Overview of Nyström high-order quadratures for boundary integral equations

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Overview

Goal: evaluate layer potential

$$u(\boldsymbol{x}) = (K\sigma)(\boldsymbol{x}) := \int_\Gamma k(\boldsymbol{x},\boldsymbol{y})\sigma(\boldsymbol{y})dS_{\boldsymbol{y}}, \quad \boldsymbol{x} \in \Omega$$

- Two routes to discretizing Γ and σ:

  Global: efficient for simple, smooth geometries

  trapezoidal rule, spherical harmonics

  Local: adaptivity for complex geometries

  G-L panels, triangular/quadrilateral elements

- Two routes to discretizing the operator:

  Galerkin: project integral operator onto a basis

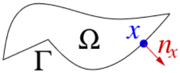
  more mature convergence theory, industrial codes

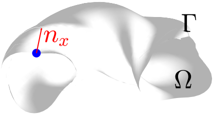
  Nyström: approx. integral operator at quadr. points

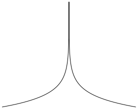
  faster set-up, basically same accuracy at same order

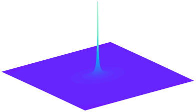
- Computational Tools:

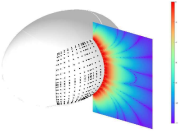
  chunkie (2D), fmm3dbie (3D), et al.









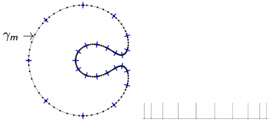


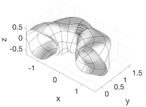
Overview: local discretization and Nyström

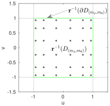
Goal: evaluate layer potential due to $\Gamma = \cup \gamma_m$

$$u(\boldsymbol{x}) = (K\sigma)(\boldsymbol{x}) = \sum_m \int_{\gamma_m} k(\boldsymbol{x}, \boldsymbol{y})\sigma(\boldsymbol{y})dS_{\boldsymbol{y}}$$

in particular, compute $u(\boldsymbol{x})$ for $\boldsymbol{x} \in \Gamma$ to get linear system for σ







- A sampling of integration ideas:
  - adaptive integration
  - generalized Gaussian quadr.
  - integration by parts
- Discretizing operator K :
  - on smooth curves is a solved problem
  - on curves with corners is also no trouble
  - on smooth surfaces currently is $10^3 - 10^4$ targs/sec/core
  - surfaces with singularities 3D corners, cones, and edges
  - related: high aspect ratio / skew panels

GGQ & adaptive integration

regularization + asymptotics $\longrightarrow$ product integration

chunkie
fmm3dbie
order

1D integral

weak: $\int_\Gamma \log|x-y|\, dy$

strong: $\int_\Gamma \frac{1}{|x-y|}\, dy$

hyper: $\int_\Gamma \frac{1}{|x-y|^2}\, dy$

super: $\int_\Gamma \frac{1}{|x-y|^3}\, dy$

2D integral

weak: $\int_\Gamma \frac{1}{|x-y|}\, dy$

strong: $\int_\Gamma \frac{1}{|x-y|^2}\, dy$

hyper: $\int_\Gamma \frac{1}{|x-y|^3}\, dy$

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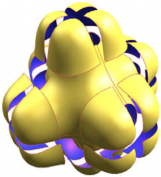
Discretization of Γ and σ

- (G) global: efficient for simple, smooth geometries

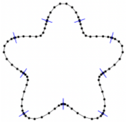
peri. trap. rule

sph. harms. (Veerapaneni et al.)

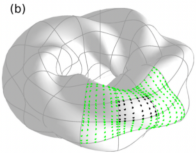


overlapping patches (Ying et al.)

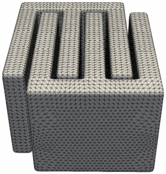
- (L) local: adaptivity for complex geometries



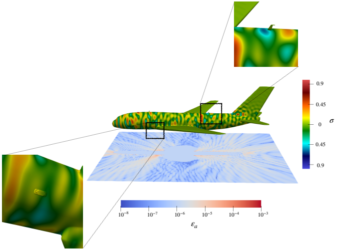
G-L panels



G-L quads (Barnett et al.)



