Boundary integral methods

for general elliptic problems

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OVERVIEW

1. First-order overdetermined systems
– Ellipticity

2. Boundary and volume integral equations
– Derivation
– Fundamental matrices and examples
– Fredholm operators

3. Fast algorithms
– Generalized Ewald summation
– Implicit local correction
– Geometric nonuniform fast Fourier transform

EXAMPLES OF ELLIPTIC PROBLEMS

Cauchy-Riemann

$$\partial_x u = \partial_y v \qquad \partial_y u = -\partial_x v$$

Low-frequency Maxwell

$$\nabla \times E = -\mathrm{i}\omega H \qquad \nabla \cdot E = 4\pi\rho$$
$$\nabla \times H = \mathrm{i}\omega E + 4\pi j \qquad \nabla \cdot H = 0$$

Linear elasticity

$$\partial_i \sigma_{ij} + F_j = 0 \qquad \sigma_{ij} - \frac{1}{2} C_{ijkl} \left(\partial_k u_l + \partial_l u_k \right) = 0$$

Laplace/Poisson/Helmholtz/Yukawa/ ...

$$\Delta u - \lambda u = f$$

Stokes

$$-\Delta u + \nabla p = f \qquad \nabla \cdot u = 0$$

PART 1. CONVERTING TO FIRST-ORDER SYSTEMS

Arbitrary-order system of partial differential equations

$$\cdots + \sum_{ijl} a_{ijkl}\partial_i\partial_j v_l + \sum_{jl} b_{jkl}\partial_j v_l + \sum_{l} c_{kl} v_l = f_k \qquad \text{in } \Omega \subset R^d$$

$$\sum_{l} \alpha_{kl} v_l + \sum_{jl} \beta_{kjl}\partial_j v_l + \cdots = g_k \qquad \text{on } \Gamma = \partial\Omega$$

Seek new solution vector $u = (v, \partial_1 v, \ldots, \partial_d v, \ldots)^T$
satisfying sparse $p \times q$ **first-order** system

$$\mathcal{A}u = \sum_{j} A_j \partial_j u + A_0 u = f \qquad \text{in } \Omega$$

and **zero-order** local linear algebraic boundary conditions

$$Bu = g \qquad \text{on } \Gamma$$

Elliptic iff principal part

$$A_n = \sum_{j} n_j A_j$$

has full rank for all unit vectors n

ELLIPTICITY AND SOLVABILITY

$$\mathcal{A}u = \sum_j A_j \partial_j u + A_0 u = f \qquad \text{in } \Omega$$

Left inverse $A_n^\dagger$ of any principal part $A_n = \sum_j n_j A_j$ determines normal derivative

$$\partial_n u = \sum_i n_i \partial_i u = A_n^\dagger (f - A_T \partial_T u - A_0 u)$$

in terms of values and tangential derivatives $A_T \partial_T u$

Could march $\partial_n u$ inward to solve boundary value problem but typical low-rank boundary conditions

$$Bu = \begin{bmatrix} \alpha & \beta n_1 & \beta n_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = g \qquad (BB^*)^2 = BB^*$$

determine only local projection $Qu = B^* Bu$

Global continuity determines complementary projection $Pu = (I - B^* B)u$ everywhere on boundary

SQUARE BUT NOT ELLIPTIC

Elliptic boundary value problem for 2D equation

$$\Delta v - \lambda v = f \qquad \text{in } \Omega$$

$$\alpha v + \beta \partial_n v = g \qquad \text{on } \Gamma$$

Obvious 3 × 3 square system

$$\mathcal{A}u = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ -\lambda & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ f \end{bmatrix}$$

$$Bu = \begin{bmatrix} \alpha & \beta n_1 & \beta n_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = g$$

anti-elliptic: principal part

$$\sum_j n_j A_j = \begin{bmatrix} n_1 & 0 & 0 \\ n_2 & 0 & 0 \\ 0 & n_1 & n_2 \end{bmatrix} \qquad \text{singular for all unit vectors } n!$$

