Symmetric Triangle Quadrature Rules for Arbitrary Functions

Brian A. Freno, William A. Johnson, Brian F. Zinser, Salvatore Campione
Sandia National Laboratories

Donald R. Wilton
University of Houston

Francesca Vipiana
Politecnico di Torino

SIAM Conference on Computational Science and Engineering
March 1, 2021

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

Outline

- Introduction to Quadrature Rules
- Quadrature Preliminaries
- Singularities
- Approach 1: Optimization for Moderate Number of Functions
- Approach 2: Quadrilateral Subdomains
- Numerical Example: The Electric-Field Integral Equation
- Summary

Outline

Overview

- Gaussian quadrature rules are useful for numerical integration
- For integrands accurately approximated by polynomials, rules are typically employed that exactly integrate polynomials

Triangles

- Quadrature rules for triangles are important for evaluating surface integrals
- Several authors have developed methods for computing symmetric quadrature rules for polynomials

  Lyness & Jespersen (1975), Dunavant (1985), Wandzura & Xiao (2003), Papanicolopulos (2015)
- Geometrically symmetric rules are desirable
  - Mapping is straightforward
  - Points are not more concentrated at a single vertex

Singularities

- Polynomial rules do not converge monotonically or rapidly for integrable functions with boundary singularities
- Such functions include unbounded derivatives at the boundary, where the function may not be defined
- For 1D, an approach has been developed to compute quadrature rules for singular functions

  Ma et al. (1996)
- For 2D, previous authors have taken the outer product of one-dimensional rules to generate asymmetric triangle rules

  Vipiana et al. (2013)

Challenges to Generate

- Regardless of dimension and function sequence, equations for computing quadrature rules are stiff and highly dependent upon initial guess
- In multiple dimensions, for a given number of points, the number of functions that can be integrated is unknown

Outline

- Introduction to Quadrature Rules
- Quadrature Preliminaries
  - Quadrature Rules
  - Symmetric Rules for Triangles
  - Polynomial Integration
- Singularities
- Approach 1: Optimization for Moderate Number of Functions
- Approach 2: Quadrilateral Subdomains
- Numerical Example: The Electric-Field Integral Equation
- Summary

Quadrature Rules

- An n-point quadrature rule exactly integrates a sequence of n_f functions $\mathbf{f}(\mathbf{x}) = \{f_1(\mathbf{x}), \dots, f_{n_f}(\mathbf{x})\}$, such that

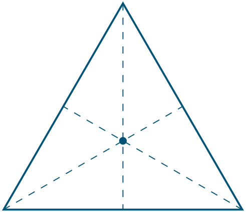
$$\int_A \mathbf{f}(\mathbf{x}) dA = \sum_{i=1}^{n} w_i \mathbf{f}(\mathbf{x}_i)$$

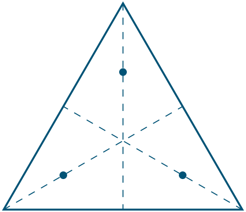
- In 1D, $n_f = 2n$ and, for polynomials, $\mathbf{f}(x) = \{1, \dots, x^{2n-1}\}$

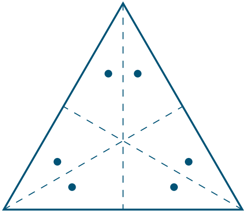
- In 2D, $n_f \stackrel{?}{=} 3n$,
  - This is unproven
  - If rules are symmetric, the efficiency can be significantly lower

Symmetric Rules for Triangles

- Invariant to rotation and reflection about the medians for equilateral triangles
- Triangles can be isoparametrically transformed to other triangles
- Rules are constructed from a combination of orbits, such that $n = n_0 + 3n_1 + 6n_2$


type-0 orbit


type-1 orbit


type-2 orbit

Polynomial Integration

- Rules that integrate polynomials of degree d exactly integrate linear combinations of $x^p y^q$
  - $0 \leq p,\, q \leq d$
  - $0 \leq p + q \leq d$
  - $n_f = (d+1)(d+2)/2$ monomials
- This can yield more equations than unknowns
  - A 3-point rule can integrate polynomials of $d = 2 \rightarrow n_f = 6$ monomials: $\mathbf{f}(x, y) = \{1,\, x,\, y,\, x^2,\, y^2,\, xy\}$
  - Number of unknowns is 2: α (position along median) and w (weight)
  - Mismatch is reconcilable; 6 quadrature equations are not linearly independent

