Code-Verification Techniques for Electromagnetic Surface Integral Equations

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Outline

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- Introduction
  - Electromagnetic Surface Integral Equations
  - Verification and Validation
  - Error Sources in Electromagnetic Surface Integral Equations
  - This Work
- The Method-of-Moments Implementation of the MFIE
- Code-Verification Approaches
- Numerical Examples
- Summary

Electromagnetic Surface Integral Equations

- Are commonly used to model electromagnetic scattering and radiation
- Relate electric surface current to incident electric and/or magnetic field
- Discretize surface of electromagnetic scatterer with elements
- Evaluate 4D reaction integrals over 2D test and source elements
- Contain singular integrands when test and source elements are near

Verification and Validation

Credibility of computational physics codes requires verification and validation

- **Validation** assesses how well models represent physical phenomena
  - Compare computational results with experimental results
  - Assess suitability of models, model error, and bounds of validity
- **Verification** assesses accuracy of numerical solutions against expectations
  - *Solution verification* estimates numerical error for particular solution
  - *Code verification* verifies correctness of numerical-method implementation

Code Verification

- Code verification most rigorously assesses rate at which error decreases
- Error requires exact solution – usually unavailable
- Manufactured solutions are popular alternative
  - Manufacture an arbitrary solution
  - Insert manufactured solution into governing equations to get residual term
  - Add residual term to equations to coerce solution to manufactured solution
- For integral equations, few instances of code verification exist
- Analytical differentiation is straightforward – analytical integration is not
- Numerical integration is necessary, generally incurs an approximation error
- Therefore, manufactured source term may have its own numerical error

Error Sources in Electromagnetic Surface Integral Equations

3 sources of numerical error:

- **Domain discretization**: Representation of curved surfaces with planar elements
  - Second-order error for curved surfaces, no error for planar surfaces
  - Error reduced with curved elements
- **Solution discretization**: Representation of solution or operators
  - Common in solution to differential, integral, and integro-differential equations
  - Finite number of basis functions to approximate solution
  - Finite samples queried to approximate underlying equation operators
- **Numerical integration**: Quadrature
  - Analytical integration is not always possible
  - For well-behaved integrands,
    - Expect integration error at least same order as solution-discretization error
    - Less rigorously, error should decrease with more quadrature points
  - For (nearly) singular integrands, monotonic convergence is not assured

This Work

Isolate solution-discretization error

- Eliminate integration error by manufacturing solution and Green's function
- Select unique solution through optimization when equations are singular

Isolate numerical-integration error

- Cancel solution-discretization error using basis functions
- Eliminate solution-discretization error by avoiding basis functions

Address domain-discretization error

- Account for curvature – integrate over curved triangular elements
- Neglect curvature – integrate over planar triangular elements

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- Introduction
- The Method-of-Moments Implementation of the MFIE
  - The Magnetic-Field Integral Equation
  - Discretization
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The Magnetic-Field Integral Equation

In time-harmonic form, scattered magnetic field $\mathbf{H}^{\mathcal{S}}$ computed from current

Scattered magnetic field $$\mathbf{H}^{\mathcal{S}}(\mathbf{x}) = \frac{1}{\mu}\nabla \times \mathbf{A}(\mathbf{x})$$

Magnetic vector potential $$\mathbf{A}(\mathbf{x}) = \mu \int_{S'} \mathbf{J}(\mathbf{x}')G(\mathbf{x},\mathbf{x}')dS'$$

Green's function $$G(\mathbf{x},\mathbf{x}') = \frac{e^{-jkR}}{4\pi R}, \qquad R = |\mathbf{x} - \mathbf{x}'|$$

Singularity when $R \to 0$

$\mathbf{J}$ is electric surface current density

$S' = S$ is surface of scatterer

μ and ϵ are permeability and permittivity of surrounding medium

$k = \omega\sqrt{\mu\epsilon}$ is wavenumber

The Magnetic-Field Integral Equation (continued)

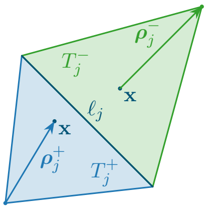
Compute $\mathbf{J}$ from incident magnetic field $\mathbf{H}^{\mathcal{I}}$ $(\mathbf{n} \times (\mathbf{H}^{\mathcal{S}} + \mathbf{H}^{\mathcal{I}}) = \mathbf{J})$:

