# Numerical Quadrature Over Smooth Closed Surfaces

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in collaboration with

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Evaluate approximately

$$\mathcal{I}_{\mathcal{S}}(f) := \iint_{\mathcal{S}} f(\mathbf{x}) d\mathcal{S}$$

S is a smooth closed surface (2D) embedded in 3D (i.e.  $\mathbf{x} \in \mathbb{R}^3$ ).

Note:

- Typically only simple integrands  $f(\mathbf{x})$  lead to explicit representations of the value of the surface integral.
- In application  $f(\mathbf{x})$  may be given only as values sampled at discrete locations.

In the case of spherical geometries applications include

- geophysics
- optics
- numerical weather prediction

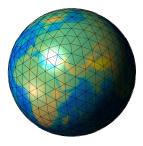
where integrated quantities such as

- total energy
- total radiance
- average temperature

are required by themselves or to supplement systems of partial differential equations.

For other geometries we imagine similar uses along with

- Surface areas
- Volumes
- etc.



On each of the N subintervals construct a constant function equal to f at the midpoint (creating many rectangular areas).

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### **Trapezoidal Approximations**

$$I_{[a,b]}(f) \approx \sum_{i=0}^{N-1} \frac{(b-a)}{N} \cdot f\left(\frac{x_i + x_{i+1}}{2}\right)$$

$$I_{[a,b]}(f) \approx \frac{(b-a)}{2N} \cdot \left(1 \cdot f(x_0) + \sum_{i=1}^{N-1} 2 \cdot f(x_i) + 1 \cdot f(x_N)\right)$$

### Extending the Approximation Idea to Spheres

In either case we approximate the integral in 1D by

$$I_{[a,b]}(f) = \int_a^b f(x) dx \approx \sum_{i=0}^N w_i f(x_i),$$

where

- $x_i$ , i = 0, 1, 2, ..., N, are discrete points in [a, b], and
- w<sub>i</sub> depend on
  - the locations of x<sub>i</sub>
  - the approximation chosen for f over each subinterval, not on f itself

#### Goal:

Find  $W_i$ ,  $i = 1, 2, \ldots, N$ , such that

$$\mathcal{I}_{S}(f) = \iint_{S} f(\mathbf{x}) dS \approx \sum_{i=1}^{N} W_{i}f(\mathbf{x}_{i})$$

where

•  $\mathbf{x}_i$ ,  $i = 1, 2, \dots, N$ , are discrete points on S

W<sub>i</sub> depend on

- the locations of the points x<sub>i</sub>
- the approximation chosen for f, not on f itself

- Required accuracy- How many points N do we need?
- Construction of node-sets- How do we place N points on the surface?
- Computational cost/run time— For a given N, how long does it take to find the W<sub>k</sub>? Can we distribute the cost to any number of processors?
- Storage requirements- For a given N, how much memory (RAM) is needed to find the W<sub>k</sub>?

### **RBF** Interpolation

RBF interpolation of a function  $f(\mathbf{x})$  at a set of points  $\{\mathbf{x}_i\}_{i=1}^N$  (all in  $\mathbb{R}^d$ ) is accomplished by enforcing

$$f(\mathbf{x}_k) pprox s(\mathbf{x}_k) := \sum_{i=1}^N c_i^{RBF} \phi(r_i(\mathbf{x}_k))$$

The interpolant is constructed by solving the linear system

$$Ac^{RBF} := \begin{bmatrix} \phi(r_{11}) & \phi(r_{12}) & \cdots & \phi(r_{1N}) \\ \phi(r_{21}) & \phi(r_{22}) & \cdots & \phi(r_{2N}) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(r_{N1}) & \phi(r_{N2}) & \cdots & \phi(r_{NN}) \end{bmatrix} \begin{bmatrix} c_1^{RBF} \\ c_2^{RBF} \\ \vdots \\ c_N^{RBF} \end{bmatrix} = \begin{bmatrix} f(\mathbf{x}_1) \\ f(\mathbf{x}_2) \\ \vdots \\ c_N^{RBF} \\ f(\mathbf{x}_N) \end{bmatrix} =: \mathbf{f}$$

(with  $r_{ji} = \|\mathbf{x}_j - \mathbf{x}_i\|_2$ ), which comes from satisfying the interpolation conditions

- The matrix A can be shown to be nonsingular in the case of GA, MQ, and IMQ RBF interpolants (see, e.g., M.D. Buhmann. "Radial basis functions." Acta Numerica, pages 1–38, 2000).
- In the case of even and odd powers the matrix (and interpolation problem) must be supplemented by multivariate polynomial terms.