Polynomial Integration (continued)

- For polynomials, an invariant sequence can be constructed to reduce number of equations
- Alternatively, we can formulate problem as unconstrained optimization problem in barycentric coordinates:

$$\underset{\boldsymbol{\alpha},\boldsymbol{\beta},\mathbf{w}}{\arg\min}\, F(\boldsymbol{\alpha},\boldsymbol{\beta},\mathbf{w}),$$

where

$$F(\boldsymbol{\alpha},\boldsymbol{\beta},\mathbf{w}) = \sum_{j=1}^{n_f}\left(\frac{\tilde{I}_{f_j} - I_{f_j}}{I_{f_j}}\right)^2,$$

$$\tilde{I}_{f_j} = \sum_{i=1}^{n} w_i' f_j(\alpha_i,\beta_i), \qquad I_{f_j} = \int_0^1\int_0^{1-\beta} f_j(\alpha,\beta)\,d\alpha\, d\beta,$$

with the expectation that $F(\boldsymbol{\alpha},\boldsymbol{\beta},\mathbf{w}) = 0$

Outline

- Introduction to Quadrature Rules
- Quadrature Preliminaries
- Singularities
  - Overview
  - One-Dimensional Characterization
  - Two-Dimensional Characterization
- Approach 1: Optimization for Moderate Number of Functions
- Approach 2: Quadrilateral Subdomains
- Numerical Example: The Electric-Field Integral Equation
- Summary

Overview

- Integrands with boundary singularities can have singularities located on edges and/or corners
  - Derivatives of integrand are unbounded
  - Integrand can be defined or undefined, provided the integrand is integrable

One-Dimensional Characterization

- Series expansion about singularity location
- Expansion alternates between monomials and singularities
- For the electric-field integral equation,

$$\mathbf{f}(x) = \{1,\, x,\, x\ln x,\, x^2,\, x^3,\, x^3\ln x,\, x^4,\, x^5,\, x^5\ln x,\, \dots\}$$

Two-Dimensional Characterization

- Expansions alternate between monomials and singularities
- If 2D characterizations of singularities are known, can use in sequence
- For the electric-field integral equation,

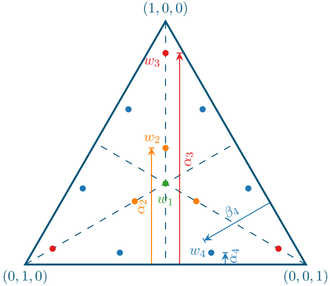
$$
\begin{gathered}
1 \\
x \\
x \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right) \\
x \ln\left(y + \sqrt{x^2 + y^2}\right) \\
x^2,\ xy \\
x^3,\ x^2 y \\
x^3 \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right) \\
x^3 \ln\left(y + \sqrt{x^2 + y^2}\right) \\
x^4,\ x^3 y,\ x^2 y^2 \\
x^5,\ x^4 y,\ x^3 y^2 \\
x^5 \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right) \\
x^5 \ln\left(y + \sqrt{x^2 + y^2}\right) \\
x^6,\ x^5 y,\ x^4 y^2,\ x^3 y^3 \\
x^7,\ x^6 y,\ x^5 y^2,\ x^4 y^3 \\
x^7 \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right) \\
x^7 \ln\left(y + \sqrt{x^2 + y^2}\right) \\
x^8,\ x^7 y,\ x^6 y^2,\ x^5 y^3,\ x^4 y^4 \\
x^9,\ x^8 y,\ x^7 y^2,\ x^6 y^3,\ x^5 y^4
\end{gathered}
$$

Outline

- Introduction to Quadrature Rules
- Quadrature Preliminaries
- Singularities
- Approach 1: Optimization for Moderate Number of Functions
  - Overview
  - Function Sequence
- Approach 2: Quadrilateral Subdomains
- Numerical Example: The Electric-Field Integral Equation
- Summary

Overview

- Goal is to efficiently integrate polynomials and singularities
- Compute points & weights through optimization – nonlinear least squares
- This approach uses polynomial rules as a baseline
  - Initial guesses near the polynomial rule
  - Same orbit counts for each n
- Replace higher polynomial degrees with singular functions
- Attempt to increase number of functions integrated



