Recursive Reduction Quadrature for the Evaluation of Laplace Layer Potentials in Three Dimensions

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Motivation and Our Contribution.

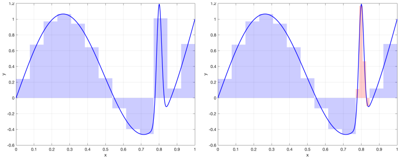
Recursive Reduction Quadrature.

A singular integral is

$$u(x) = \int_\Gamma K(x,y)\mu(y)\, d\Gamma$$

such that $K(x,y) = \mathcal{O}(|x-y|^{-\lambda})$, $\lambda > 0$. Γ represents the integration domain. $d\Gamma$ is the differential element on Γ. Take the Laplace equation for example, $K(x,y) = \frac{1}{4\pi|x-y|}$.

Quadrature is a numerical integration rule, $u(x) \approx \sum_j K(x,y_j)\mu(y_j)\, w_j$:



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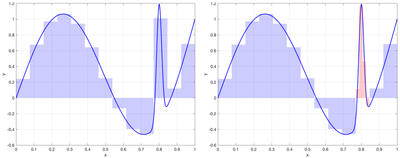
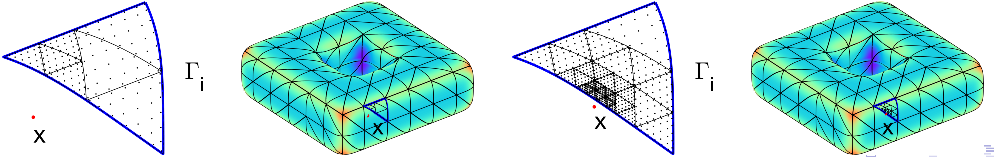
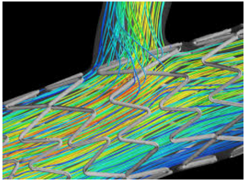


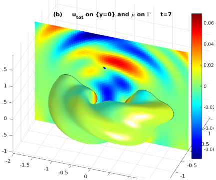
Adaptive quadrature on a surface element Γ_i:



- Singular integrals are mathematically interesting.
- Singular integrals arise in critical applications across science and engineering.

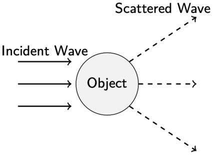


Blood flow

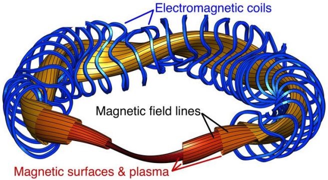


Direct scattering

(Barnett, Greengard, Hagstrom, '20)



Inverse scattering



Electromagnetism

(Simons Collaboration on Hidden Symmetries and Fusion Energy)

$K(\boldsymbol{r}', \boldsymbol{r})$:

$$\frac{1}{8\pi}\left(I\frac{1}{|\boldsymbol{r}'-\boldsymbol{r}|} + \frac{(\boldsymbol{r}'-\boldsymbol{r})\otimes(\boldsymbol{r}'-\boldsymbol{r})}{|\boldsymbol{r}'-\boldsymbol{r}|^3}\right), \qquad \frac{e^{ik|\boldsymbol{r}'-\boldsymbol{r}|}}{4\pi|\boldsymbol{r}'-\boldsymbol{r}|}, \qquad \frac{(\boldsymbol{r}'-\boldsymbol{r})(1-ik|\boldsymbol{r}'-\boldsymbol{r}|)}{4\pi|\boldsymbol{r}'-\boldsymbol{r}|^3}e^{ik|\boldsymbol{r}'-\boldsymbol{r}|}$$

This is due to several reasons:

- Different singularity types:

$$\log|\boldsymbol{r}' - \boldsymbol{r}|, \quad 1/|\boldsymbol{r}' - \boldsymbol{r}|, \quad 1/|\boldsymbol{r}' - \boldsymbol{r}|^2, \quad \cdots$$

- Different interaction types ($\boldsymbol{r}' \in \Gamma_i$ or not):
  self interaction, on-boundary near interaction, off-boundary close interaction
- Complicated mesh elements, i.e. non-flat Γ_i.

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Large literature on quadrature problem:

(Duffy '82) (Bruno, et al. '01) (Ying, et al. '06) (Rokhlin, et al. '10) (Tornberg, et al. '18) (Greengard, et al. '21) (Zorin, et al. '21) (Barnett, et al. '22) ...

