# First-order overdetermined systems

# for elliptic problems

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# OVERVIEW

Convert elliptic problems to first-order overdetermined form
– Control error via residuals
– Understand solvability of boundary value problem

Generalize classical ADI iteration
– Essentially optimal in simple domains
– Eliminate symmetry and commutativity restrictions

Reconstruct classical potential theory
– Employ Fourier analysis and Ewald summation
– Build fast boundary integral solvers in complex domains

# EXAMPLES OF ELLIPTIC PROBLEMS

## Cauchy-Riemann

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

## Low-frequency Maxwell

$$\nabla \times E = -\frac{i\omega}{c} H \qquad \nabla \cdot E = 4\pi\rho$$

$$\nabla \times H = \frac{i\omega}{c} E + \frac{4\pi}{c} j \qquad \nabla \cdot H = 0$$

## 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/ ...

$$\Delta u + su = f$$

## Stokes

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

## PART 1. CONVERTING TO FIRST-ORDER SYSTEMS

**Higher-order system of partial differential equations**

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

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

**Seek new solution vector** $u = (v, \partial_1 v, \ldots, \partial_d v, \ldots)^T$

**Vector** $u$ **satisfies first-order system**

$$Au = \sum_{j} A_j \partial_j u + A_0 u = f \qquad \textbf{in } \Omega$$

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

**Sparse matrices** $A_j$, $A_0$, $B$ **localize algebraic structure**

# SQUARE BUT NOT ELLIPTIC

**Robin boundary value problem for 2D Poisson equation**

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

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

**$3 \times 3$ square system**

$$Au = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ 0 & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ f \end{bmatrix}$$

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

**System not elliptic (in sense of Protter): principal part**

$$\sum_j k_j A_j = \begin{bmatrix} k_1 & 0 & 0 \\ k_2 & 0 & 0 \\ 0 & k_1 & k_2 \end{bmatrix} \qquad \text{singular for all } k!$$

# OVERDETERMINED BUT ELLIPTIC

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

**Overdetermined** $4 \times 3$ **elliptic system**

$$Au = \begin{bmatrix} \partial_1 & -1 & 0 \\ \partial_2 & 0 & -1 \\ 0 & -\partial_2 & \partial_1 \\ 0 & \partial_1 & \partial_2 \end{bmatrix} \begin{bmatrix} v \\ \partial_1 v \\ \partial_2 v \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ f \end{bmatrix}$$

**Compatibility conditions** $\Rightarrow$ **overdetermined but elliptic**

$$\sum_j k_j A_j = \begin{bmatrix} k_1 & 0 & 0 \\ k_2 & 0 & 0 \\ 0 & -k_2 & k_1 \\ 0 & k_1 & k_2 \end{bmatrix}$$

**full-rank** $\Rightarrow$ **injective for** $k \neq 0$

**Analysis: controls derivatives** $\partial_j u$ **in terms of** $u$ **and** $f$

**Computation: controls error via residuals**

# LOCAL SOLVABILITY FOR NORMAL DERIVATIVE

**Ellipticity** of first-order system

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

implies any normal part $A_n = \sum_j n_j A_j$ is left-invertible

$$A_n^\dagger = (A_n^* A_n)^{-1} A_n^* \qquad \longrightarrow \qquad A_n^\dagger A_n = I$$

Determines any **directional derivative**

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

in terms of tangential derivatives

$$A_T \partial_T u = \sum_j A_j \partial_j u - A_n \partial_n u = \sum_{ij} A_i \left(\delta_{ij} - n_i n_j\right) \partial_j u$$

and zero-order data

# SOLVE BOUNDARY VALUE PROBLEM

**With full tangential data plus elliptic system can integrate**

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

**inward to solve boundary value problem**

**Boundary conditions**

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

**determine local projection** $B^* B u = B^* g$ **on the boundary**

**Boundary value problem constrains** $(I - B^* B)u$ **on boundary**

**Contrast: hyperbolic systems blind** $\perp$ **characteristics**

# PART 2. ALTERNATING DIRECTION IMPLICIT

**Separable second-order equations in rectangles**

$$-\Delta u = Au + Bu = -\partial_1^2 u - \partial_2^2 u = f$$

**efficiently solved by essentially optimal ADI iteration**

$$(h + A)(h + B)u^{m+1} = (h - A)(h - B)u^m + 2f$$

**when $A$ and $B$ are commuting positive Hermitian operators**

**Fast damping over geometric range**

$$a \geq 0 \quad \rightarrow \quad \left|\frac{h-a}{h+a}\right| \leq 1$$

$$\frac{1}{2} \leq \frac{b}{h} \leq 2 \quad \rightarrow \quad \left|\frac{h-b}{h+b}\right| \leq \frac{1}{3}$$

**implies $O(\epsilon)$ error reduction in $O(\log N \log \epsilon)$ sweeps**

## ADI FOR POISSON SYSTEM

**Choose arbitrary sweep direction** $n$ **and normalize**

$$\sum_j A_j \partial_j u = \sum_{ij} A_i (n_i n_j + \delta ij - n_i n_j) \partial_j u = A_n \partial_n u + A_T \partial_T u$$

**Left-invert** $A_n$ **by ellipticity and damp on scale** $1/h$

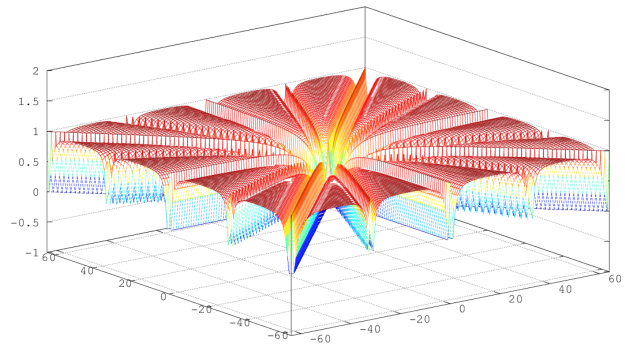
$$h u^{m+1} + \partial_n u^{m+1} + B_0 u^{m+1} = h u^m - B_T \partial_T u^m + A_n^\dagger f$$