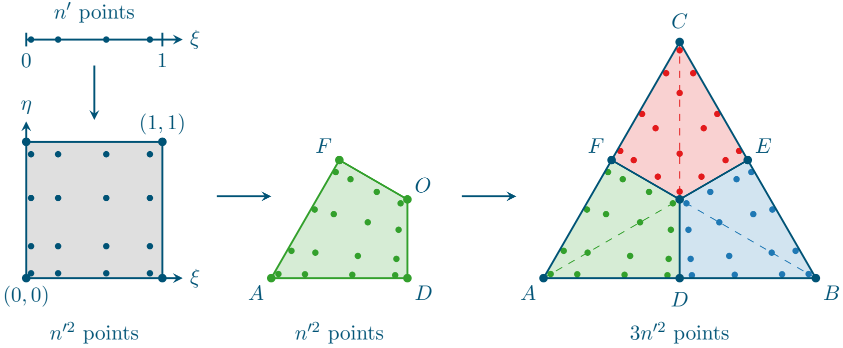
Function Sequence

- Weigh number of singular functions against maximum polynomial degree
- Ability to integrate polynomials includes ability to integrate cross terms (e.g., x^3 includes x^2y)
- Ability to integrate singular functions does not extend to cross terms
- Three approaches to address this issue:
  - Use 2D characterization of singularity, if available
  - Use 1D characterization of singularity, assume cross terms are not essential
  - Include cross terms for 1D characterization and reduce polynomial degree
- Alternatively, one can use Approach 2

Outline

Overview

- In multiple dimensions, number of integrable functions not straightforward
- Computation is expensive and multiple solutions exist
- For lengthy function sequences, we employ n'-point 1D rules that integrate 1D function sequences, such that $n = 3n'^2$



Outline

Overview

Scalar Potential

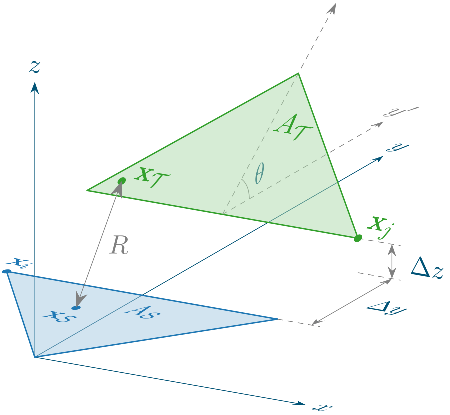
$$I_{s,c} = \int_{A_\mathcal{T}} \int_{A_\mathcal{S}} \frac{\cos(2\pi R)}{R} dA_\mathcal{S} dA_\mathcal{T}$$

$$I_{s,s} = \int_{A_\mathcal{T}} \int_{A_\mathcal{S}} \frac{\sin(2\pi R)}{R} dA_\mathcal{S} dA_\mathcal{T}$$

Vector Potential

$$I_{v,c} = \int_{A_\mathcal{T}} (\mathbf{x}_\mathcal{T} - \mathbf{x}_j) \cdot \int_{A_\mathcal{S}} \frac{\cos(2\pi R)}{R} (\mathbf{x}_\mathcal{S} - \mathbf{x}_i) dA_\mathcal{S} dA_\mathcal{T}$$

$$I_{v,s} = \int_{A_\mathcal{T}} (\mathbf{x}_\mathcal{T} - \mathbf{x}_j) \cdot \int_{A_\mathcal{S}} \frac{\sin(2\pi R)}{R} (\mathbf{x}_\mathcal{S} - \mathbf{x}_i) dA_\mathcal{S} dA_\mathcal{T}$$



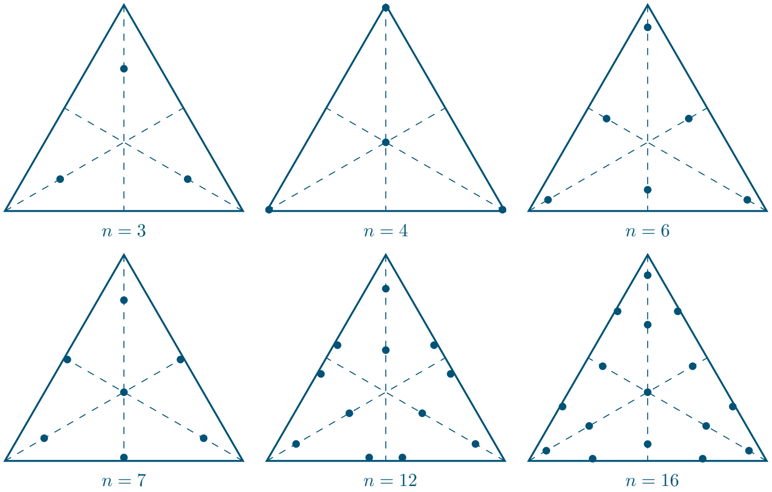
$A_\mathcal{S}$ has vertices $(0\,\text{m}, 0\,\text{m})$, $(1/20\,\text{m}, 1/20\,\text{m})$, and $(-1/20\,\text{m}, 1/20\,\text{m})$