### **RBF** Interpolation with Polynomial Terms

When multivariate polynomial terms must be included the interpolant is modified to be

$$f(\mathbf{x}) pprox \hat{s}(\mathbf{x}) = \sum_{i=1}^{N} c_i^{RBF} \phi(r_i(\mathbf{x})) + \sum_{l=1}^{M} c_l^m \pi_l(\mathbf{x}),$$

where  $\{\pi_l\}_{l=1}^M$  is the set of all polynomial terms up to degree *m*. In  $\mathbb{R}^2$ ,  $M = \frac{(m+1)(m+2)}{2}$  and this set includes the terms

$$\underbrace{1}, \underbrace{x, y}, \underbrace{x^{2}, xy, y^{2}}, \underbrace{x^{3}, x^{2}y, xy^{2}, y^{3}}, \dots, \underbrace{x^{m}, x^{m-1}y, x^{m-2}y^{2}, \dots, x^{2}y^{m-2}, xy^{m-1}, y^{m}}$$

Once augmented, the linear system becomes

$$\hat{A}\hat{c} = \begin{bmatrix} A & P^m \\ (P^m)^T & 0 \end{bmatrix} \begin{bmatrix} c^{RBF} \\ c^m \end{bmatrix} = \begin{bmatrix} f \\ 0 \end{bmatrix} = \hat{f} \quad \text{where} \quad c^m = \begin{bmatrix} c_1^m & c_2^m & \cdots & c_M^m \end{bmatrix}^T$$

and (again, in  $\mathbb{R}^2$ )

The last M equations come from the conditions

$$\sum_{i=1}^{N} c_i^{RBF} \pi_I(\mathbf{x}_i) = 0, \ I = 1, 2, \dots, M.$$

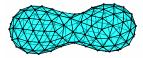
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Given: N nodes on the surface, S, and a (flat) triangulation, T, of the node set

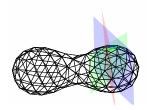
Concept Illustration



Given: N nodes on the surface, S, and a (flat) triangulation, T, of the node set

For each of the flat triangles in T, find a projection point.

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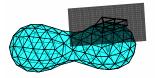


5

Given: N nodes on the surface, S, and a (flat) triangulation, T, of the node set

- For each of the flat triangles in T, find a projection point.
- Project a neighborhood (on S) of the three vertices of the triangle into the plane containing the vertices, including *n* nodes from S<sub>N</sub>.

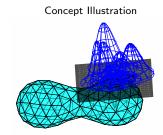
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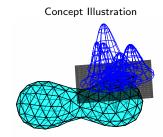
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- Find quadrature weights over the local projected node set for the definite integral over the projected central flat planar triangle.



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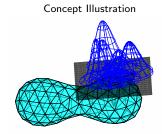
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- Convert quadrature weights in each plane to corresponding weights for the surface.



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- Convert quadrature weights in each plane to corresponding weights for the surface.
- Combine the weights for the individual curved triangles to obtain the full weight set for the surface.



### Initialization

Given a set  $S_N := {\mathbf{x}_i}_{i=1}^N \subset S$ , we associate to the set  $T = {t_{A_k B_k C_k}}_{k=1}^K$  of flat triangles a set of curved triangles,  $T = {\tau_{A_k B_k C_k}}_{k=1}^K$ , such that

- the curved triangle vertices are the elements of  $S_N$ ,
- the curved triangle edges are projections of the flat triangle edges to the surface,
- no curved triangle contains an element of S<sub>N</sub> other than its vertices,
- the interiors of the curved triangles are pairwise disjoint, and
- the union of the set  $\mathcal{T}$  covers S.

The requirements on  $\mathcal{T}$  allow

$$\mathcal{I}_{S}(f) = \iint_{S} f(\mathbf{x}) dS = \sum_{k=1}^{K} \iint_{\tau_{A_{k}} B_{k} C_{k}} f(\mathbf{x}) dS$$

Flat Triangles in T



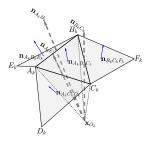
Curved Triangles in T



For each edge of a flat triangle in T define a unique "cutting" plane so that both of the two triangles containing a given edge will define the same plane.