4th-ord tri's (Greengard et al.)



industrial geoms.

Quadrature literature

Auxiliary nodes/patches: (Barnett-Greengard-Hagstrom '20, Greengard-O'Neil-Rachh-Vico '21)

GGQ: (Ma-Rokhlin-Wandzura '96; Yarvin-Rokhlin '98; Bremer '12; Bremer-Gimbutas-Rokhlin '10, Bremer-Gimbutas '12, ...)

QBX and hedgehog: (Klöckner-Barnett-Greengard-O'Neil '13; Morse-Rahimian-Zorin '21; Af Klinteberg-Tornberg '16; Siegel-Tornberg '18; Wala-Klöckner '18, ...)

Change of variable/singularity cancelation: (Ying-Biros-Zorin '06; Malhotra-Cerfon-Imbert-Gérard-O'Neil '19; Erichsen-Sauter '98; Gimbutas-Veerapaneni '13, ...)

Kernel regularization: (Beale '01; Tlupova-Beale '19; Pérez-Arancibia-Faria-Turc '18; Dong-Lai-Li '20; Bao-Xu-Yin '17 ...)

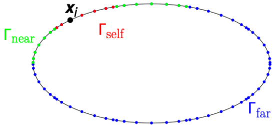
Corner/Open surface: (Helsing-Ojala '08; Helsing '11; Helsing-Jiang '18; Helsing-Jiang '22; Rachh-Serkh '17; Hoskins-Rachh '19; Bremer-Rokhlin-Sammis '10; Bremer-Rokhlin-Sammis '10; Serkh-Rokhlin '16; Gopal-Trefethen 19; Kress '90 ...)

Kernel Split: (Helsing-Karlsson '14; Helsing-Holst '15; Fryklund-Af Klinteberg-Tornberg '19 ...)

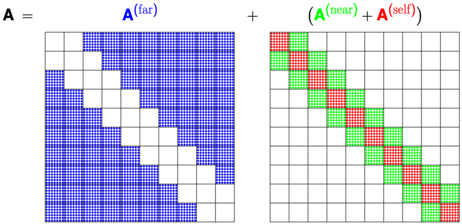
And many more: (Kress '91; Alpert '95; Kapur-Rokhlin '97; Duan-Rokhlin '08; Kolm-Rokhlin '01; Wu-Martinsson '22; Xiao-Gimbutas '10; Bremer-Gimbutas '12; Barnett-Wu-Veerapaneni '15; Stein-Barnett '22; Af Klinteberg-Barnett '21; Af Klinteberg '23; Bao-Hua-Lai-Zhang '23; Malhotra-Barnett '23 ...)

Quadrature tasks and categories

- task A) fill A^{far}: $|\boldsymbol{x}_i - \boldsymbol{x}_j| > d$, use smooth quadr, $A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)w_j$
- task B) fill A^{near}: $|\boldsymbol{x}_i - \boldsymbol{x}_j| < d$, need near-singular quadr, $A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j)w_{ij}$
- task C) fill A^{self}: $\boldsymbol{x}_i = \boldsymbol{x}_j$, need singular quadr, $A_{ii} = k(\boldsymbol{x}_i, \boldsymbol{x}_i)w_{ii}$



(Martinsson '14 CBMS)



Quadrature wish list:

- dimension independent 2D and 3D
- kernel independent
- high order accurate to industrial mesh
- setup speed

  on-the-fly for moving geometry

- robust to target location
- robust to patch deformation
- parallel implementation
- easy to use for non-expert

  soln. anywhere

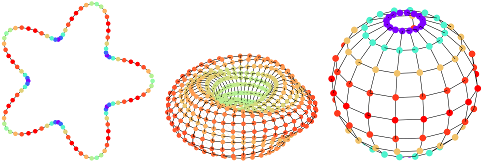
Quadrature task A) fill A^{far}

$A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) w_j$, w_j independent of $\boldsymbol{x}_i$

$u(\boldsymbol{x}) = \int_0^{2\pi} k(\boldsymbol{x}, \boldsymbol{y}(t)) \sigma(t) |\boldsymbol{y}'(t)| \, dt$

parametric $\boldsymbol{x}(t)$: $(0, 2\pi) \to \Gamma$

global: axisymmetric geoms.



peri. trap. rule for peri. func.