$A_\mathcal{T}$ has same shape

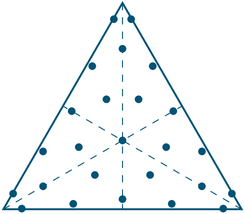
Approach 1 Function Sequences

1D Singularities	2D Singularities
1	1
x	x
$x \ln x$	$x \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right)$
$x^2,\ xy$	$x \ln\left(y + \sqrt{x^2 + y^2}\right)$
$x^3,\ x^2y$	$x^2,\ xy$
$x^3 \ln x$	$x^3,\ x^2y$
$x^4,\ x^3y,\ x^2y^2$	$x^3 \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right)$
$x^5,\ x^4y,\ x^3y^2$	$x^3 \ln\left(y + \sqrt{x^2 + y^2}\right)$
$x^5 \ln x$	$x^4,\ x^3y,\ x^2y^2$
$x^6,\ x^5y,\ x^4y^2,\ x^3y^3$	$x^5,\ x^4y,\ x^3y^2$
$x^7,\ x^6y,\ x^5y^2,\ x^4y^3$	$x^5 \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right)$
$x^7 \ln x$	$x^5 \ln\left(y + \sqrt{x^2 + y^2}\right)$
$x^8,\ x^7y,\ x^6y^2,\ x^5y^3,\ x^4y^4$	$x^6,\ x^5y,\ x^4y^2,\ x^3y^3$
$x^9,\ x^8y,\ x^7y^2,\ x^6y^3,\ x^5y^4$	$x^7,\ x^6y,\ x^5y^2,\ x^4y^3$
$x^9 \ln x$	$x^7 \ln\left(y - 1 + \sqrt{x^2 + (y-1)^2}\right)$
$x^{10},\ x^9y,\ x^8y^2,\ x^7y^3,\ x^6y^4,\ x^5y^5$	$x^7 \ln\left(y + \sqrt{x^2 + y^2}\right)$

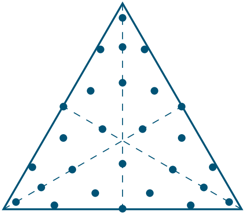
Approach 1, 1D Singularities



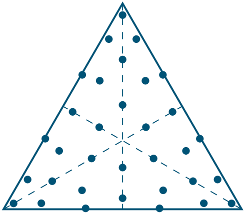
Approach 1, 1D Singularities (continued)