Challenge: type specific, low order or slow

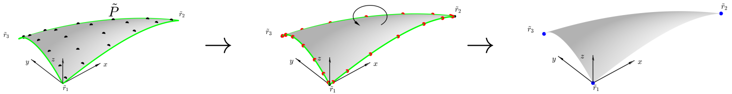
Efficiently and accurately compute $u(\boldsymbol{r}') = \int_{\Gamma_i} K(\boldsymbol{r}', \boldsymbol{r})\mu(\boldsymbol{r})\, dS$ for arbitrary shape:

Main Contribution: Unified framework

Efficiently and accurately compute $u(\boldsymbol{r}') = \int_{\Gamma_i} K(\boldsymbol{r}', \boldsymbol{r})\mu(\boldsymbol{r})\, dS$ for arbitrary shape:

Main procedure:

surface integral $\rightarrow$ line integrals $\rightarrow$ function evaluations



- Fast: recursive dimension reduction
- Accurate: high-order analytic integration

(Zhu, Veerapaneni, '22 SISC) (Jiang, Zhu, '24 arxiv)

Motivation and Our Contribution.

Recursive Reduction Quadrature.

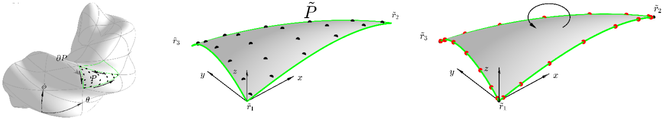
Key ideas for computing $\int_P \frac{(\boldsymbol{r}'-\boldsymbol{r})\cdot\boldsymbol{n}(\boldsymbol{r})}{|\boldsymbol{r}'-\boldsymbol{r}|^3}\mu(\boldsymbol{r})dS$ (will come back to $\int_P \frac{1}{|\boldsymbol{r}'-\boldsymbol{r}|}\sigma(\boldsymbol{r})dS$):

- adapt a differential geometric approach for 2-to-1 form reduction: $\int_P \alpha = \int_{\partial P} \omega$
- develop a quaternion function approximation: $\underbrace{(\mu, \mathbf{0})}_{quaternion} \approx \sum(0, \nabla H)(c_0, \boldsymbol{c})$
- derive complete reduction to 0-form evaluation: $\int_{\partial P} \tilde{\omega} = \int_{\partial(\partial P)} \tilde{\zeta}$

High-order elements

$$\boxed{\int_P \frac{(\mathbf{r}'-\mathbf{r})\cdot \mathbf{n}(\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}\mu(\mathbf{r})dS = \int_{\partial P}\omega} \quad \Rightarrow \quad \int_{\partial P}\tilde{\omega} = \tilde{\zeta}\Big|_{\mathbf{r}_i}$$

$$\alpha = d\omega \quad \Leftarrow \quad \tilde{\omega} = d\tilde{\zeta}$$



Theorem: 2-to-1 form (Jiang-Zhu '24) (Zhu-Veerapaneni '22)

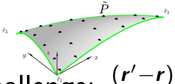
On a contractible domain P, the differential 2-form

$$\alpha = \boldsymbol{f}(\boldsymbol{r})\cdot\boldsymbol{n}(\boldsymbol{r})dS \text{ is exact } \Leftrightarrow \alpha \text{ is closed } (\nabla\cdot\boldsymbol{f}=0),$$

where dS is the area differential. Assume $\nabla\cdot\boldsymbol{f}=0$, then for any $\boldsymbol{r}'\in\mathbb{R}^3$,

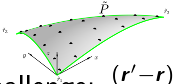
$$\alpha = d\omega \text{ (surface-to-line)},$$

where 1-form $\omega = \left(-\int_0^1 t(\boldsymbol{r}-\boldsymbol{r}')\times\boldsymbol{f}(\boldsymbol{r}'+t(\boldsymbol{r}-\boldsymbol{r}'))dt\right)\cdot d\boldsymbol{r}$.



$$\boxed{\int_P \frac{(\boldsymbol{r}'-\boldsymbol{r})\cdot\boldsymbol{n}(\boldsymbol{r})}{|\boldsymbol{r}'-\boldsymbol{r}|^3}\mu(\boldsymbol{r})dS = \int_{\partial P}\omega} \quad \Rightarrow \quad \int_{\partial P}\tilde{\omega} = \tilde{\zeta}\Big|_{\boldsymbol{r}_i}$$

Challenge: $\frac{(\boldsymbol{r}'-\boldsymbol{r})\cdot\boldsymbol{n}(\boldsymbol{r})}{|\boldsymbol{r}'-\boldsymbol{r}|^3}\mu(\boldsymbol{r})dS$ is not closed, $\mu(\boldsymbol{r})$ is not even known outside surface P!!