$t_j = 2\pi j/N, \sigma_j = \sigma(t_j)$, for $j = 1, \cdots, N$

$w_j = |\boldsymbol{x}'(t_j)| \cdot 2\pi/N$, arc length

$A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) w_j$, if $|\boldsymbol{x}_i - \boldsymbol{x}_j| > d$

Quadrature task A) fill A^{far}

$A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) w_j$, w_j independent of $\boldsymbol{x}_i$

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parametric $\boldsymbol{x}(t) : (0, 2\pi) \to \Gamma$

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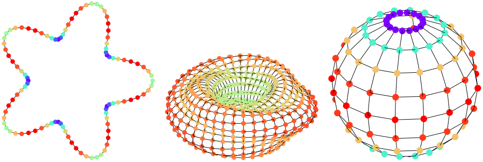
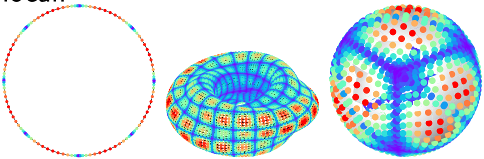


local:



(Vioreanu-Rokhlin)

peri. trap. rule for peri. func.

$t_j = 2\pi j/N, \sigma_j = \sigma(t_j)$, for $j = 1, \cdots, N$

$w_j = |\boldsymbol{x}'(t_j)| \cdot 2\pi/N$, arc length

$A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) w_j$, if $|\boldsymbol{x}_i - \boldsymbol{x}_j| > d$

$p-$point G-L nodes and weights

$\Gamma = \cup \gamma_m$, each $\gamma_m : [a_{m-1}, a_m] \to \gamma_m$

$\sum_m \int_{a_{m-1}}^{a_m} k(\boldsymbol{x}, \boldsymbol{y}(t)) \sigma(t) |\boldsymbol{y}'(t)| \, dt$

$t_j^{(m)}$, $\sigma_j^{(m)} = \sigma(t_j^{(m)})$, for $j = 1, \cdots, p$

$w_j^{(m)} = |\boldsymbol{x}'(t_j^{(m)})| \cdot (a_m - a_{m-1}) w_j^{\text{std}}$

$\{\boldsymbol{x}_\ell\}$ denotes the entire set of quadr. nodes

$A_{\ell,\ell'} = k(\boldsymbol{x}_\ell, \boldsymbol{x}_{\ell'}) w_{\ell'}$, if $|\boldsymbol{x}_\ell - \boldsymbol{x}_{\ell'}| > d$

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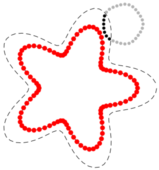
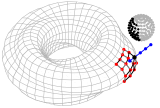
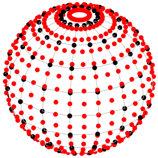
Quadrature task B) fill A^{near}: peri. trap. rule for peri. func.

$A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) w_{ij}$, w_{ij} depends of $\boldsymbol{x}_i$

global: vesicle simulation







(Helsing et al.) (Malhotra et al.) (Veerapaneni et al.)

$t_j = 2\pi j/N$, $w_j = |\boldsymbol{x}'(t_j)| \cdot 2\pi/N$

Associate $\mathbb{C}$ with $\mathbb{R}^2$, $dy = i n_y \, ds_y$

$$u(x) := \frac{1}{2\pi} \int_\Gamma \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot \boldsymbol{n_y}}{|\boldsymbol{x}-\boldsymbol{y}|^2} ds_{\boldsymbol{y}} = \mathrm{Re} \frac{1}{2\pi i} \int_\Gamma \frac{\sigma(y)}{x-y} dy$$