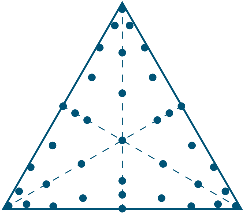
$n = 25$



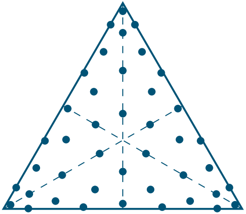
$n = 27$



$n = 33$

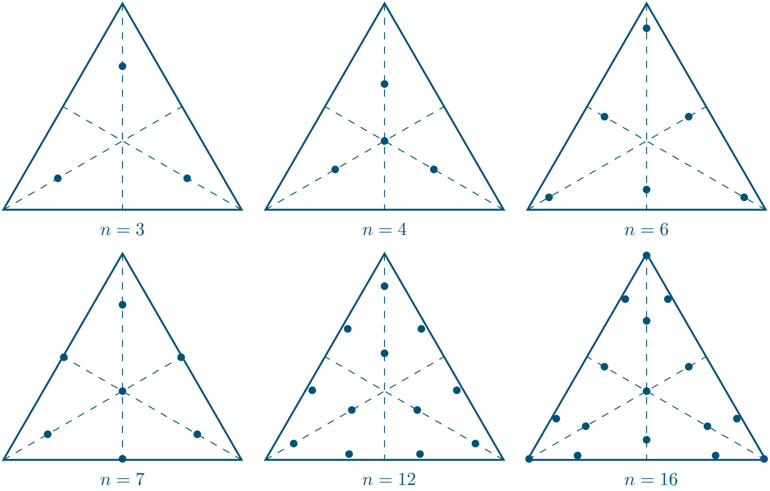


$n = 37$

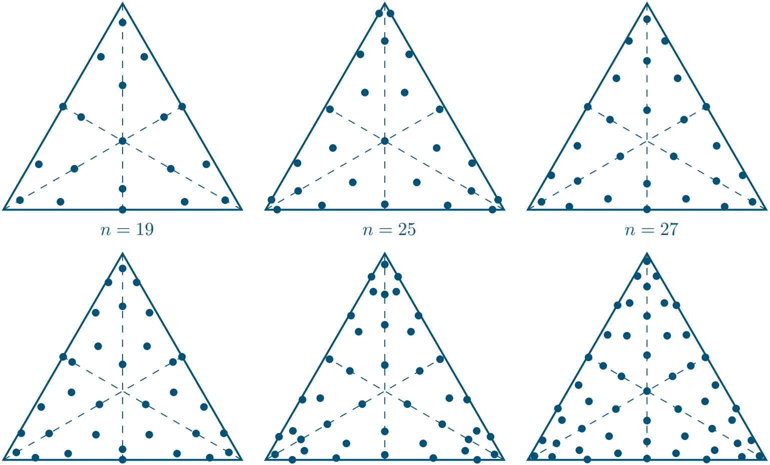


$n = 42$

Approach 1, 2D Singularities



Approach 1, 2D Singularities (continued)



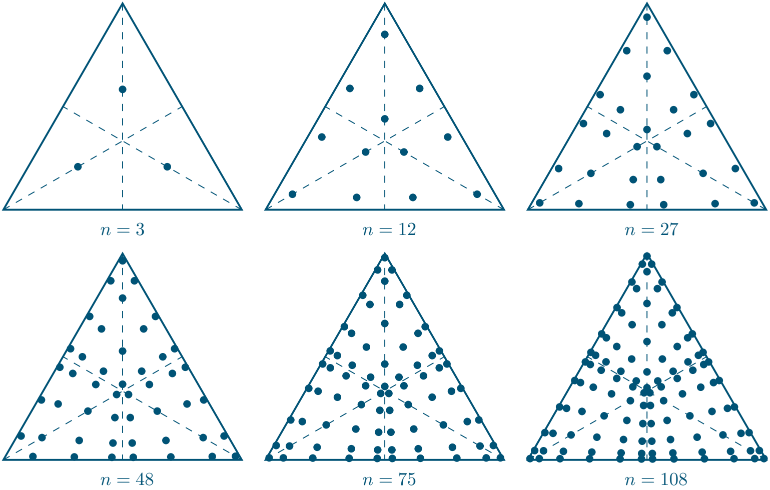
$n = 19$ $n = 25$ $n = 27$

$n = 33$ $n = 42$ $n = 52$

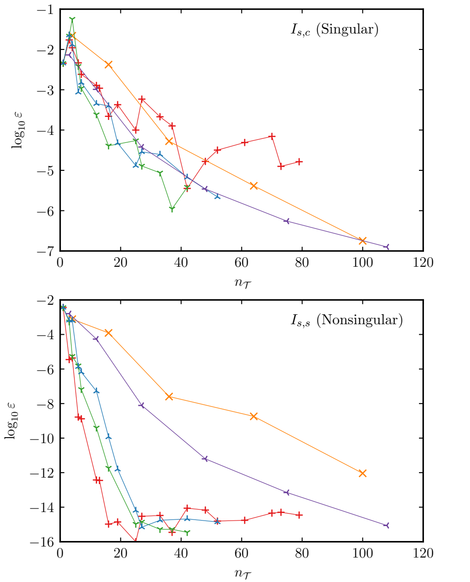
Approach 2 Function Sequence

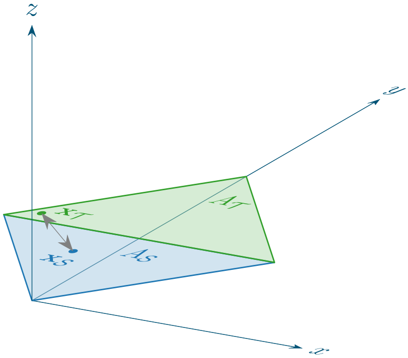
$$\mathbf{f}(x) = \{1,\, x,\, x\ln x,\, x^2,\, x^3,\, x^3\ln x,\, x^4,\, x^5,\, x^5\ln x, \ldots\}$$