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Quaternions are

$$a + bi + cj + dk = (a, b, c, d), \text{ where } a, b, c, d \in \mathbb{R}, \text{ and } i^2 = j^2 = k^2 = ijk = -1$$

The multiplication rule for $f = (f_0, \boldsymbol{f})$ and $g = (g_0, \boldsymbol{g})$ is

$$fg = (f_0 g_0 - \boldsymbol{f}\cdot\boldsymbol{g}, f_0\boldsymbol{g} + g_0\boldsymbol{f} + \boldsymbol{f}\times\boldsymbol{g}).$$

Lemma: Quaternion approx./extension (Jiang-Zhu '24) (Zhu-Veerapaneni '22)

We construct a basis consisting of harmonic polynomials

$$H^{(l,m)}: \mathbb{R}^3 \to \mathbb{R}, \text{ such that } \operatorname{span}\{H_z^{(l,m)}|_{\mathbb{R}^2\times\{0\}}\} = \operatorname{span}\{x^l y^m\}$$

$0 \le l + m \le p - 1$, and for any smooth $\mu: \mathbb{R}^2 \to \mathbb{R}$, $\exists!$ quaternion $\{c^{(l,m)}\}$

$$(\mu, \mathbf{0}) \approx -\sum_{l,m}(0, \nabla H^{(l,m)})\Big|_P (c_0^{(l,m)}, \boldsymbol{c}^{(l,m)})$$

$$H^{(l,m)}(x,y,z) := \mathrm{Im}\left(R_l^m(y,z,x)\right). \tag{1}$$

The regular solid harmonic polynomials R_l^m ($1 \leq m \leq l \leq p$) are defined by the formula

$$R_l^m(\boldsymbol{r}) = \frac{1}{\sqrt{2l+1}} r^l Y_l^m(\theta,\phi), \tag{2}$$

where (r,θ,ϕ) are the spherical polar coordinates of $\boldsymbol{r}$. The spherical harmonic polynomials Y_l^m are defined by the formula

$$Y_l^m(\theta,\phi) = \sqrt{2l+1}\sqrt{\frac{(l-m)!}{(l+m)!}} P_l^m(\cos(\theta)) e^{im\phi}, \tag{3}$$

The associated Legendre polynomials P_l^m are defined by the formula

$$P_l^m(x) = \frac{1}{2^l l!}(1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l. \tag{4}$$

$$\boxed{\int_P \frac{(\mathbf{r}'-\mathbf{r})\cdot\mathbf{n}(\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}\nabla H^{(l,m)}(\mathbf{r})dS = \int_{\partial P}\omega^{(l,m)}} \quad \Rightarrow \quad \int_{\partial P}\tilde{\omega} = \tilde{\zeta}\Big|_{\mathbf{r}_i}$$

Theorem: quaternion 2-to-1 form with translation (Jiang-Zhu '24)

Let $\alpha^{(l,m)}$ be the quaternion differential 2-forms defined by

$$\alpha^{(l,m)}(\mathbf{r}',\mathbf{r}) = (0, \underbrace{\nabla K(\mathbf{r}',\mathbf{r})}_{\frac{(\mathbf{r}'-\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}})(0,\mathbf{n}(\mathbf{r}))(0, \underbrace{\nabla H^{(l,m)}(\mathbf{r})}_{(\mathbf{r}'+t(\mathbf{r}-\mathbf{r}'))^{(l,m)}})dS, \quad \underbrace{\nabla H^{(l,m)}(\mathbf{r})}_{\to((1-t)\mathbf{r}'+t\mathbf{r})^{(l,m)}}$$

where $\mathbf{r}$ in $\alpha^{(l,m)}(\mathbf{r}',\mathbf{r})$ are source points on P, then $\alpha^{(l,m)}$ are closed, and the differential 1-forms $\omega^{(l,m)}$ such that $\alpha = d\omega$ are defined by

$$\omega^{(l,m)}(\mathbf{r}',\mathbf{r}) = \sum_{j,k}\frac{(j-2)!(l-j)!}{(l-1)!}\left(0, d\left(\frac{\mathbf{r}'-\mathbf{r}}{|\mathbf{r}'-\mathbf{r}|}\right)\right)\left(0,\nabla H^{(j,k)}(\mathbf{r})\right)H^{(l-j,m-k)}(\mathbf{r}')T_{jk,lm},$$

where $\mathbf{r}$ in $\omega^{(l,m)}(\mathbf{r}',\mathbf{r})$ are source points on ∂P.