Cauchy's formula:

$$\frac{1}{2\pi i} \int_\Gamma \frac{u(y)}{y-x} dy = \begin{cases} u(x), & x \in \Omega \\ 0, & x \in \Omega^c \end{cases}$$

special case for $u(x) \equiv 1$:

$$\frac{1}{2\pi i} \int_\Gamma \frac{1}{y-x} dy = 1, \text{ for } x \in \Omega$$

combine:

$$\int_\Gamma \frac{u(y)-u(x)}{y-x} dy = 0, \text{ for } x \in \Omega$$

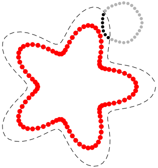
$$u(x) \approx \frac{\sum u_j/(y_j-x) w_j}{\sum 1/(y_j-x) w_j} \quad \text{(see BIE2D)}$$

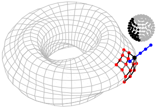
(Helsing et al.) (Barnett et al.)

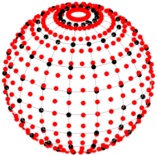
Quadrature task B) fill A^{near}: G-L panel, kernel-split quadrature

$A_{ij} = k(\boldsymbol{x}_i, \boldsymbol{x}_j) w_{ij}$, w_{ij} depends of $\boldsymbol{x}_i$

global:

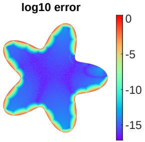


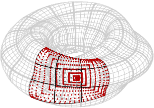


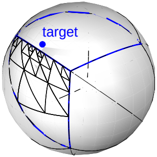


(Helsing et al.) (Malhotra et al.) (Veerapaneni et al.)

local:







(Helsing et al.) (Barnett et al.) (Greengard et al.)

rewrite into complex Cauchy integral

$$u^{(m)}(\boldsymbol{x}) = \frac{1}{2\pi} \int_{\gamma_m} \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot \boldsymbol{n_y}}{|\boldsymbol{x}-\boldsymbol{y}|^2} \sigma(\boldsymbol{y})\, ds_{\boldsymbol{y}}$$
$$= \mathrm{Re} \frac{1}{2\pi i} \int_{\gamma_m} \frac{\sigma(y)}{x-y}\, dy$$

On γ_m, $\sigma(x)$ is smooth. So expand $\sigma(x)$ as a polynomial in x

$$\sigma(x) \approx \sum_{k=0}^{n} c_k x^k$$

plug it in to get

$$u^{(m)}(\boldsymbol{x}) \approx \mathrm{Re} \frac{1}{2\pi i} \sum_{k=0}^{n} c_k \int_{\gamma_m} \frac{y^k}{x-y}\, dy$$
$$= \mathrm{Re} \frac{1}{2\pi i} \sum_{k=0}^{n} c_k p_k$$

2−term recurrence for $p_k = \int_{-1}^{1} \frac{y^k}{x-y} \mathrm{d}y$

$$p_{k+1} = z_0 p_k + \frac{1-(-1)^k}{k}$$

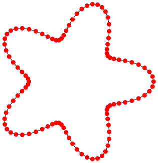
kernel-split

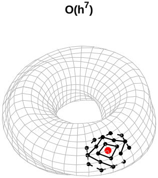
$$k(\boldsymbol{x}, \boldsymbol{y}) = k_o(\boldsymbol{x}, \boldsymbol{y}) + \log|\boldsymbol{x}-\boldsymbol{y}| k_L(\boldsymbol{x}, \boldsymbol{y})$$
$$+ \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot \boldsymbol{n_y}}{|\boldsymbol{x}-\boldsymbol{y}|^2} k_C(\boldsymbol{x}, \boldsymbol{y})$$ (Helsing et al.)

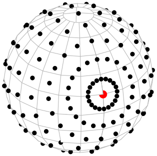
Quadrature task C) fill A^{self}

$A_{ii} = k(\boldsymbol{x}_i, \boldsymbol{x}_i) w_{ii}$, $k(\boldsymbol{x}_i, \boldsymbol{x}_i) = \infty$

global:

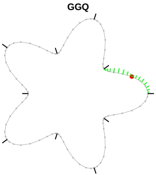


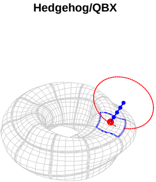


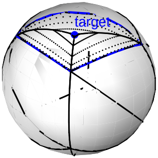


(Kress, Kapur-Rokhlin) (Wu et al.) (Veerapaneni et al.)

local:





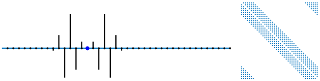


(Kolm-Rokhlin) (Morse et al.) (Bremer-Gimbutas)

(Alpert) (Barnett Klöckner et al.)