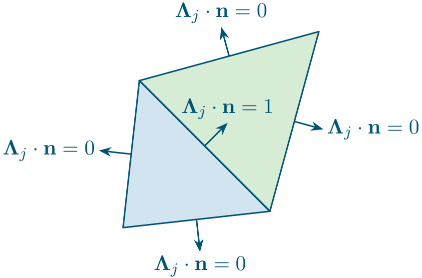
$$\frac{1}{2}\mathbf{J} - \mathbf{n} \times \int_{S'} [\mathbf{J}(\mathbf{x}') \times \nabla' G(\mathbf{x}, \mathbf{x}')] dS' = \mathbf{n} \times \mathbf{H}^{\mathcal{I}}$$

Discretize surface with triangles, approximate $\mathbf{J}$ with RWG basis functions:

$$\mathbf{J}_h(\mathbf{x}) = \sum_{j=1}^{n_b} J_j \boldsymbol{\Lambda}_j(\mathbf{x})$$

Project MFIE onto vector-valued RWG basis functions





Discretized Problem

In matrix–vector form, solve for $\mathbf{J}^h$:

$$\mathbf{Z}\mathbf{J}^h = \mathbf{V}$$

$$\underset{\text{Impedance matrix}}{Z_{i,j} = a(\boldsymbol{\Lambda}_j, \boldsymbol{\Lambda}_i)}, \qquad \underset{\text{Current vector}}{J_j^h = J_j}, \qquad \underset{\text{Excitation vector}}{V_i = b(\mathbf{H}^{\mathcal{I}}, \boldsymbol{\Lambda}_i)}$$

$$a(\mathbf{u},\mathbf{v}) = \frac{1}{2}\int_S \bar{\mathbf{v}}(\mathbf{x}) \cdot \mathbf{u}(\mathbf{x}) dS - \int_S \bar{\mathbf{v}}(\mathbf{x}) \cdot \left(\mathbf{n}(\mathbf{x}) \times \int_{S'} \left[\mathbf{u}(\mathbf{x}') \times \nabla' G(\mathbf{x},\mathbf{x}')\right] dS'\right) dS$$

$$b(\mathbf{u},\mathbf{v}) = \int_S \bar{\mathbf{v}}(\mathbf{x}) \cdot \left[\mathbf{n}(\mathbf{x}) \times \mathbf{u}(\mathbf{x})\right] dS$$

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  - Manufactured Surface Current and Green's Function
  - Solution-Discretization Error
  - Numerical-Integration Error
  - Domain-Discretization Error
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Manufactured Surface Current

Continuous equations: $r_i(\mathbf{J}\ \ ) = a(\mathbf{J}\ \ , \boldsymbol{\Lambda}_i) - b(\mathbf{H}^{\mathcal{I}}, \boldsymbol{\Lambda}_i) = 0$

Discretized equations: $r_i(\mathbf{J}_h) = a(\mathbf{J}_h, \boldsymbol{\Lambda}_i) - b(\mathbf{H}^{\mathcal{I}}, \boldsymbol{\Lambda}_i) = 0$

Method of manufactured solutions modifies discretized equations:

$$\mathbf{r}(\mathbf{J}_h) = \mathbf{r}(\mathbf{J}_{\text{MS}}),$$

$\mathbf{J}_{\text{MS}}$ is manufactured solution, $\mathbf{r}(\mathbf{J}_{\text{MS}})$ is computed exactly

Modified discretized equations: $a(\mathbf{J}_h, \boldsymbol{\Lambda}_i) = \underbrace{a(\mathbf{J}_{\text{MS}}, \boldsymbol{\Lambda}_i)}_{= b\big(\mathbf{H}^{\mathcal{I}}, \boldsymbol{\Lambda}_i\big)\text{: implement via } \mathbf{H}^{\mathcal{I}}}$

$$\mathbf{H}^{\mathcal{I}} = \frac{1}{2}\mathbf{J}_{\text{MS}} \times \mathbf{n} - \int_{S'} \left[\mathbf{J}_{\text{MS}}(\mathbf{x}') \times \nabla' G(\mathbf{x}, \mathbf{x}')\right] dS'$$