Approach 2

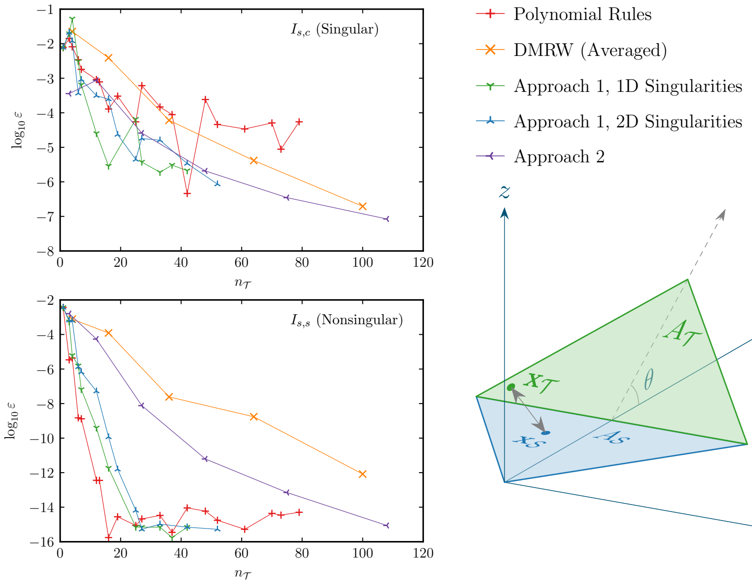


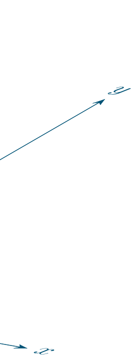
Case 1: Scalar potential, singular interaction, $\theta = 0°$, $\Delta y = 0$, and $\Delta z = 0$



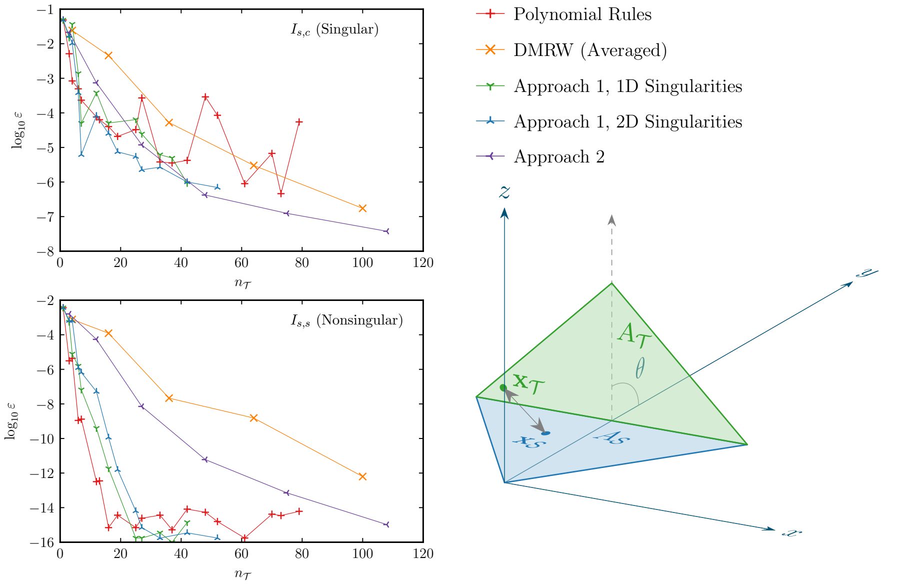


Case 2: Scalar potential, singular interaction, $\theta = 45°$, $\Delta y = 0$, and $\Delta z = 0$

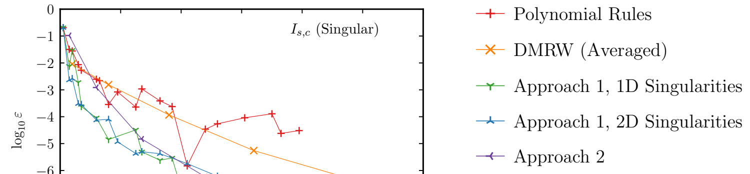


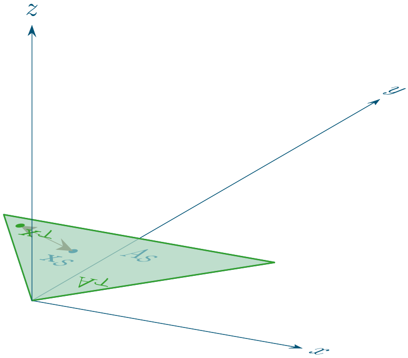


Case 3: Scalar potential, singular interaction, $\theta = 90°$, $\Delta y = 0$, and $\Delta z = 0$

