

- Therefore the formula for the Three-Point Gauss Quadrature is

$$\int_{-1}^1 f(x) dx \approx \frac{5}{9}f\left(-\sqrt{3/5}\right) + \frac{8}{9}f(0) + \frac{5}{9}f\left(\sqrt{3/5}\right)$$



Nodes and Weights



- The bold ticks show location of the nodes are placed
- The numbers above them show the weight
- Both the node locations and weights are symmetric



Quadrature Nodes

- In practice, programmers use a look-up table for the x_i and w_i

```
1  if(n==0)
2      x = 0;    w = 2;
3  if(n==1)
4      x(1) = -1/sqrt(3);    x(2) = -x(1);
5      w(1) = 1;            w(2) = w(1);
6  if(n==2)
7      x(1) = -sqrt(3/5);    x(2) = 0;    x(3) = -x(1);
8      w(1) = 5/9;          w(2) = 8/9;    w(3) = w(1);
9  if(n==3)
10     x(1) = -0.861136311594053;    x(4) = -x(1);
11     x(2) = -0.339981043584856;    x(3) = -x(2);
12     w(1) = 0.347854845137454;    w(4) = w(1);
13     w(2) = 0.652145154862546;    w(3) = w(2);
14  if(n==4)
15     x(1) = -0.906179845938664;    x(5) = -x(1);
16     x(2) = -0.538469310105683;    x(4) = -x(2);
17     x(3) = 0;
18     w(1) = 0.236926885056189;    w(5) = w(1);
19     w(2) = 0.478628670499366;    w(4) = w(2);
20     w(3) = 0.568888888888889;
21  if(n==5)
22     x(1) = -0.932469514203152;    x(6) = -x(1);
23     x(2) = -0.661209386466265;    x(5) = -x(2);
24     x(3) = -0.238619186083197;    x(4) = -x(3);
25     w(1) = 0.171324492379170;    w(6) = w(1);
26     w(2) = 0.360761573048139;    w(5) = w(2);
27     w(3) = 0.467913934572691;    w(4) = w(3);
```



Degree of Precision

Question

How good is the 3-point Gauss?

Example

What is the degree of precision of the quadrature

$$\int_{-1}^1 f(x) dx \approx \frac{5}{9}f\left(-\sqrt{3/5}\right) + \frac{8}{9}f(0) + \frac{5}{9}f\left(\sqrt{3/5}\right)?$$

- This is a $n + 1 = 3$ point quadrature which means $n = 2$
- Degree of precision is

$$2n + 1 = 5$$

- The 3-point Newton-Cotes (Simpson's Rule) has degree of precision 3



Example

Example

Consider the integral

$$\int_{-1}^1 (3x^{13} + 4x + 7) dx$$

Which Gaussian quadrature rule will find the exact value of the integral?

- The function being integrated is a 12th degree polynomial
- Let $2n + 1 = 13$ so

$$n = 6$$

- Since $n + 1 = 7$, integral is exact for the

7-point Gaussian quadrature

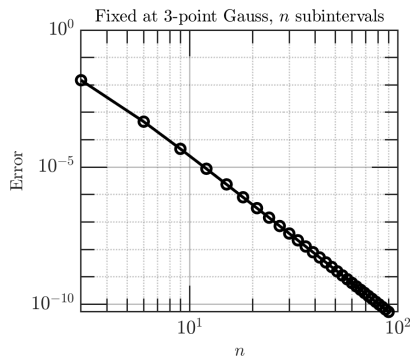
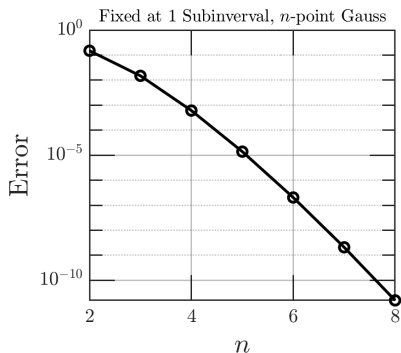


Let's run some code

int_gauss_test.m

This script uses int_gauss.m to integrate $\int_0^5 xe^{-x} dx$ with

- 1 subinterval, increasing number of nodes
- 3 nodes, increases number of intervals



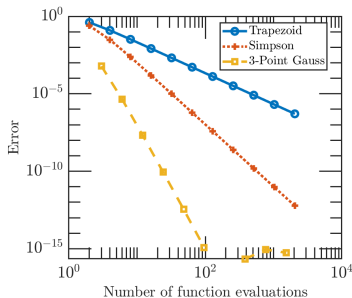
Let's run some code

int_compare_gauss_trapezoid_simpson.m

Compare the numerical experiment for integrating $\int_0^5 xe^{-x} dx$ with

- 1 Trapezoid
- 2 Simpson
- 3 Gauss

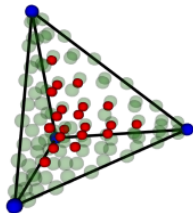
Result: Gauss quadrature is much more accurate for the same number of function evals.