The cutting plane along the edge  $A_k B_k$  of triangle  $t_{A_k B_k C_k}$  is defined to contain the edge and to be parallel to

$$\mathbf{n}_{A_k B_k} = \frac{1}{2} \left( \mathbf{n}_{A_k B_k C_k} + \operatorname{sign} \left( \mathbf{n}_{A_k B_k C_k}^{\mathsf{T}} \mathbf{n}_{A_k B_k E_k} \right) \mathbf{n}_{A_k B_k E_k} \right).$$

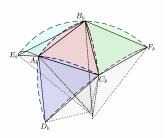


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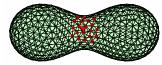
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Local projection of a point  $\mathbf{x}$  on S into a plane occurs

in 4 steps







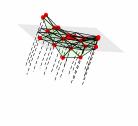


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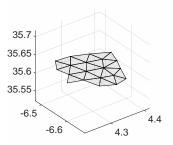
Local projection of a point  $\mathbf{x}$  on S into a plane occurs in 4 steps

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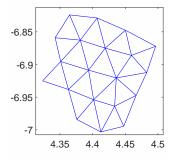
- Determine the intersection of the plane containing the triangle and the line through projection point in the direction of (x - x<sub>O<sub>k</sub></sub>).
- Translate the projection point to the origin in 3D and rotate the coordinate system so that the normal of the current triangle points vertically.



3

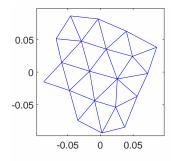
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- Orop the third coordinate.



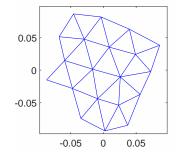
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Local projection of a point  $\mathbf{x}$  on S into a plane occurs in 4 steps

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- Orop the third coordinate.
- Translate so that the midpoint of the current triangle is at the origin in 2D.

These four steps can be completed using

$$\boldsymbol{\chi}_{k} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \boldsymbol{R}_{k} \frac{1}{\boldsymbol{n}_{A_{k}B_{k}C_{k}} \cdot (\boldsymbol{\mathsf{x}} - \boldsymbol{\mathsf{x}}_{O_{k}})} \left( \boldsymbol{n}_{A_{k}B_{k}C_{k}} \times \left( (\boldsymbol{\mathsf{x}} - \boldsymbol{\mathsf{x}}_{O_{k}}) \times (\boldsymbol{\mathsf{x}}_{M_{k}} - \boldsymbol{\mathsf{x}}_{O_{k}}) \right) \right)$$

### Projection and Change of Variables

The projection amounts to a local parameterization and a change of variables in the integral over  $\tau_{A_k B_k C_k}$ , so that

$$\begin{split} \mathcal{I}_{S}(f) &= \sum_{k=1}^{K} \iint\limits_{\tau_{A_{k}}B_{k}C_{k}} f(\mathbf{x})dS \\ &= \sum_{k=1}^{K} \iint\limits_{\tau_{A_{k}}B_{k}C_{k}} f(\mathbf{x}(\boldsymbol{\chi}_{k})) \frac{\mathbf{n}_{P_{k}} \cdot (\mathbf{x}(\boldsymbol{\chi}_{k}) - \mathbf{x}_{O_{k}})}{\mathbf{n}_{S}(\mathbf{x}(\boldsymbol{\chi}_{k})) \cdot (\mathbf{x}(\boldsymbol{\chi}_{k}) - \mathbf{x}_{O_{k}})} \left( \frac{\mathbf{n}_{A_{k}}B_{k}C_{k} \cdot (\mathbf{x}(\boldsymbol{\chi}_{k}) - \mathbf{x}_{O_{k}})}{\mathbf{n}_{A_{k}}B_{k}C_{k} \cdot (\mathbf{x}_{A_{k}} - \mathbf{x}_{O_{k}})} \right)^{2} dA, \end{split}$$

where

$$\mathbf{n}_{\mathsf{S}}(\mathsf{x}) := \frac{\nabla h(\mathsf{x})}{\|\nabla h(\mathsf{x})\|_{2}} \text{ or } \mathbf{n}_{\mathsf{S}}(\mathsf{x}) := \frac{\frac{\partial}{\partial u}\mathsf{x}(u,v) \times \frac{\partial}{\partial v}\mathsf{x}(u,v)}{\left\|\frac{\partial}{\partial u}\mathsf{x}(u,v) \times \frac{\partial}{\partial v}\mathsf{x}(u,v)\right\|_{2}}$$

and

$$\mathbf{n}_{P_k} := \frac{\mathbf{n}_{A_k B_k C_k}}{\left\| \mathbf{n}_{A_k B_k C_k} \right\|_2}.$$

If a global parameterization,  $\mathbf{x}(u, v)$ , of S is not available, then the local projection  $\mathbf{x}(\boldsymbol{\chi}_k)$  provides a local parameterization that is known at  $\mathbf{x}(\boldsymbol{\chi}_{k,j})$ , j = 1, 2, ..., n.