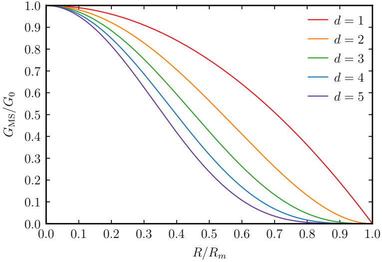
MMS incorporated through $\mathbf{H}^{\mathcal{I}}$ – no additional source term required

Manufactured Green's Function

Integrals with G cannot be computed analytically or, when $R \to 0$, accurately

Inaccurately computing $\mathbf{H}^{\mathcal{I}}$ contaminates convergence studies

Manufacture Green's function: $G_{\mathrm{MS}}(R) = G_0\left(1 - \frac{R^2}{R_m^2}\right)^d$, $R_m = \max_{\mathbf{x},\mathbf{x}'\in S} R$ and $d \in \mathbb{N}$



Reasoning:
1) Even powers of R permit integrals to be computed analytically for many $\mathbf{J}_{\mathrm{MS}}$
2) G_{MS} increases when R decreases, as with actual G

Solution-Discretization Error

- Error due to basis-function approximation of solution: $\mathbf{J}_h(\mathbf{x}) = \sum_{j=1}^{n_b} J_j \mathbf{\Lambda}_j(\mathbf{x})$
- Measured with discretization error: $\mathbf{e_J} = \mathbf{J}^h - \mathbf{J}_n$

$$\|\mathbf{e_J}\| \leq C_\mathbf{J} h^{p_\mathbf{J}}$$

J_{n_j}: component of $\mathbf{J}_{\text{MS}}$ flowing from T_j^+ to T_j^-
$C_\mathbf{J}$: function of solution derivatives
h : measure of mesh size
$p_\mathbf{J}$: order of accuracy

- Compute $p_\mathbf{J}$ from $\|\mathbf{e_J}\|$ across multiple meshes (expect $p_\mathbf{J} = 2$ for RWG)
- Avoid numerical-integration error contamination → integrate exactly (G_{MS})

Solution-Discretization Error: Solution Uniqueness

For terms with G_{MS}, $\mathbf{Z}$ is practically singular $\rightarrow$ infinite solutions for $\mathbf{J}^h$

Choose $\mathbf{J}^h$ closest to $\mathbf{J}_n$ (J_{n_j}: $\mathbf{J}_{\text{MS}}$ from $T_j^+ \rightarrow T_j^-$) that satisfies $\mathbf{Z}\mathbf{J}^h = \mathbf{V}_{\text{MS}}$

Compute pivoted QR factorization of $\mathbf{Z}^H$ to determine rank

Express $\mathbf{J}^h$ in terms of basis $\mathbf{Q}$:

$$\mathbf{J}^h = \mathbf{Q}_1\mathbf{u} + \mathbf{Q}_2\mathbf{v}$$

$\mathbf{u}$: coefficients that satisfy $\mathbf{Z}\mathbf{J}^h = \mathbf{V}_{\text{MS}}$
$\mathbf{v}$: coefficients that bring $\mathbf{J}^h$ closest to $\mathbf{J}_n$, given $\mathbf{u}$

Compute $\mathbf{v}$ by minimizing

- $\|\mathbf{e}_\mathbf{J}\|_2$: closed-form solution
  may require finer meshes when measuring $\|\mathbf{e}_\mathbf{J}\|_\infty$
- $\|\mathbf{e}_\mathbf{J}\|_\infty$: more expensive (linear programming)
  does not require finer meshes when measuring $\|\mathbf{e}_\mathbf{J}\|_\infty$

Numerical-Integration Error

- Error due to quadrature evaluation of integrals on both sides of equation
- Measured by functionals

$$e_a(\mathbf{u}) = a^q(\mathbf{u},\mathbf{u}) - a(\mathbf{u},\mathbf{u}) \qquad e_b(\mathbf{u}) = b^q(\mathbf{H}_{\text{MS}}^{\mathcal{I}},\mathbf{u}) - b(\mathbf{H}_{\text{MS}}^{\mathcal{I}},\mathbf{u})$$

$$|e_a| \leq C_a h^{p_a} \qquad |e_b| \leq C_b h^{p_b}$$

a^q, b^q: quadrature evaluation of a and b
C_a, C_b: functions of integrand derivatives
p_a, p_b: order of accuracy of quadrature rules