To derive the target-centered 1-forms, we use the translation of solid harmonic polynomials. The translation of $H^{(l,m)}$ is,

$$\begin{aligned} H^{(l,m)}(\boldsymbol{r}' + t(\boldsymbol{r} - \boldsymbol{r}')) &= H^{(l,m)}\left((1-t)\boldsymbol{r}' + t\boldsymbol{r}\right) \\ &= \sum_{j=0}^{l}\sum_{k=-j}^{j} H^{(j,k)}(t\boldsymbol{r}) H^{(l-j,m-k)}((1-t)\boldsymbol{r}')\, T_{jk,lm} \\ &= \sum_{j=0}^{l} t^j (1-t)^{l-j} \sum_{k=-j}^{j} H^{(j,k)}(\boldsymbol{r}) H^{(l-j,m-k)}(\boldsymbol{r}')\, T_{jk,lm}. \end{aligned} \tag{5}$$

where $T_{jk,lm}$ denotes the translation operator of local expansions.

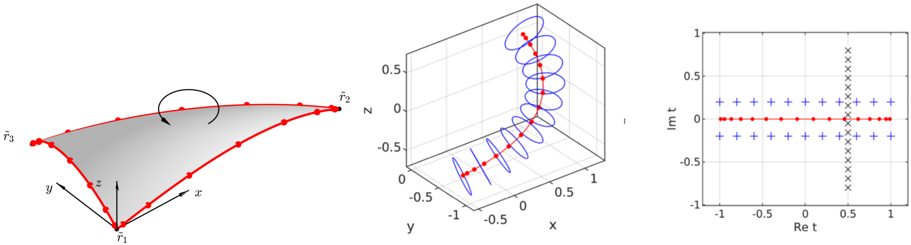
$$\int_P \frac{(\mathbf{r}'-\mathbf{r})\cdot\mathbf{n}(\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^3}\nabla H^{(l,m)}(\mathbf{r})dS = \int_{\partial P}\omega^{(l,m)} \quad \Rightarrow \quad \boxed{\int_{\partial P}\tilde{\omega}^{(j,k)} = \tilde{\zeta}^{(j,k)}\Big|_{\mathbf{r}_i}}$$

Essentially, we care about

$$\tilde{\zeta}^{(j,k)}(\mathbf{r}') = \int_{\partial P}\tilde{\omega}^{(j,k)} = \int_{\partial P}\frac{g^{(j,k)}(\mathbf{r})}{|\mathbf{r}'-\mathbf{r}|^{\lambda}}\,|d\mathbf{r}|.$$

Assume ∂P is parameterized by $t \in [-1,1]$, we have:

$$\tilde{\zeta}^{(j,k)}(\mathbf{r}') = \int_{-1}^{1}\frac{F(t)}{((t-t_0)(t-\overline{t_0}))^{\lambda/2}}dt.$$



singularity swap quadrature

(af Klinteberg, Barnett '21)

The above framework also works for higher order derivatives. However, for $\frac{1}{|\boldsymbol{r}'-\boldsymbol{r}|}\sigma(\boldsymbol{r})dS$

- We need another closed 2-form (involving both $1/|\boldsymbol{r}' - \boldsymbol{r}|$ and $\nabla(1/|\boldsymbol{r}' - \boldsymbol{r}|)$)

Lemma: Closed 2-form (Jiang-Zhu '24)

On a contractible domain P, suppose u and v satisfy Laplace equation, then

$$(u\nabla v - v\nabla u) \cdot \boldsymbol{n} dS$$

is closed, and thus exact on P, where dS is the area differential.