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After projecting into the plane we consider evaluating

$$I_{t_{A_k}B_kC_k}(g) := \iint_{t_{A_k}B_kC_k} g(\boldsymbol{\chi}_k) \, dA$$

Notice: integrating the RBF interpolant of  $g(\chi_k)$ 

$$\begin{split} l_{t_{A_{k}B_{k}C_{k}}}\left(g\right) &\approx l_{t_{A_{k}B_{k}C_{k}}}\left(\hat{s}\right) = l_{t_{A_{k}B_{k}C_{k}}}\left(\sum_{j=1}^{n}c_{j}^{RBF}\phi\left(r_{j}\left(\boldsymbol{\mathbf{x}}_{k}\right)\right) + \sum_{l=1}^{M}c_{l}^{M}\pi_{l}\left(\boldsymbol{\mathbf{x}}_{k}\right)\right) \\ &= \sum_{j=1}^{n}c_{j}^{RBF}l_{t_{A_{k}B_{k}C_{k}}}\left(\phi\left(r_{j}\left(\boldsymbol{\mathbf{x}}_{k}\right)\right)\right) + \sum_{l=1}^{M}c_{l}^{M}l_{t_{A_{k}B_{k}C_{k}}}\left(\pi_{l}\left(\boldsymbol{\mathbf{x}}_{k}\right)\right) \\ &= \hat{\mathbf{c}}^{T}\hat{\mathbf{1}}, \end{split}$$

where

$$\hat{\mathbf{I}} = \begin{bmatrix} \mathbf{I}_{m}^{RBF} \\ \mathbf{I}_{m}^{m} \end{bmatrix}, \mathbf{I}_{m}^{RBF} = \begin{bmatrix} t_{t_{A_{k}B_{k}C_{k}}}(\phi(r_{1})) \\ t_{t_{A_{k}B_{k}C_{k}}}(\phi(r_{2})) \\ \vdots \\ t_{t_{A_{k}B_{k}C_{k}}}(\phi(r_{n})) \end{bmatrix}, \text{ and } \mathbf{I}^{m} = \begin{bmatrix} t_{t_{A_{k}B_{k}C_{k}}}(\pi_{1}) \\ t_{t_{A_{k}B_{k}C_{k}}}(\pi_{2}) \\ \vdots \\ t_{t_{A_{k}B_{k}C_{k}}}(\pi_{M}) \end{bmatrix}$$

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Recall that if  $\hat{A}$  is invertible, then  $\hat{\mathbf{c}} = \hat{A}^{-1} \hat{\mathbf{g}}$ . So

$$\begin{aligned} l_{t_{ABC}}\left(g\right) &\approx l_{t_{ABC}}\left(\hat{g}\right) = \hat{\mathbf{c}}^{T}\hat{\mathbf{i}} \\ &= \left(\hat{A}^{-1}\hat{\mathbf{g}}\right)^{T}\hat{\mathbf{i}} \\ &= \hat{\mathbf{g}}^{T}\left(\left(\hat{A}^{-1}\right)^{T}\hat{\mathbf{i}}\right) \\ &= \hat{\mathbf{g}}^{T}\left(\left(\hat{A}^{T}\right)^{-1}\hat{\mathbf{i}}\right) \\ &= \hat{\mathbf{c}}^{T}\hat{\mathbf{\omega}} \end{aligned}$$

Here 
$$\hat{A}^T \hat{\mathbf{w}} = \hat{\mathbf{I}}$$
 and  $\hat{\mathbf{g}} = \begin{bmatrix} g(\boldsymbol{\chi}_{k,1}) & g(\boldsymbol{\chi}_{k,2}) & \cdots & g(\boldsymbol{\chi}_{k,n}) & 0 & \cdots & 0 \end{bmatrix}^T$ 

Let w be the first n entries in the solution of this system of equations so that we have

$$I_{t_{A_k B_k C_k}}(g) \approx \mathbf{g}^T \mathbf{w} = \sum_{j=1}^n w_{k,j} g\left( \boldsymbol{\chi}_{k,j} \right).$$

Finding the weights  $w_{k,j}$ , j = 1, 2, ..., n requires two pieces of information The (hopefully closed form) integrals (j = 1, 2, ..., n and l = 1, 2, ..., M)

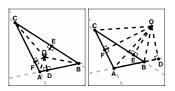
$$I_{t_{A_{k}B_{k}C_{k}}}\left(\phi\left(r_{j}\right)\right) = \iint_{t_{A_{k}B_{k}C_{k}}}\phi\left(r_{j}\left(\boldsymbol{\chi}_{k}\right)\right)dA$$

and

$$I_{t_{A_{k}}B_{k}C_{k}}(\pi_{I}) = \iint_{t_{A_{k}}B_{k}C_{k}} \pi_{I}(\boldsymbol{\chi}_{k}) dA \text{ (Elementary)}$$