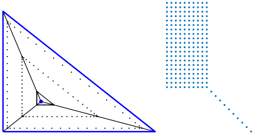
GGQ

- peri. trap. rule for peri. func.



(Kapur-Rokhlin) for log singularity: $k(t) = \phi(t) \log|\sin \frac{t\pi}{T}| + \phi(t)$

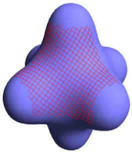
- tri. panels (Bremer-Gimbutas)

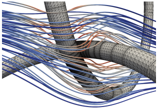


interp. mat.

sph. harms. $r\,dr\,d\theta$

hybrid



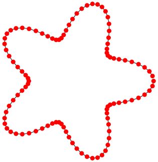


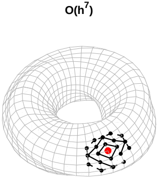
(Ying et al.) (Malhotra et al.)

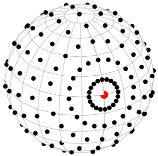
Quadrature task C) fill A^{self}: Kress

$A_{ii} = k(\boldsymbol{x}_i, \boldsymbol{x}_i) w_{ii}$, $k(\boldsymbol{x}_i, \boldsymbol{x}_i) = \infty$

global:

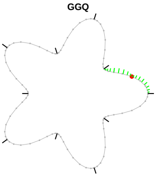


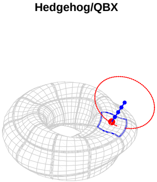


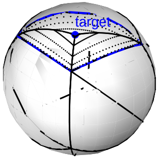


(Kress, Kapur-Rokhlin) (Wu et al.) (Veerapaneni et al.)

local:







(Kolm-Rokhlin) (Morse et al.) (Bremer-Gimbutas)

(Alpert) (Barnett, Klöckner et al.)

$\int_0^{2\pi} g(s)\sigma(s)\,ds = 2\pi \sum \bar{g}_n \sigma_n$

use trapezoid rule to evaluate σ_n

$$\sigma_n = \frac{1}{N} \sum_{j=1}^{N} e^{-int_j} \sigma(t_j)$$

use Fourier series

$$g(s) = \log\left(4 \sin^2 \frac{s}{2}\right) \Leftrightarrow g_n = \begin{cases} 0, n = 0 \\ \frac{-1}{|n|}, n \neq 0 \end{cases}$$

translate g by t corresponds to multiplication of g_n by e^{-int}

$$u(t) = \int_0^{2\pi} \log\left(4 \sin^2 \frac{t-s}{2}\right) \sigma(s)\,ds \approx \sum_{j=0}^{2n-1} R_j(t)\sigma(t_j)$$

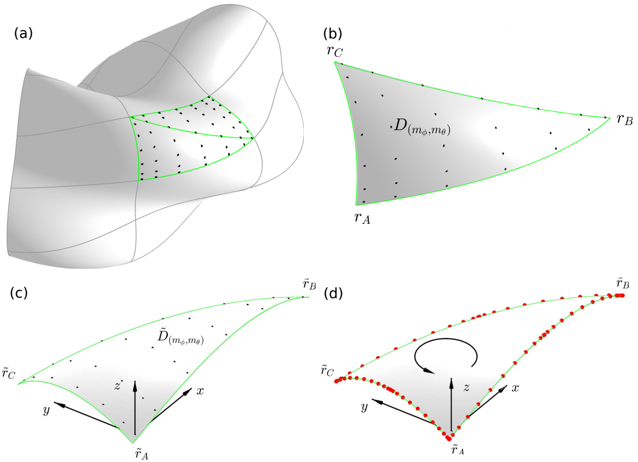
where the weights, which depend on the target location t, are

$$R_j(t) = -\frac{4\pi}{N}\left(\sum_{n=1}^{N/2-1} \frac{1}{n} \cos n(x_j - t) + \frac{1}{N} \cos \frac{N}{2}(x_j - t)\right)$$