Higher Dimensions



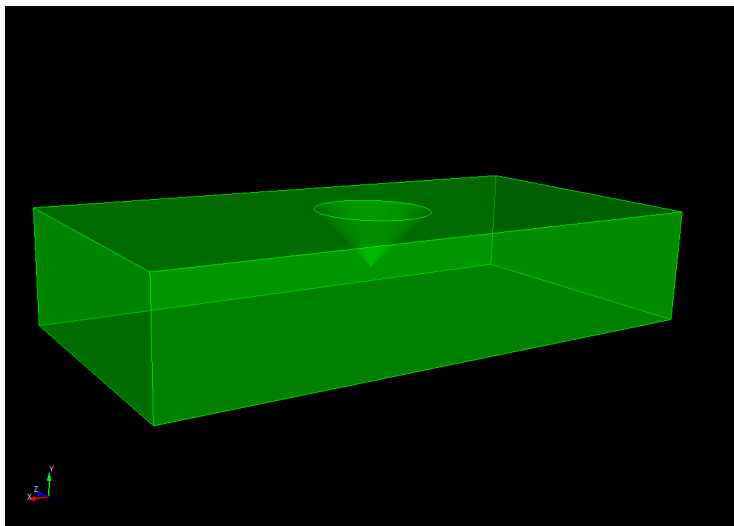
Something interesting...



- Gaussian quadrature also works for $\iint f(x, y) dA$
- Also works for $\iiint f(x, y, z) dV$
- Gauss nodes in other shapes are not easy

Quadrature

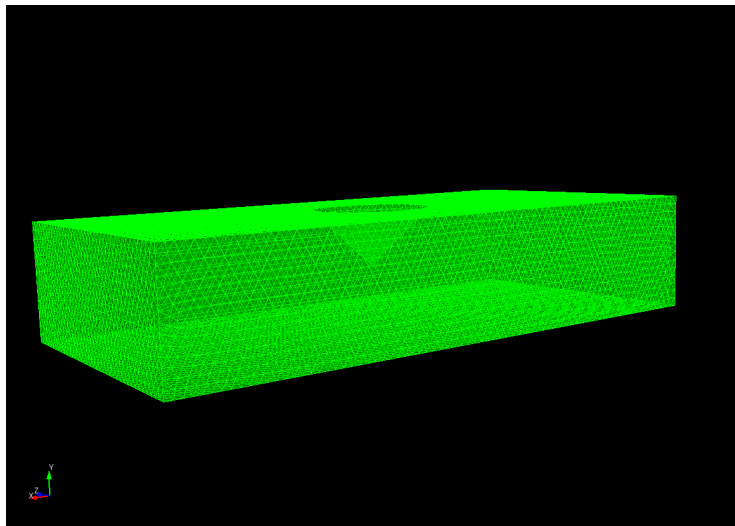
Consider quadrature over “interesting” 3D domain



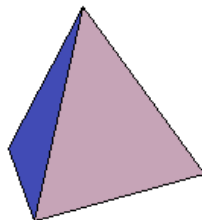
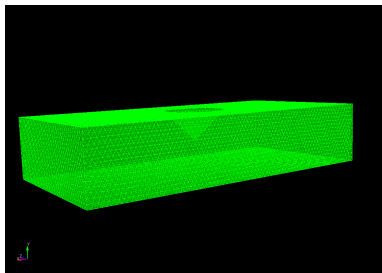
Quadrature

Consider quadrature over “interesting” 3D domain

- Break into "subintervals" of 40K tetrahedrons, and integrate each tet



Quadrature



- 40K tetrahedrons.
- Need to integrate a function $f(x)$ over each tet Ω_i : $\int_{\Omega_i} f(x) dx$
- Needs quadrature
- Map the integration to a reference tetrahedron
- Perform Gauss Quadrature using $(n+1)(n+2)(n+3)/6$ quadrature points (where n is the 1-D number of points).
- Results in # of tetrahedrons $\times n^3/6$ function evaluations



Meet Legendre



This is the only picture of Adrien-Marie Legendre (1752-1833)