ALGEBRA TO THE RESCUE

$$\Delta v - \lambda v = f \qquad \text{in } \Omega$$

Overdetermined 4×3 **system**

$$\mathcal{A}u = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ 0 & -\partial_2 & \partial_1 \\ -\lambda & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ f \end{bmatrix}$$

adds compatibility condition to enforce ellipticity:

$$A_n = \sum_j n_j A_j = \begin{bmatrix} n_1 & 0 & 0 \\ n_2 & 0 & 0 \\ 0 & -n_2 & n_1 \\ 0 & n_1 & n_2 \end{bmatrix}$$

full-rank for all unit vectors n

Cancellations determine original v **from** $\mathcal{A}^*\mathcal{A}u = \mathcal{A}^* f$**:**

$$\left(\Delta + \lambda^2\right) v - (\lambda + 1)\partial_1 v_1 - (\lambda + 1)\partial_2 v_2 = \lambda f$$

PART 2. POTENTIAL THEORY

Given fundamental matrix $G_x(y)$ **of adjoint system**

$$\mathcal{A}^* G_x = -\sum_{j=1}^{d} \partial_j G_x(y) A_j + G_x(y) A_0 = \delta_x(y) I \qquad \text{in } Q \supset \Omega,$$

Gauss theorem (and $\delta_x \to \frac{1}{2}\delta_\gamma$ **as** $x \to \gamma \in \Gamma$**)**

$$\int_\Omega \partial_j \Big(G_x(y) A_j u(y) \Big) \, \mathrm{d}y = \int_\Gamma n_j(\gamma) G_x(\gamma) A_j u(\gamma) \, \mathrm{d}\gamma$$

implies simple boundary integral equation

$$\frac{1}{2} u(\gamma) + \int_\Gamma G_\gamma(\sigma) A_n(\sigma) u(\sigma) \, \mathrm{d}\sigma = \mathcal{G} f(\gamma) \quad \text{on } \Gamma$$

with volume potential

$$\mathcal{G} f(\gamma) = \int_\Omega G_\gamma(y) f(y) \, \mathrm{d}y$$

Alternatively, homogeneous fundamental matrix $F_x(y)$ **of** principal part $\mathcal{A} - A_0$ **gives** volume integral equation

$$\frac{1}{2} u(\gamma) + \int_\Gamma F_\gamma(\sigma) A_n(\sigma) u(\sigma) \, \mathrm{d}\sigma + \mathcal{F} A_0 u(\gamma) = \mathcal{F} f(\gamma) \quad \text{on } \Gamma$$

PROJECTED INTEGRAL EQUATION

Project out boundary condition $Bu = g$ **with** $P = I - B^*B$

Solve square integral equation

$$\frac{1}{2}\mu(\gamma) + \int_\Gamma P(\gamma)G_\gamma(\sigma)A_n(\sigma)\mu(\sigma)\mathrm{d}\sigma = \rho(\gamma)$$

for locally projected unknown $\mu = Pu$ **with data**

$$\rho(\gamma) = P(\gamma)\mathcal{G}f(\gamma) - P(\gamma)\mathcal{L}B^*g(\gamma)$$

and single layer potential

$$\mathcal{L}h(\gamma) = \int_\Gamma G_\gamma(\sigma)A_n(\sigma)h(\sigma)\,\mathrm{d}\sigma$$

Recover $u = \mu + B^*g$ **locally on** Γ **and then globally**

$$u(x) = \mathcal{G}f(x) + \mathcal{L}u(x) \qquad \text{in } \Omega$$

Volume integral is compact correction

EXAMPLE 1: LAPLACE ...