- With multiple meshes, compute p_a and p_b from $|e_a|$ and $|e_b|$
- Avoid solution-discretization error contamination → cancel or eliminate it

Numerical-Integration Error: Solution-Discretization Error Avoidance

2 complementary approaches to avoiding solution-discretization error:

- Solution-discretization error cancellation

$$e_a(\mathbf{J}_{h_{\text{MS}}}) = a^q(\mathbf{J}_{h_{\text{MS}}}, \mathbf{J}_{h_{\text{MS}}}) - a(\mathbf{J}_{h_{\text{MS}}}, \mathbf{J}_{h_{\text{MS}}})$$
$$e_b(\mathbf{J}_{h_{\text{MS}}}) = b^q(\mathbf{H}^{\mathcal{I}}_{\text{MS}}, \mathbf{J}_{h_{\text{MS}}}) - b(\mathbf{H}^{\mathcal{I}}_{\text{MS}}, \mathbf{J}_{h_{\text{MS}}})$$

$\mathbf{J}_{h_{\text{MS}}}$ is the basis-function representation of $\mathbf{J}_{\text{MS}}$

$e_a(\mathbf{J}_{h_{\text{MS}}})$ and $e_b(\mathbf{J}_{h_{\text{MS}}})$ are proportional to their influence on $\mathbf{e}_{\mathbf{J}} = \mathbf{J}^h - \mathbf{J}_n$

- Solution-discretization error elimination

$$e_a(\mathbf{J}_{\text{MS}}) = a^q(\mathbf{J}_{\text{MS}}, \mathbf{J}_{\text{MS}}) - a(\mathbf{J}_{\text{MS}}, \mathbf{J}_{\text{MS}})$$
$$e_b(\mathbf{J}_{\text{MS}}) = b^q(\mathbf{H}^{\mathcal{I}}_{\text{MS}}, \mathbf{J}_{\text{MS}}) - b(\mathbf{H}^{\mathcal{I}}_{\text{MS}}, \mathbf{J}_{\text{MS}})$$

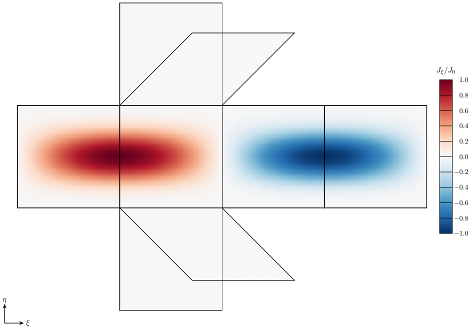
Domain-Discretization Error

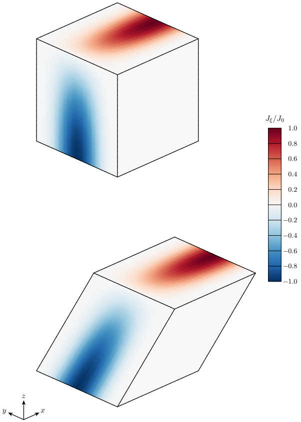
Triangular elements approximate curved S with faceted approximation S_h

- Accounting for curvature
  - Integrate over curved triangles that conform to S instead of planar triangles
  - Use solution-discretization error elimination approach
  - Assess curvature implementation and numerical integration
- Neglecting curvature
  - Use solution-discretization error cancellation approach
  - Assess numerical integration by computing integrals on S_h instead of S

Outline

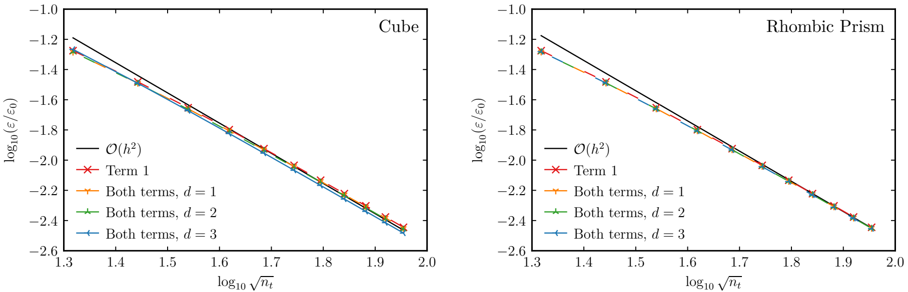
Manufactured Surface Current $\mathbf{J}_{\mathrm{MS}}$ for Cube and Rhombic Prism