2 The solution of the linear system  $\hat{A}^T \hat{w} = \hat{I}$ 

For the RBF terms, consider integration over right triangles only:



Define (minding the order of  $A_k B_k C_k$  and likewise for the other triangles)

$$s_{t_{A_kB_k}C_k} := sign\left(\left(\left[\begin{array}{cc} 0 & -1\\ 1 & 0 \end{array}\right] \left(\boldsymbol{\chi}_{k,B_k} - \boldsymbol{\chi}_{k,A_k}\right)\right) \cdot \left(\boldsymbol{\chi}_{k,C_k} - \boldsymbol{\chi}_{k,A_k}\right)\right)$$

The integral over an arbitrary triangle is the sum of integrals over six right triangles:

$$\begin{split} & t_{A_k B_k C_k}(\phi) = & s_{t_{A_k} B_k C_k} \left( s_{t_{O_k A_k D_k}} t_{t_{O_k A_k D_k}}(\phi) + s_{t_{O_k D_k B_k}} t_{t_{O_k D_k B_k}}(\phi) + \\ & s_{t_{O_k B_k} E_k} t_{t_{O_k B_k E_k}}(\phi) + s_{t_{O_k} E_k C_k} t_{t_{O_k} E_k C_k}(\phi) + \\ & s_{t_{O_k C_k F_k}} t_{t_{O_k C_k F_k}}(\phi) + s_{t_{O_k F_k A_k}} t_{t_{O_k F_k A_k}}(\phi) \right). \end{split}$$

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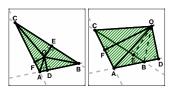
$$I_{t_{A_{k}B_{k}C_{k}}}\left(\phi\left(r_{j}\right)\right) = \iint_{t_{A_{k}B_{k}C_{k}}}\phi\left(r_{j}\left(\boldsymbol{\chi}_{k}\right)\right)dA$$

and

$$I_{t_{A_{k}}B_{k}C_{k}}(\pi_{I}) = \iint_{t_{A_{k}}B_{k}C_{k}} \pi_{I}(\boldsymbol{\chi}_{k}) \, dA \text{ (Elementary)}$$

2 The solution of the linear system  $\hat{A}^T \hat{w} = \hat{I}$ 

For the RBF terms, consider integration over right triangles only:



Define (minding the order of  $A_k B_k C_k$  and likewise for the other triangles)

$$\mathsf{s}_{\mathsf{t}_{\mathsf{A}_k\mathsf{B}_k\mathsf{C}_k}} := \mathsf{sign}\left(\left(\left[\begin{array}{cc} 0 & -1\\ 1 & 0 \end{array}\right]\left(\boldsymbol{\chi}_{k,\mathsf{B}_k} - \boldsymbol{\chi}_{k,\mathsf{A}_k}\right)\right) \cdot \left(\boldsymbol{\chi}_{k,\mathsf{C}_k} - \boldsymbol{\chi}_{k,\mathsf{A}_k}\right)\right)$$

The integral over an arbitrary triangle is the sum of integrals over six right triangles:

$$\begin{split} & t_{A_{k}B_{k}C_{k}}(\phi) = & s_{t_{A_{k}B_{k}C_{k}}} \left( s_{t_{O_{k}A_{k}D_{k}}} l_{t_{O_{k}A_{k}D_{k}}}(\phi) + s_{t_{O_{k}D_{k}B_{k}}} l_{t_{O_{k}D_{k}B_{k}}}(\phi) + \\ & s_{t_{O_{k}B_{k}E_{k}}} l_{t_{O_{k}B_{k}E_{k}}}(\phi) + s_{t_{O_{k}E_{k}C_{k}}} l_{t_{O_{k}E_{k}C_{k}}}(\phi) + \\ & s_{t_{O_{k}C_{k}F_{k}}} l_{t_{O_{k}C_{k}F_{k}}}(\phi) + s_{t_{O_{k}F_{k}A_{k}}} l_{t_{O_{k}F_{k}A_{k}}}(\phi) \right). \end{split}$$

Finding the weights  $w_{k,j}$ , j = 1, 2, ..., n requires two pieces of information The (hopefully closed form) integrals (j = 1, 2, ..., n and l = 1, 2, ..., M)