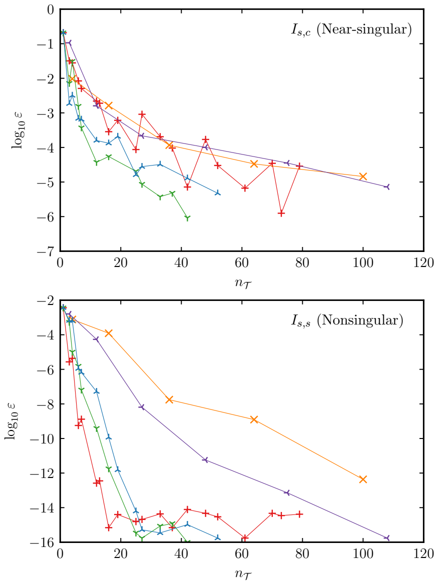


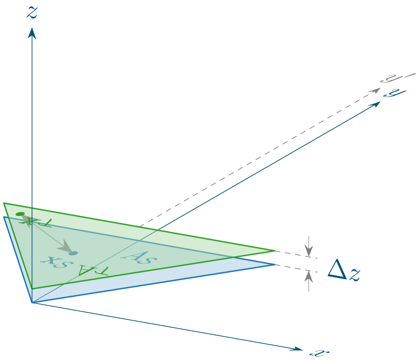
Case 4: Scalar potential, singular interaction, $\theta = 180°$, $\Delta y = 0$, and $\Delta z = 0$





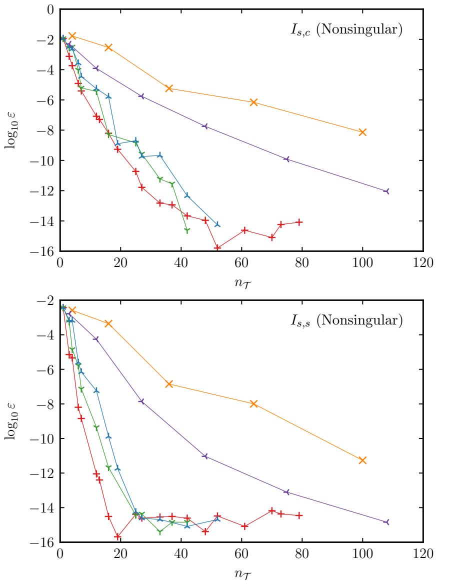
Case 5: Scalar potential, near-singular interaction, $\theta = 180°$, $\Delta y = 0$, and $\Delta z = \delta_z$

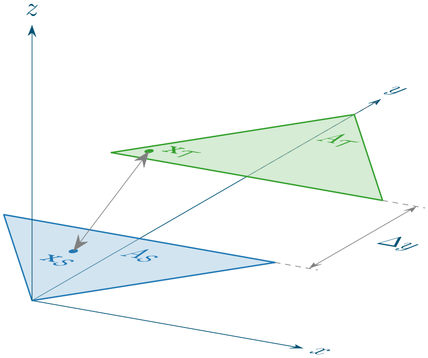




$\delta_z = 1/200$ of maximum edge length

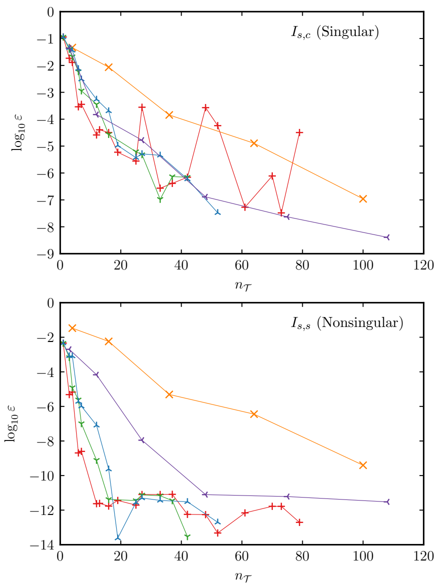
Case 6: Scalar potential, far interaction, $\theta = 0°$, $\Delta y = \delta_y$, and $\Delta z = 0$