- Manufacture solution for 2D strip of class C^2
- Wrap strip around lateral surfaces of prisms
- Solution is product of ξ and η dependencies
  - ξ dependency: sinusoid with a single period
  - η dependency: cubed sinusoid with a half period
- Current flows along ξ

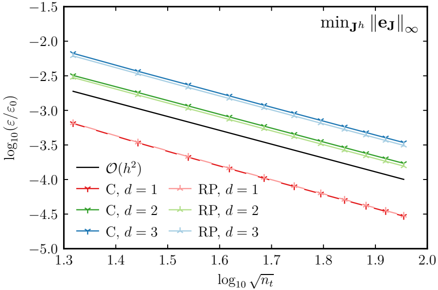
Solution-Discretization Error: $\varepsilon = \|\mathbf{e_J}\|_\infty$

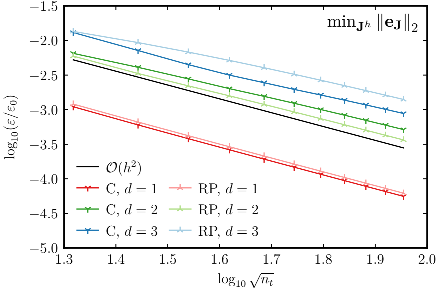


$$a(\mathbf{J}_h, \mathbf{\Lambda}_i) = \underbrace{\frac{1}{2}\int_S \mathbf{\Lambda}_i(\mathbf{x}) \cdot \mathbf{J}_h(\mathbf{x}) dS}_{\text{Term 1}} + \underbrace{\int_S \mathbf{\Lambda}_i(\mathbf{x}) \cdot \left(\mathbf{n}(\mathbf{x}) \times \int_{S'} \left[\nabla' G_{\text{MS}}(\mathbf{x}, \mathbf{x}') \times \mathbf{J}_h(\mathbf{x}')\right] dS'\right) dS}_{\text{Term 2}}$$

$$G_{\text{MS}}(\mathbf{x}, \mathbf{x}') = \left(1 - \frac{R^2}{R_m^2}\right)^d$$

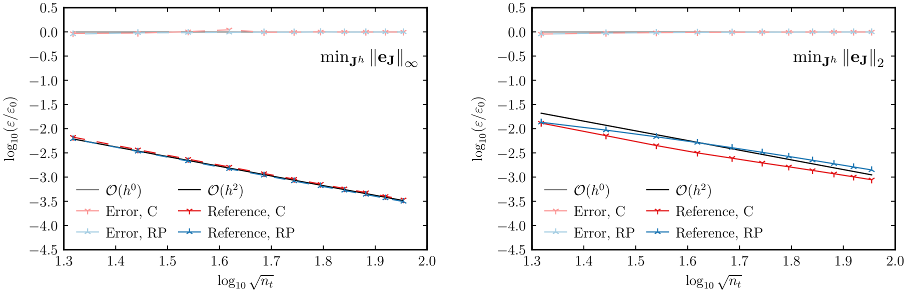
Solution-Discretization Error: $\varepsilon = \|\mathbf{e}_\mathbf{J}\|_\infty$, Term 2