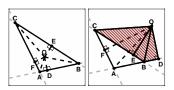
$$I_{t_{A_{k}B_{k}C_{k}}}\left(\phi\left(r_{j}\right)\right) = \iint_{t_{A_{k}B_{k}C_{k}}}\phi\left(r_{j}\left(\boldsymbol{x}_{k}\right)\right)dA$$

and

$$I_{t_{A_{k}}B_{k}C_{k}}(\pi_{I}) = \iint_{t_{A_{k}}B_{k}C_{k}} \pi_{I}(\boldsymbol{\chi}_{k}) \, dA \text{ (Elementary)}$$

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### Step 3: Find Quadrature Weights Locally in the Tangent Plane

Finding the weights  $w_{k,j}$ , j = 1, 2, ..., n requires two pieces of information The (hopefully closed form) integrals (j = 1, 2, ..., n and l = 1, 2, ..., M)

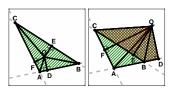
$$I_{t_{A_{k}B_{k}C_{k}}}\left(\phi\left(r_{j}\right)\right) = \iint_{t_{A_{k}B_{k}C_{k}}}\phi\left(r_{j}\left(\boldsymbol{x}_{k}\right)\right)dA$$

and

$$I_{t_{A_k}B_kC_k}(\pi_l) = \iint_{t_{A_k}B_kC_k} \pi_l(\boldsymbol{\chi}_k) \, dA \text{ (Elementary)}$$

2 The solution of the linear system  $\hat{A}^T \hat{w} = \hat{I}$ 

For the RBF terms, consider integration over right triangles only:



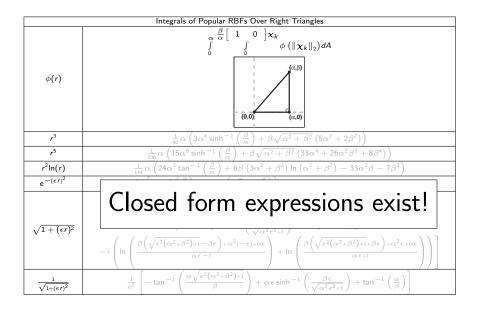
Define (minding the order of  $A_k B_k C_k$  and likewise for the other triangles)

$$\mathsf{s}_{\mathsf{t}_{\mathsf{A}_k\mathsf{B}_k\mathsf{C}_k}} := \mathsf{sign}\left(\left(\left[\begin{array}{cc} 0 & -1\\ 1 & 0 \end{array}\right]\left(\boldsymbol{\chi}_{k,\mathsf{B}_k} - \boldsymbol{\chi}_{k,\mathsf{A}_k}\right)\right) \cdot \left(\boldsymbol{\chi}_{k,\mathsf{C}_k} - \boldsymbol{\chi}_{k,\mathsf{A}_k}\right)\right)$$

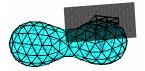
The integral over an arbitrary triangle is the sum of integrals over six right triangles:

$$\begin{split} & t_{A_k B_k C_k}(\phi) = & s_{t_{A_k} B_k C_k} \left( s_{t_{O_k A_k D_k}} t_{t_{O_k A_k D_k}}(\phi) + s_{t_{O_k D_k B_k}} t_{t_{O_k D_k B_k}}(\phi) + \\ & s_{t_{O_k B_k} E_k} t_{t_{O_k B_k E_k}}(\phi) + s_{t_{O_k} E_k C_k} t_{t_{O_k} E_k C_k}(\phi) + \\ & s_{t_{O_k C_k F_k}} t_{t_{O_k C_k F_k}}(\phi) + s_{t_{O_k F_k A_k}} t_{t_{O_k F_k A_k}}(\phi) \right). \end{split}$$

# Integrating RBFs Over Right Triangles



When approximating  $g(\boldsymbol{\chi}_k)$  we interpolate over n points  $\{\boldsymbol{\chi}_{k,j}\}_{j=1}^n$ 



These points are taken to be the projections of the *n* nearest quadrature nodes (in  $S_N$ ) to the midpoint of  $t_{A_k B_k C_k}$ .

For each midpoint, the *n* nearest neighbors in Euclidean distance are found at the initialization of the proposed method using the kd-tree algorithm in  $O(N \ n \log N)$  operations (see e.g., J. H. Friedman, J. L. Bentley, and R. A. Finkel. "An algorithm for finding best matches in logarithmic expected time." *ACM Trans Math Softw*, 3(3), 1977).