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- We need another approximation/extension (scalar approximation using $\boldsymbol{n}$)

Theorem: Scalar approx./extension (Jiang-Zhu '24)

We construct a basis consisting of harmonic polynomials $H^{(l,m)} : \mathbb{R}^3 \to \mathbb{R}$. such that for any smooth $\sigma : \mathbb{R}^2 \to \mathbb{R}$, $\exists!$ scalar $\{d^{(l,m)}\}$, $0 \le l + m \le p - 1$

$$\sigma \approx \sum_{l,m} \left(\nabla H^{(l,m)} \cdot \boldsymbol{n}\right)\Big|_P d^{(l,m)}$$

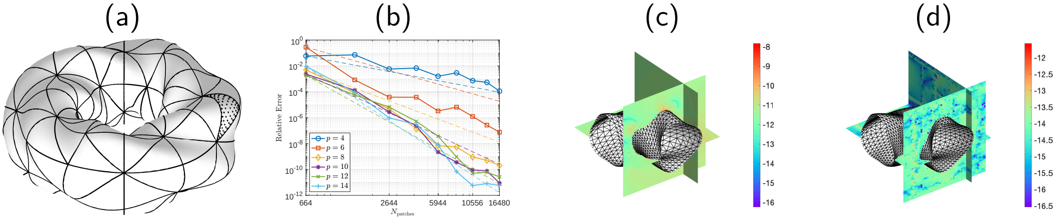
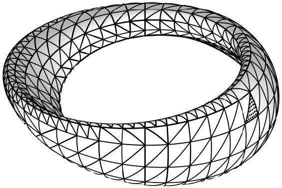


Figure: (a) triangulated warped torus boundary; (b) relative l_∞ errors as functions of N_{patches} for various orders p; Slice plots of $\log_{10}$ of the pointwise relative errors for the warped torus. (c) $p = 8,\ n_\theta = 36,\ n_\phi = 72$. (d) $p = 14,\ n_\theta = 48,\ n_\phi = 96$.



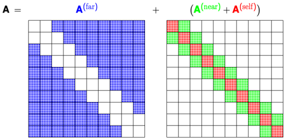
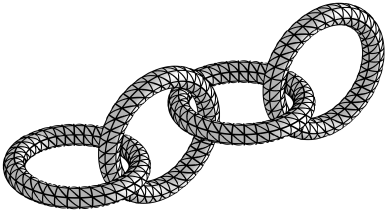
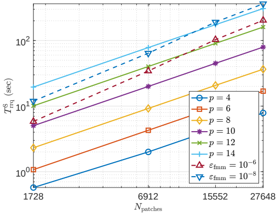
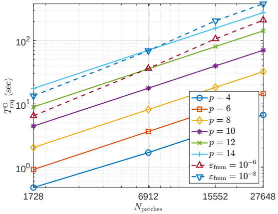


Table: Throughput in points processed per second per core during the solve phase. "FMM" for far speed, "rrq" for self and near speed. "S" for single layer, "D" for double layer.

p	X^S_{FMM}	X^D_{FMM}	X^S_{rrq}	X^D_{rrq}	ε_{FMM}	E_∞
4	26894	24144	21285	27212	1e-04	1.1e-04
6	20445	17494	15065	21376	1e-06	2.1e-05
8	13983	11646	9921	15017	1e-08	2.8e-07
10	13341	10803	6621	10449	1e-09	3.2e-08
12	9888	8089	4324	6845	1e-10	7.6e-10
14	9113	7178	2907	4534	1e-12	9.7e-12







Computation time in seconds in the quadrature correction part for the volumetric evaluation of Laplace layer potentials, on a corresponding uniform grid of $101 \times 101 \times 101$, $201 \times 201 \times 201$, $301 \times 301 \times 301$, and $401 \times 401 \times 401$ points, for the interlocking-tori for $p = 4, 6, \ldots, 14$. Middle: Computation time T_{rrq} for the Laplace single layer potential operator. Right: Computation time T_{rrq} for the Laplace double layer potential operator. In both figures, the dashed lines show the computation time on a single FMM call on the same set of source points on the boundary and target points in the volume.

S. Jiang and H. Zhu, “Recursive reduction quadrature for the evaluation of Laplace layer potentials in three dimensions," *arXiv preprint arXiv:2411.08342*, 2024.

H. Zhu and S. Veerapaneni, “High-order close evaluation of Laplace layer potentials: A differential geometric approach," ***SIAM Journal on Scientific Computing***, vol. 44, no. 3, pp. A1381–A1404, 2022.

L. af Klinteberg and A. Barnett, “Accurate quadrature of nearly singular line integrals in two and three dimensions by singularity swapping," ***BIT Numerical Mathematics***, vol. 61, no. 1, pp. 83–118, 2021

J. Helsing and R. Ojala, “On the evaluation of layer potentials close to their sources," ***Journal of Computational Physics***, vol. 227, no. 5, pp. 2899–2921, 2008

The journey continues ...

Thank you!