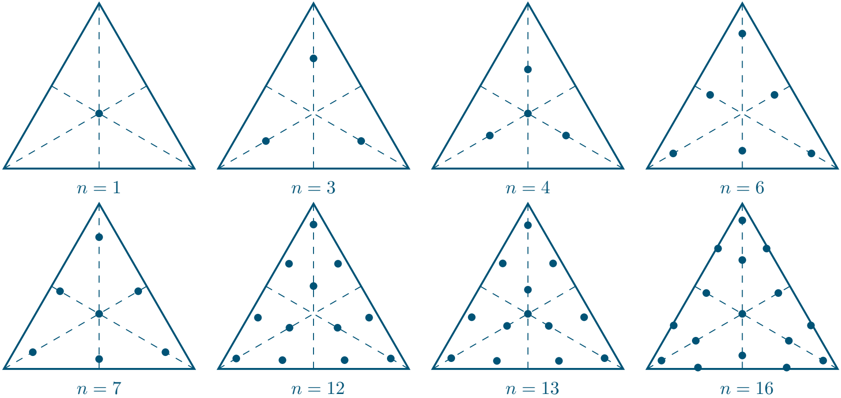
	$\min_{\mathbf{J}^h} \|\mathbf{e}_\mathbf{J}\|_\infty$		$\min_{\mathbf{J}^h} \|\mathbf{e}_\mathbf{J}\|_2$	
Mesh	C	RP	C	RP
1–2	2.0800	2.0653	2.0811	1.2935
2–3	2.0141	2.0529	2.1055	1.4193
3–4	2.0303	2.0193	1.9159	1.5150
4–5	2.0196	2.0163	1.6421	1.5847
5–6	2.0061	2.0242	1.6677	1.6372
6–7	2.0133	2.0158	1.5800	1.6779
7–8	2.0113	2.0167	1.6282	1.7104
8–9	2.0037	2.0122	1.6664	1.7369
9–10	2.0086	2.0117	1.6974	1.7589
10–11	2.0053	2.0118	1.7231	1.7776

Solution-Discretization Error: $\varepsilon = \|\mathbf{e_J}\|_\infty$ for Coding Error ($d = 3$)



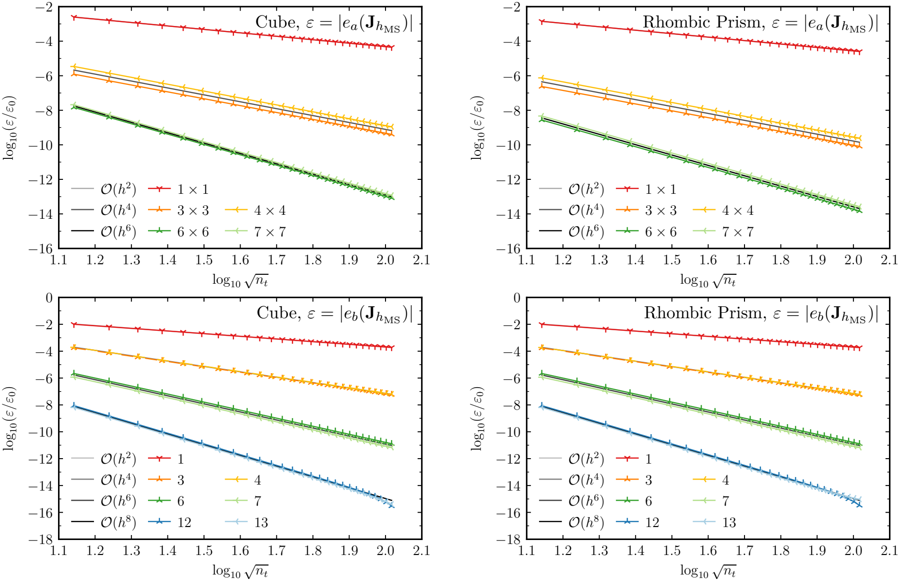
Both norms are able to detect the coding error

Numerical-Integration Error: Polynomial Quadrature Rules

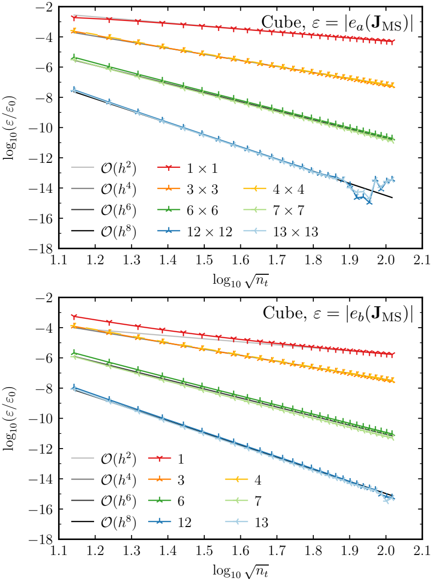


n	1	3	4	6	7	12	13	16
Max. integrand degree	1	2	3	4	5	6	7	8
Convergence rate	$\mathcal{O}(h^2)$	$\mathcal{O}(h^4)$	$\mathcal{O}(h^4)$	$\mathcal{O}(h^6)$	$\mathcal{O}(h^6)$	$\mathcal{O}(h^8)$	$\mathcal{O}(h^8)$	$\mathcal{O}(h^{10})$