#### Steps 4 and 5: Convert and Combine Quadrature Weights

Applying step 3 to the double integral over each of the triangles  $t_{A_k B_k C_k}$  gives (with  $\mathbf{x}_{k,j} := \mathbf{x}(\boldsymbol{\chi}_k)$ )

$$\iint_{\tau_{A_{k}B_{k}}C_{k}} f(\mathbf{x})dS = \iint_{t_{A_{k}B_{k}}C_{k}} f(\mathbf{x}(\boldsymbol{\chi}_{k})) \frac{\mathbf{n}_{P_{k}} \cdot (\mathbf{x}(\boldsymbol{\chi}_{k}) - \mathbf{x}_{O_{k}})}{\mathbf{n}_{S}(\mathbf{x}(\boldsymbol{\chi}_{k})) \cdot (\mathbf{x}(\boldsymbol{\chi}_{k}) - \mathbf{x}_{O_{k}})} \left( \frac{\mathbf{n}_{A_{k}B_{k}}C_{k} \cdot (\mathbf{x}(\boldsymbol{\chi}_{k}) - \mathbf{x}_{O_{k}})}{\mathbf{n}_{A_{k}B_{k}}C_{k} \cdot (\mathbf{x}_{A_{k}} - \mathbf{x}_{O_{k}})} \right)^{2} dA$$

$$\approx \sum_{j=1}^{n} w_{k,j}f(\mathbf{x}_{k,j}) \frac{\mathbf{n}_{P_{k}} \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})}{\mathbf{n}_{S}(\mathbf{x}_{k,j}) \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})} \left( \frac{\mathbf{n}_{A_{k}B_{k}}C_{k} \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})}{\mathbf{n}_{A_{k}B_{k}}C_{k} \cdot (\mathbf{x}_{A_{k}} - \mathbf{x}_{O_{k}})} \right)^{2}.$$

Hence,

$$\mathcal{I}_{S}(f) \approx \sum_{k=1}^{K} \sum_{j=1}^{n} w_{k,j}^{\mathsf{RBF}} f(\mathbf{x}_{k,j}) \frac{\mathbf{n}_{P_{k}} \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})}{\mathbf{n}_{S}(\mathbf{x}_{k,j}) \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})} \left( \frac{\mathbf{n}_{A_{k}} B_{k} c_{k} \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})}{\mathbf{n}_{A_{k}} B_{k} c_{k} \cdot (\mathbf{x}_{A_{k}} - \mathbf{x}_{O_{k}})} \right)^{2}.$$

Weights in the plane and on the surface differ only by a factor.

Let  $\mathcal{K}_i$ , i = 1, 2, ..., N be the set of all pairs (k, j) such that  $\chi_{k,j} \mapsto \mathbf{x}_i$ . Then the surface integral over S can be written as

$$\mathcal{I}_{S}(f) \approx \sum_{i=1}^{N} \left( \sum_{(k,j) \in \mathcal{K}_{i}} w_{k,j} \frac{\mathbf{n}_{P_{k}} \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})}{\mathbf{n}_{S}(\mathbf{x}_{k,j}) \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})} \left( \frac{\mathbf{n}_{A_{k}B_{k}C_{k}} \cdot (\mathbf{x}_{k,j} - \mathbf{x}_{O_{k}})}{\mathbf{n}_{A_{k}B_{k}C_{k}} \cdot (\mathbf{x}_{A_{k}} - \mathbf{x}_{O_{k}})} \right)^{2} \right) f(\mathbf{x}_{i}) = \sum_{i=1}^{N} W_{i}f(\mathbf{x}_{i}) =: \tilde{\mathcal{I}}_{\mathbb{S}^{2}}(f).$$

Results are presented for quasi-uniform node sets on three test surfaces and three test integrands.

Note: Present method default settings when computing quadrature weights for each spherical triangle:

- $\phi(r) = r^7$
- 80 nearest neighbors
- Bivariate polynomial terms up to degree 7

Worst case error shown when the test function has been randomly rotated 1,000 times.

## Test Surfaces

We consider the rotated Cassini Ovals defined by

$$h(\mathbf{x}) = h(x, y, z) = (x^2 + y^2 + z^2)^2 - 2\lambda^2 b^2 (x^2 - y^2 - z^2) + b^4 (\lambda^4 - 1) = 0$$

which can also be parameterized explicitly via

$$\begin{split} & x(\theta, \phi) = \rho(\phi) cos(\phi) \\ & y(\theta, \phi) = \rho(\phi) sin(\phi) sin(\theta) \\ & z(\theta, \phi) = \rho(\phi) sin(\phi) cos(\theta) \\ & \rho(\phi) = b \sqrt{\sqrt{1 + \lambda^4 (cos^2(2\phi) - 1)} + \lambda^2 cos(2\phi)} \\ & \theta \in [0, 2\pi) \\ & \phi \in [0, \pi] \end{split}$$