(Kress) (Kussmaul-Martensen)

More on fill A^{near} and A^{self}: kernel split quadrature

surface-to-line integral conversion: $\int_{\Gamma_i} \frac{1}{4\pi} \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot \boldsymbol{n_y}}{|\boldsymbol{x}-\boldsymbol{y}|^3} \sigma(\boldsymbol{y})\, dS_{\boldsymbol{y}} = \sum \int_{\partial\Gamma_i}$ something $ds_{\boldsymbol{y}}$



More on fill A^{near} and A^{self}: kernel split quadrature

- construct a harmonic polynomial approximation/extension to $\sigma(\boldsymbol{y})$ on Γ_i:

  $(\sigma(\boldsymbol{y}), \mathbf{0}) \approx -\sum_{n=1}^{p} \sum_{m=1}^{n} (0, \nabla H^{(nm)}) c^{(nm)}$

where $H^{(nm)}(\boldsymbol{y}) = Y_n^m(\theta, \phi) r^n$ are spherical harmonics of degree n.

- divergence free integrand to apply surface-to-line integral conversion:

  $(0, \frac{\partial}{\partial \boldsymbol{n_y}} \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|})(0, \boldsymbol{n_y})(0, \nabla H^{(nm)}) ds_{\boldsymbol{y}}$

- analytical integration along "radial" direction:

  $M_n(\boldsymbol{x}, \boldsymbol{y}) = \int_0^1 \frac{t^{n+1}}{|\boldsymbol{x}-t\boldsymbol{y}|^3} \mathrm{d}t$

via recursion

  $M_n = \frac{\boldsymbol{x}\cdot\boldsymbol{y}}{|\boldsymbol{y}|^2} M_{n-1} + \frac{n-1}{|\boldsymbol{y}|^2} N_{n-2} - \frac{1}{|\boldsymbol{y}|^2} \frac{t^{n-1}}{|\boldsymbol{x}-t\boldsymbol{y}|}\Big|_0^1$

- numerical integration along $\partial\Gamma_i$

  (Zhu-Veerapaneni '22)

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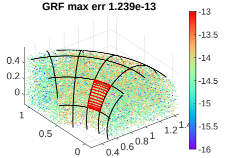
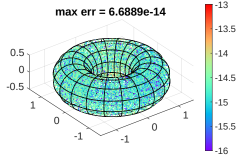
- numerical integration along $\partial\Gamma_i$

  (Zhu-Veerapaneni '22)

work in progress:

- Helmholtz, Stokes kernels (Zhu-Jiang et al.)
- high aspect ratio patches, quadrilateral elements, proper single layer potential treatment (Zhu-Jiang)
- quadrature via complete reduction (Zhu-Jiang)





Computational tools

- chunkie (Askham, et al.)
- fmm3dbie (Rachh, et al.)
- BIE2D, BIE3D (Barnett)
- pyBIE2D (Stein)
- SCTL, BIEST (Malhotra)
- ves3d (Malhotra, Lu, et al.)
- Bempp (Betcke et al.)
- ...

Resources

Many numerical analysis (mathematics heavy). Somewhat accessible:

- *Linear Integral Equations*, R. Kress, (1999, Springer). Ch. 6 & 12.
- *The Numerical Solution of Integral Equations of the Second Kind*, K. E. Atkinson, (1997, CUP).

Fewer on the practical/tutorial side, few with last 15 years of progress:

- "High-order accurate methods for Nyström discretization of integral equations on smooth curves in the plane", S Hao, AH Barnett, PG Martinsson, P Young. *Adv. Comput. Math.* **40**, 245–272 (2014).

  various quadratures for logarithmic singularities, for, eg, SLP, Helmholtz

- "Solving integral equations on piecewise smooth boundaries using the RCIP method: a tutorial", J Helsing. (2013).
- `https://users.flatironinstitute.org/~ahb/BIE/`
- `https://github.com/ahbarnett/BIEbook` in progress...

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