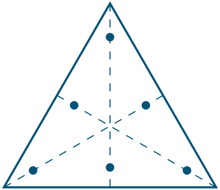
Numerical-Integration Error: Cancellation ($d = 3$)



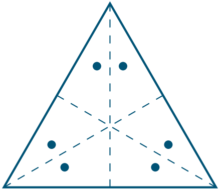
Numerical-Integration Error: Elimination ($d = 3$)



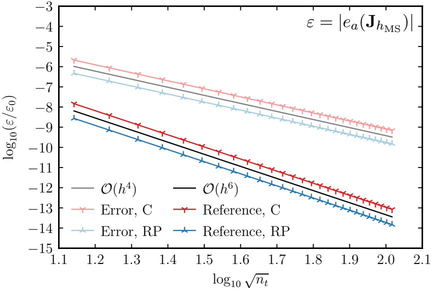
Numerical-Integration Error: Coding Error, Cancellation ($d = 3$)

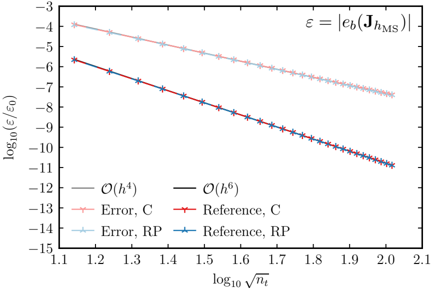


Maximum polynomial degree: 4

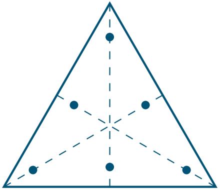


Maximum polynomial degree: 3

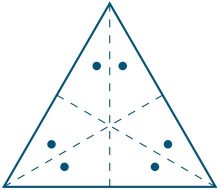




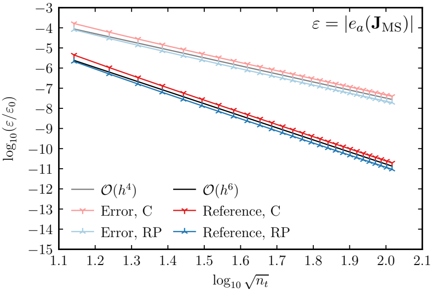
Numerical-Integration Error: Coding Error, Elimination ($d = 3$)

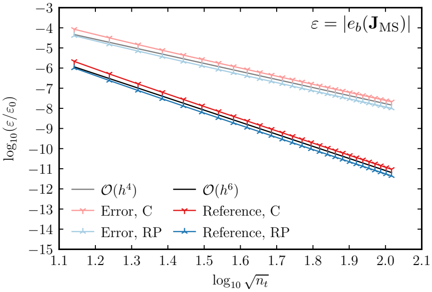


Maximum polynomial degree: 4



Maximum polynomial degree: 3





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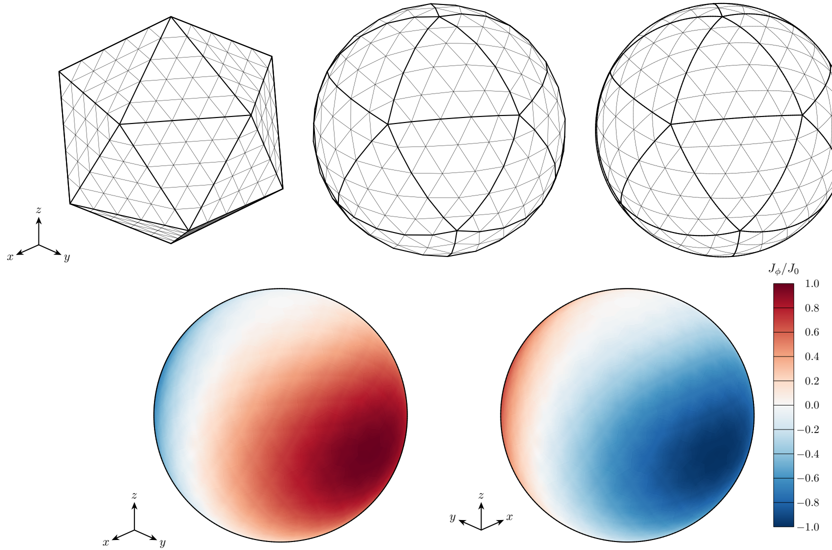
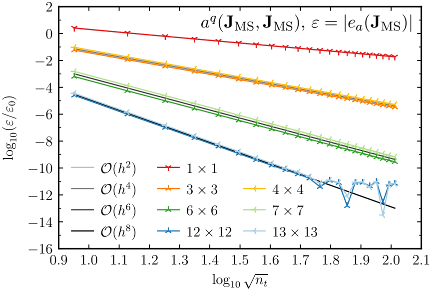
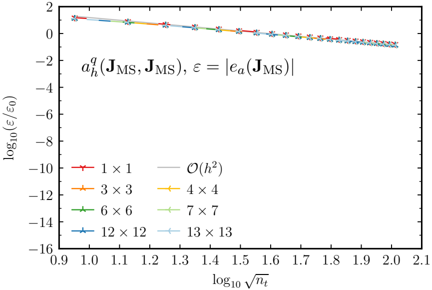
Manufactured Surface Current $\mathbf{J}_{\mathrm{MS}}$ and Mesh ($n_t = 500$) for Sphere