$$\Delta v - \lambda v = f$$

Fundamental matrix

$$G = \begin{bmatrix} \partial_1 R_\lambda & \partial_2 R_\lambda & 0 & R_\lambda \\ (\lambda+1)\partial_1^2 R_{-1} R_\lambda - R_{-1} & (\lambda+1)\partial_1\partial_2 R_{-1} R_\lambda & -\partial_2 R_{-1} & \partial_1 R_\lambda \\ (\lambda+1)\partial_1\partial_2 R_{-1} R_\lambda & (\lambda+1)\partial_2^2 R_{-1} R_\lambda - R_{-1} & \partial_1 R_{-1} & \partial_2 R_\lambda \end{bmatrix}$$

with kernel R_z of resolvent $(\Delta - z)^{-1}$
for two values $z = \lambda$ and $z = -1$ (due to scaling)

Nonclassical integral equations for Dirichlet problem

$$\begin{aligned} \frac{1}{2} v_{,n} + n \cdot \int_\Gamma \partial R_\lambda v_{,n} - t \cdot \int_\Gamma \partial R_{-1} v_{,t} &= \rho_n \\ \frac{1}{2} v_{,t} + n \cdot \int_\Gamma \partial R_{-1} v_{,t} - t \cdot \int_\Gamma \partial R_\lambda v_{,n} &= \rho_t \end{aligned}$$

determine usual normal derivative $v_{,n}$ and
unusual tangential derivative $v_{,t}$ of solution v

EXAMPLE 2: MAXWELL

$$
\begin{aligned}
\nabla \times E &= -\mathrm{i}\omega H & \qquad \nabla \cdot E &= 4\pi\rho \\
\nabla \times H &= \mathrm{i}\omega E + 4\pi j & \qquad \nabla \cdot H &= 0
\end{aligned}
$$

Homogeneous fundamental matrix

$$
F = \begin{bmatrix}
0 & \partial_3 & -\partial_2 & \partial_1 & 0 & 0 & 0 & 0 \\
-\partial_3 & 0 & \partial_1 & \partial_2 & 0 & 0 & 0 & 0 \\
\partial_2 & -\partial_1 & 0 & \partial_3 & 0 & 0 & 0 & 0 \\
-0 & 0 & 0 & 0 & 0 & \partial_3 & -\partial_2 & \partial_1 \\
0 & -0 & 0 & 0 & -\partial_3 & 0 & \partial_1 & \partial_2 \\
0 & 0 & -0 & 0 & \partial_2 & -\partial_1 & 0 & \partial_3
\end{bmatrix} R_0
$$

with kernel R_0 of resolvent Δ^{-1}

Volume integral equation

$$
\frac{1}{2}u(\gamma) + \int_\Gamma F_\gamma(\sigma) A_n(\sigma) u(\sigma)\, \mathrm{d}\sigma + \mathcal{F}A_0 u(\gamma) = \mathcal{F}f(\gamma) \quad \textbf{on } \Gamma
$$

employs layer potential independent of frequency and sequesters frequency ω into compact volume potential $\mathcal{F}A_0$

GENERAL FUNDAMENTAL MATRIX

Fourier analysis in box $Q \supset \Omega$ gives fundamental matrix

$$G_x(y) = \sum_{k \in Z^d} \mathrm{e}^{-\mathrm{i}k^T x} s(k)^{-1} a^*(k) \mathrm{e}^{\mathrm{i}k^T y}$$

with $s = a^* a$ positive definite Hermitian and symbol

$$a(k) = \mathrm{i} \sum_{j=1}^{d} k_j A_j + A_0$$

Homogeneity of principal part makes box potential

$$\mathcal{A}^\dagger f(x) = \int_Q G_x(y) f(y) \, \mathrm{d}y$$

a bounded Fredholm operator from any $H^{s-1}(Q)$ to $H^s(Q)$

Trace $\gamma : H^s(Q) \hookrightarrow H^{s-1/2}(\Gamma)$ restricts volume potential $\mathcal{G}f = \gamma \mathcal{A}^\dagger f$ to $H^{s-1/2}(\Gamma)$ where $g = Bu$ lives