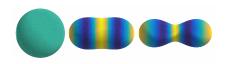






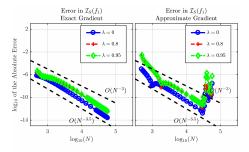
In all cases b is chosen so that the surface area is equal to 1 by finding numerically the root of

$$R(b) = 1 - 8 \int_{0}^{b\sqrt{\lambda^{2}+1}\sqrt{b\sqrt{b^{2}+4\lambda^{2}x^{2}} - \lambda^{2}b^{2} - x^{2}}} \int_{0}^{\sqrt{\lambda^{2}b^{6} - b^{3}(b^{2} + 4\lambda^{2}x^{2})^{\frac{3}{2}} + 4\lambda^{2}b^{3}x^{2}\sqrt{b^{2} + 4\lambda^{2}x^{2}}}} \sqrt{\frac{\lambda^{2}b^{6} - b^{3}(b^{2} + 4\lambda^{2}x^{2})^{\frac{3}{2}} + 4\lambda^{2}b^{3}x^{2}\sqrt{b^{2} + 4\lambda^{2}x^{2}}}{\lambda^{2}b^{6} - b^{3}(b^{2} + 4\lambda^{2}x^{2})^{\frac{3}{2}} + 4\lambda^{2}b^{2}x^{4} + 4\lambda^{4}b^{4}x^{2} + b^{4}x^{2} + b^{4}y^{2} + 4\lambda^{2}b^{2}x^{2}y^{2}}}} dydx$$



Integrand:

$$f_1(\mathbf{x}) = \frac{1}{3}\mathbf{x} \cdot \frac{\nabla h(\mathbf{x})}{\|\nabla h(\mathbf{x})\|_2}$$



Features: Infinitely smooth, computes the volume of the surface of revolution.



Integrand:

$$f_2(\mathbf{x}) = \frac{2}{\pi} \tan^{-1} (100 \mathbf{e}_3^T \mathbf{x})$$

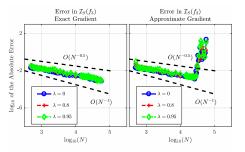
Error in  $\mathcal{I}_S(f_2)$ Error in  $\mathcal{I}_S(f_2)$ Exact Gradient Approximate Gradient log<sub>10</sub> of the Absolute Error  $O(N^{-3})$ -6  $\lambda = 0$  $-\lambda = 0$ -10  $O(N^{-3.5})$  $O(N^{-3.5})$  $\lambda = 0.8$  $\leftarrow \lambda = 0.8$  $- - \lambda = 0.95$  $- \mathbf{0} \cdot \mathbf{0} = 0.95$ -14 3  $\mathbf{5}$ 3  $\mathbf{5}$ 4  $\log_{10}(N)$  $\log_{10}(N)$ 

Features: Infinitely smooth with a steep gradient near where the third coordinate of x is zero.



Integrand:

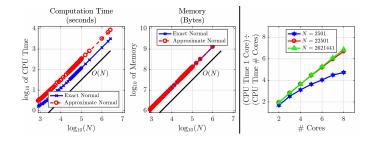
$$f_3(\mathbf{x}) = \mathsf{sign}(\mathbf{e}_3^T\mathbf{x})$$



Features: Discontinuous where the third coordinate of **x** is zero.

# **Timing Results**

All computations were performed in Matlab on machines with dual Intel Xeon E5-2687W 3.1 GHz, 8-core processors.



Figures indicate for the proposed method:

- O(N) cost and memory for up to at least millions of nodes
- $O(N \log N)$  cost is expected when the nearest neighbor search starts to dominate the computation.
- 'Embarrassingly parallel' scalability with number of cores

- A high order accurate algorithm has been developed for quadrature over smooth closed surfaces
- The node sets can feature any types of density variations (e.g. local refinement in certain areas, etc.), demonstrated for the sphere in "Numerical quadrature over the surface of a sphere" (J.A. Reeger and B. Fornberg)
- The total cost is O(N log N) operations and O(N) memory for finding weights for N nodes.
- The algorithm is 'embarrassingly parallel', making it trivial to use any number of available processors.
- Even on a standard PC, it can be run for *N*-values in the millions. This eliminates the need for tabulating weights for specific node distributions.

Publications:

- J. A. Reeger and B. Fornberg. "Numerical quadrature over the surface of a sphere." *Stud. Appl. Math.*, 137(2): 174-188, 2016.
- J. A. Reeger, B. Fornberg, and M. L. Watts. "Numerical quadrature over smooth, closed surfaces." P. Roy. Soc. Lon. A Mat., 472:20160401, 2016. (doi:10.1098/rspa.2016.0401).
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Implementations Available: http://www.jonahareeger.com (MATLAB, Julia, and Python)

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