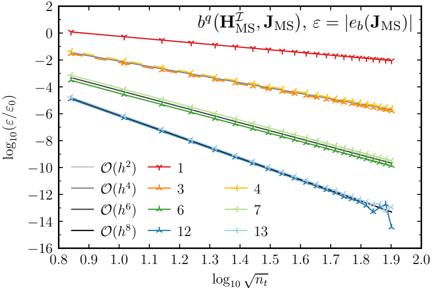


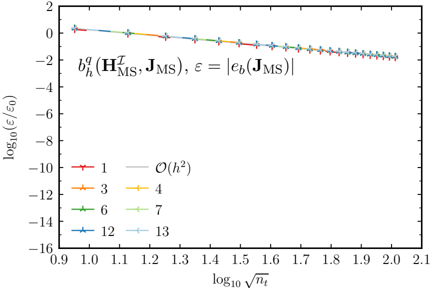
Manufactured surface current $\mathbf{J}_{\mathrm{MS}}(\mathbf{x}) = J_\phi(\theta,\phi)\mathbf{e}_\phi = (J_0 \sin^2\theta \sin\phi)\mathbf{e}_\phi$ (ϕ around z)

Domain-Discretization Error: Elimination ($d = 3$)

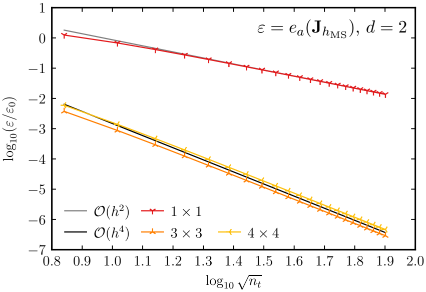


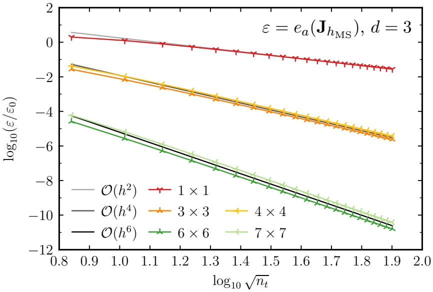






Domain-Discretization Error: Cancellation, No Curvature





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  - Closing Remarks

Closing Remarks

3 error sources in integral equations:

- **Solution-discretization error** – isolated
  - Integrated exactly
  - Optimized to select unique solution when equations were singular
- **Numerical-integration error** – isolated
  - Canceled solution-discretization error – used basis functions
  - Eliminated solution-discretization error – did not use basis functions
- **Domain-discretization error** – addressed
  - Accounted for curvature – integrated over curved triangular elements
  - Neglected curvature – integrated over planar triangular elements

Achieved expected orders of accuracy with and without coding errors

Questions? bafreno@sandia.gov brianfreno.github.io

Additional Information

- B. Freno, N. Matula, W. Johnson
  Manufactured solutions for the method-of-moments implementation of the EFIE
  Journal of Computational Physics (2021) arXiv:2012.08681
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  Code-verification techniques for the method-of-moments implementation of the EFIE
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  Manufactured solutions for an electromagnetic slot model
  Journal of Computational Physics (2024) arXiv:2406.14573