Dual trace $\gamma^* : H^{1/2-s}(\Gamma) \hookrightarrow H^{-s}(Q)$ yields layer potential $\mathcal{L}g = \gamma \mathcal{A}^\dagger \gamma^* g$ mapping $H^{1/2-s}(\Gamma)$ to itself

Repaired at endpoint $s = 1/2$ by homogeneity

PART 3. GENERALIZED EWALD SUMMATION

Matrix filter $\mathrm{e}^{-\tau s}$ gives exponential convergence

$$\begin{aligned} G_x(y) &= \sum_{|k|\le N} \mathrm{e}^{-\mathrm{i}k^T x} \mathrm{e}^{-\tau s(k)} s(k)^{-1} a^*(k) \mathrm{e}^{\mathrm{i}k^T y} \\ &+ \quad \text{tiny } O(\mathrm{e}^{-\tau N^2}) \text{ truncation error} \\ &+ \quad \text{big } O(\tau) \text{ but local filtering error} \end{aligned}$$

Fundamental matrix G is smooth rapidly-converging series

$$G_\tau(x) = \sum \mathrm{e}^{-\tau s(k)} s(k)^{-1} a^*(k) \mathrm{e}^{-\mathrm{i}k^T x} \sim \mathrm{e}^{-\tau \mathcal{S}} \mathcal{S}^{-1} \mathcal{A}^*$$

corrected by local asymptotic series

$$\mathcal{G} - \mathcal{G}_\tau = (I - \mathrm{e}^{-\tau \mathcal{S}}) \mathcal{S}^{-1} \mathcal{A}^* = \left(\tau - \frac{\tau^2}{2!} \mathcal{S} + \frac{\tau^3}{3!} \mathcal{S}^2 - \cdots \right) \mathcal{A}^*$$

with local differential operators $\mathcal{A}^*$ and $\mathcal{S} = \mathcal{A}^* \mathcal{A}$

Includes many classical local corrections and Ewald formulas (with special function kernels) for Laplace, Stokes, . . .

LOCAL CORRECTION IN A BOX

$\mathcal{A}^\dagger f(x) = (\mathcal{G}_\tau + \mathcal{C}_\tau)\, f(x)$ **solves** $\mathcal{A}u = f$ **in periodic box** Q

Rapidly converging Fourier series $\mathcal{G}_\tau f$ **approximated by FFT**

Explicit local correction

$$\mathcal{C}_\tau f(x) = \left(\tau - \frac{\tau^2}{2!}\mathcal{S} + \frac{\tau^3}{3!}\mathcal{S}^2 - \cdots \pm \frac{\tau^m}{m!}\mathcal{S}^{m-1}\right)\mathcal{A}^* f(x) + O(\tau^{m+1})$$

approximated by $(2p+1)^d$**-point stencil with matrix weights**

$$C_\tau f(x) = \sum_{|k|\le p} W_k(x) f(x+kh) + O(\tau^{m+1}) + O(\tau h^{2p}).$$

High-order accuracy with minimal smoothness requirements

LOCALLY-CORRECTED VOLUME POTENTIALS

Gauss theorem differentiates indicator function $\omega(x)$ of set Ω

$$\int_\Omega \partial_j u \, \mathrm{d}x = \int_\Gamma n_j u \, \mathrm{d}\gamma \qquad \Leftrightarrow \qquad \partial_j \omega = n_j \delta_\Gamma$$

Second-order derivatives involve curvature

$$\partial_j \partial_k \omega(x) = (\partial_j n_k)\delta_\Gamma + n_j n_k \partial_n \delta_\Gamma$$

Volume potential of discontinuous source $f\omega$ splits

$$\mathcal{G}f(x) = \int_\Omega G_x(y) f(y) \, \mathrm{d}y = \mathcal{A}^\dagger(f\omega) = \mathcal{G}_\tau(f) + \mathcal{C}_\tau(f\omega)$$