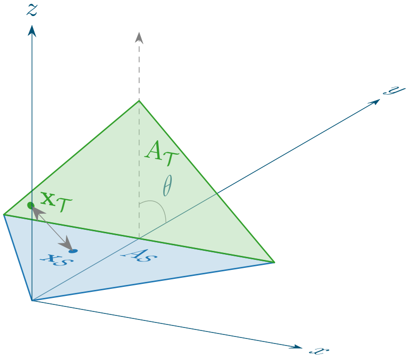




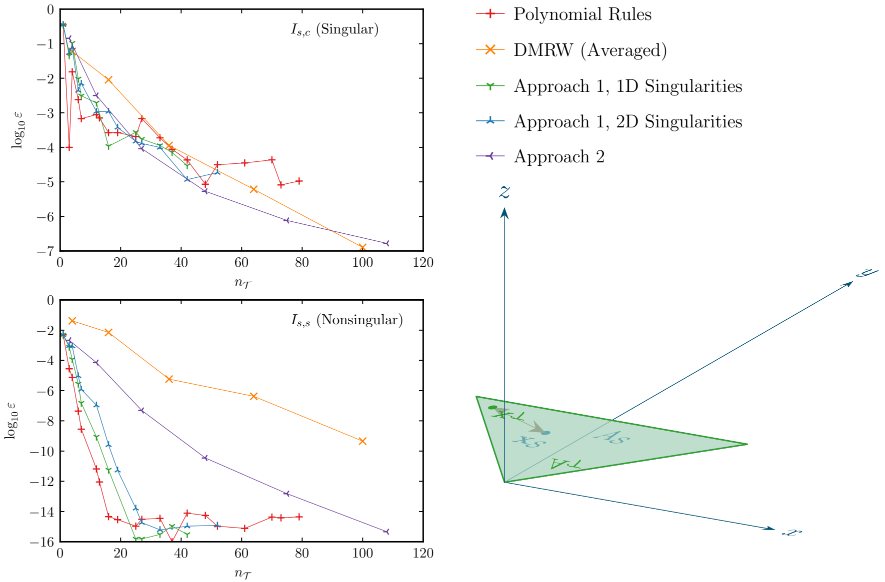
$\delta_y \approx 1.25 \times$ (maximum edge length)

Case 7: Vector potential, singular interaction, $\theta = 90°$, $\Delta y = 0$, and $\Delta z = 0$





Case 8: Vector potential, singular interaction, $\theta = 180°$, $\Delta y = 0$, and $\Delta z = 0$



Outline

Summary

- Introduced 2 symmetric quadrature approaches for arbitrary functions
- Motivated by need to integrate singular integrands
- Approach 1
  - Generally most efficient for singular integrands – outperformed polynomial rules by orders of magnitude
  - Similar efficiency to polynomial rules for nonsingular integrands
- Approach 2
  - More efficient than polynomial rules for singular integrands
  - Error decreases monotonically relative to number of integration points
  - Points are cheap to compute (from 1D rules)

References

- **B. Freno, W. Johnson, B. Zinser, S. Campione**
  Symmetric triangle quadrature rules for arbitrary functions
  ***Computers & Mathematics with Applications* (2020)** `arXiv:1909.01480`

- **B. Freno, W. Johnson, B. Zinser, D. Wilton, F. Vipiana, S. Campione**
  Characterization and integration of the singular test integrals in the method-of-moments implementation of the electric-field integral equation
  ***Engineering Analysis with Boundary Elements* (2021)** `arXiv:1911.02107`

- D. A. Dunavant
  High degree efficient symmetrical Gaussian quadrature rules for the triangle
  International Journal for Numerical Methods in Engineering (1985)

- J. N. Lyness and D. Jespersen
  Moderate degree symmetric quadrature rules for the triangle
  IMA Journal of Applied Mathematics (1975)

- J. Ma, V. Rokhlin, S. Wandzura
  Generalized Gaussian quadrature rules for systems of arbitrary functions
  SIAM Journal on Numerical Analysis (1996)

- S.-A. Papanicolopulos
  Computation of moderate-degree fully-symmetric cubature rules on the triangle using symmetric polynomials and algebraic solving
  Computers & Mathematics with Applications (2015)

- F. Vipiana, D. R. Wilton, W. A. Johnson
  Advanced numerical schemes for the accurate evaluation of 4-D reaction integrals in the method of moments
  IEEE Transactions on Antennas and Propagation (2013)

- S. Wandzura, H. Xiao
  Symmetric quadrature rules on a triangle
  Computers & Mathematics with Applications (2003)

Questions?

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.