For a set of collocation points $\boldsymbol{r}^{(i,j)}$ $(0 \le i+j \le p-1)$ on the triangular patch P, the quaternion coefficients $c^{(l,m)} = (c_0^{(l,m)}, \boldsymbol{c}^{(l,m)})$ are then obtained by solving the following linear system:

$$\sum_{l=1}^{p} \sum_{m=1}^{l} (0, \nabla H^{(l,m)}(\boldsymbol{r}^{(i,j)}))(c_0^{(l,m)}, \boldsymbol{c}^{(l,m)}) = (\mu(\boldsymbol{r}^{(i,j)}), \mathbf{0}), \quad 0 \le i+j \le p-1. \tag{6}$$

Writing out explicitly, (6) is equivalent to the following equations with only the usual vector calculus involved:

$$\begin{aligned} -\sum_{l,m} \nabla H^{(l,m)}(\boldsymbol{r}^{(i,j)}) \cdot \mathbf{c}^{(l,m)} &= \mu(\boldsymbol{r}^{(i,j)}), \\ \sum_{l,m} c_0^{(l,m)} \nabla H^{(l,m)}(\boldsymbol{r}^{(i,j)}) + \nabla H^{(l,m)}(\boldsymbol{r}^{(i,j)}) \times \mathbf{c}^{(l,m)} &= \mathbf{0}. \end{aligned} \tag{7}$$

Let $\nabla H = (F_1, F_2, F_3)$. Then in block matrix form, we have

$$\begin{pmatrix} 0 & -F_1 & -F_2 & -F_3 \\ F_1 & 0 & -F_3 & F_2 \\ F_2 & F_3 & 0 & -F_1 \\ F_3 & -F_2 & F_1 & 0 \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} \mu \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{8}$$

where the length of c_k $(k = 0, 1, 2, 3)$ is n_{p} with $n_{\mathrm{p}} = \frac{p(p+1)}{2}$, the size of each block is $n_{\mathrm{p}} \times n_{\mathrm{p}}$.

For a target point $\boldsymbol{r}'$, we approximate $F(t)$ by its polynomial interpolant with $\tilde{p}$ Gauss-Legendre nodes,

$$F(t) = \sum_{i=0}^{\tilde{p}-1} \tilde{c}_i t^i, \quad \tilde{c} = UF, \tag{9}$$

where

$$\tilde{c} = \begin{bmatrix} \tilde{c}_0 \\ \vdots \\ \tilde{c}_{\tilde{p}-1} \end{bmatrix}, \quad F = \begin{bmatrix} F(t_1) \\ \vdots \\ F(t_{\tilde{p}}) \end{bmatrix}, \quad U = \begin{bmatrix} 1 & t_1 & \cdots & t_1^{\tilde{p}-1} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_{\tilde{p}} & \cdots & t_{\tilde{p}}^{\tilde{p}-1} \end{bmatrix}^{-1}. \tag{10}$$

The integrals

$$\mathcal{I}_i(\boldsymbol{r}') = \int_{-1}^{1} \frac{t^i}{((t - t_0)(t - \overline{t_0}))^{\lambda/2}} dt \tag{11}$$

can be calculated by a recurrence relation (af Klinteberg, Barnett '21) (Tornberg, Gustavsson '06).

Conversion of the BVP to a Boundary Integral Equation (BIE).

↓

Discretization of BIE using Nyström, collocation, BEM, . . .

↓

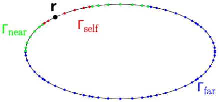
$N \times N$ discrete linear system. Dense, well-conditioned.

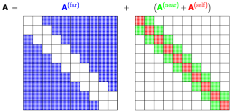
↓

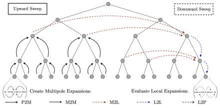
Iterative solver accelerated by fast matrix-vector framework, for example, FMM and DMK, in $O(N)$. Then evaluate solution in the domain.

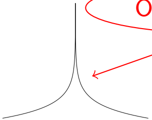
$$\begin{cases} -\Delta u(\mathbf{r}) = 0, & \mathbf{r} \in \Omega, \\ u(\mathbf{r}) = g(\mathbf{r}), & \mathbf{r} \in \Gamma, \end{cases}$$

$$\Rightarrow \quad \alpha\mu(\mathbf{r}') + \int_\Gamma K(\mathbf{r}', \mathbf{r})\mu(\mathbf{r})\, dS \quad = \quad g(\mathbf{r})$$









Our contribution