Explicit local correction $\mathcal{C}_\tau$ satisfies product rule

$$\mathcal{C}_\tau(f\omega)(x) = \tau\left[(\mathcal{A}^* f(x))\omega(x) - A_n^* f(x)\delta_\Gamma(x)\right] + O(\tau^2)$$

and localizes Galerkin computations

IMPLICIT LOCAL CORRECTION

Volume potential

$$u = \mathcal{G}f(x) = \mathcal{G}_\tau f + (I - \mathrm{e}^{-\tau\mathcal{S}})u$$

since $\mathcal{A}^* f = \mathcal{A}^*\mathcal{A}u = \mathcal{S}u$

Sharpen $\mathcal{G}_\tau f$ **into** u **with local backward heat flow**

$$u = \mathrm{e}^{+\tau\mathcal{S}}\mathcal{G}_\tau f$$

Analogous to Gaussian nonuniform fast Fourier transform: smooth rough sources, uniform transform, unsmooth

Overcomes Gibbs phenomenon?

SPECTRAL INTEGRAL EQUATION

Fourier series for fundamental solution separates variables

$$G_\tau(x-y) = \sum \mathrm{e}^{-\mathrm{i}k^T x} \mathrm{e}^{-\tau s(k)} a^\dagger(k) \mathrm{e}^{\mathrm{i}k^T y}$$

Converts integral equation to semi-separated form

$$\left(\frac{1}{2} + MRT\right) \mu(\gamma) = \rho(\gamma)$$

- T **computes Fourier coefficients of** $(A_n \mu)\delta_\Gamma$
- R **applies** $\mathrm{e}^{-\tau s} a^\dagger$ **to Fourier modes**
- M **evaluates Fourier series on** Γ

Solve in Fourier space by identity

$$\left(\frac{1}{2} + MRT\right)^{-1} = 2 - 2MR\left(\frac{1}{2} + TMR\right)^{-1} T$$

Compresses integral operator to low-rank matrix

$$(TMR)_{kq} = \int_\Gamma A_n(\sigma) P(\sigma) \mathrm{e}^{-\mathrm{i}(k-q)^T \sigma} \, \mathrm{d}\sigma \, \mathrm{e}^{-\tau s(q)} a^\dagger(q)$$

Randomize Fourier transform

NONUNIFORM FAST FOURIER TRANSFORM

Standard FFT works on uniform equidistant mesh

Nonuniform FFT works on arbitrary point sources:
– form coefficients from small source to large target spans
– butterfly: merge source and shorten target span recursively
– evaluate large source fields in small target spans

Integral equation requires Fourier coefficients
of soup of piecewise polynomials P_j on simplices T_j
(points, segments, triangles, tetrahedra, . . .)

$$\widehat{f}(k) = \sum_j \int_{T_j} \mathrm{e}^{\mathrm{i}k^T x} P_j(x)\,\mathrm{d}x$$

Similar to semiconductor mask computations

GEOMETRIC NONUNIFORM FFT

Geometric NUFFT evaluates Fourier coefficients of soup in arbitrary dimension and codimension

Still a butterfly but
– integrate polynomials over d-dimensional source simplices
– and d-dimensional target simplices
– to apply exact transform in D dimensions

Dimensional recursion evaluates matrix element

$$F(k, d, S, P, \alpha, \sigma) = \int_S (x - \sigma)^\alpha \, \mathrm{e}^{\mathrm{i}k^T x} P(x) \, \mathrm{d}x$$

in terms of
– lower-dimensional simplex faces $F(k, d-1, \partial_j S, P, \alpha, \sigma)$
– lower-degree differentiated polynomials $F(k, d, S, \partial_j P, \alpha, \sigma)$
– lower-order moments $F(k, d, S, P, \alpha - e_j, \sigma)$

Numerically stable for large $|k|$, quadrature for small $|k|$

CONCLUSION

Solve general elliptic problems

in first-order overdetermined form with

– projected boundary integral equation

– generalized Ewald summation

– geometric nonuniform fast Fourier transforms