**Error mode** $\mathrm{e}^{\mathrm{i} k^T x}$ **damped by matrix symbol**

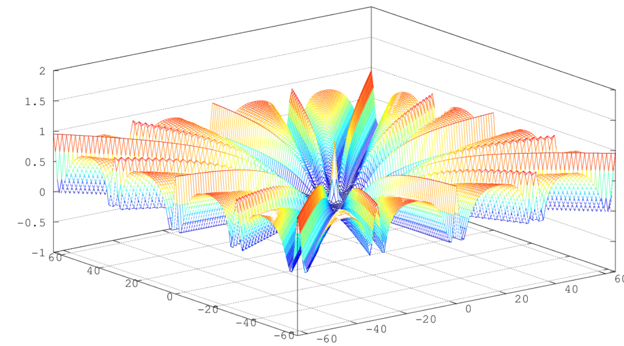
$$\rho(k) = \prod_h \prod_n \left(h + \mathrm{i} k_n + B_0\right)^{-1} \left(h - \mathrm{i} k_T B_T\right)$$

**Spectral radius** $0.9^M$ **with** $M = O(\log N)$ **sweeps**

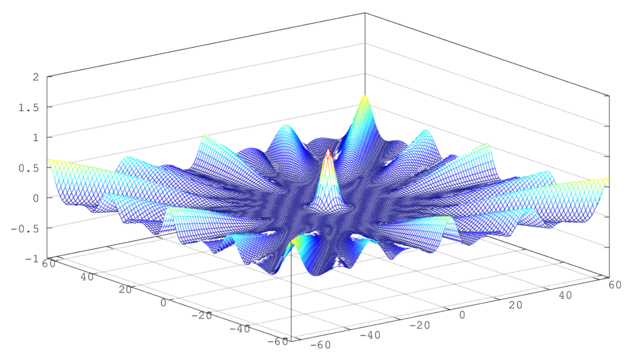
# SPECTRAL RADIUS FOR POISSON SYSTEM



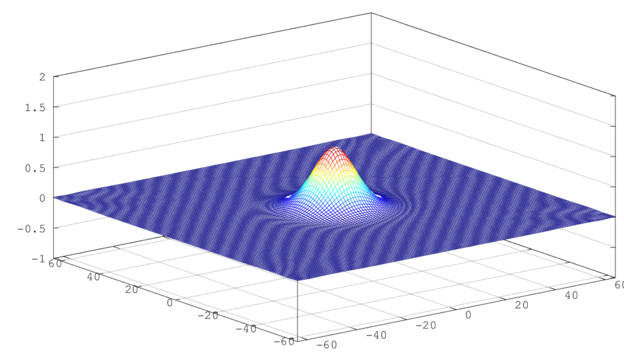
$h = 1$



$h = 4$



$h = 16$



$h = 64$

# BIG PICTURE

**Given operators $A$ and $B$ with**
**cheap resolvents $(hI - A)^{-1}$ and $(hI - B)^{-1}$**
**find an efficient scheme for the solution of**

$$(A + B)u = f$$

**Underlies many computational problems where either**
**– $A$ is sparse and $B$ is low-rank or**
**– $A$ and $B$ are both sparse but in different bases or**
**– fast schemes deliver $A^{-1}$ and $B^{-1}$ or . . .**

**Challenging when $A$ and $B$ don't commute**

**Solution very unlikely in this generality**

# ADI SQUARED

$A$ and $B$ may not be invertible (or even square), so square

$$(A+B)^*(A+B)u = (A+B)^* f = g$$

Solve corresponding heat equation

$$\partial_t u = -(A+B)^*(A+B)u + g$$

to get $u$ as $t \to \infty$

Discretize time and split

$$(I + hA^*A)\,(I + hB^*B)\,u^{m+1} = (I - h(A^*B + B^*A))\,u^m + g$$

to get $u + O(h)$ as $t \to \infty$

Alternate directions for symmetric symbol

$$\rho = (I + hB^*B)^{-1}\,(I + hA^*A)^{-1}\,(I - 2h(A^*B + B^*A))\,(I + hA^*A)^{-1}\,(I + hB^*B)^{-1}$$

Similar with more operators $A$, $B$, $C$, $D$, . . .

# POISSON/YUKAWA/HELMHOLTZ

**Second-order equation $\to$ overdetermined first-order system**

$$\Delta u + su = f \quad \to \quad (A + B + C)u = A_1\partial_1 u + A_2\partial_2 u + A_0 u = f$$

**with high-frequency zero-order operator $C = O(s)$**

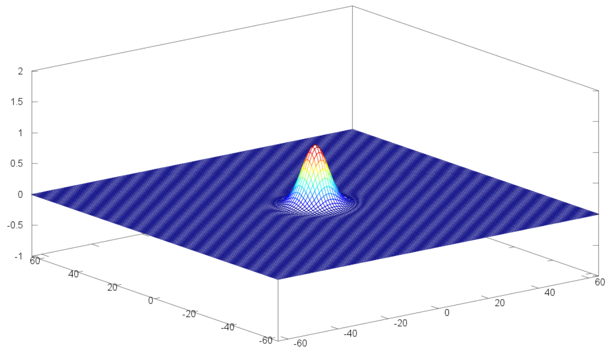
**Fourier mode $(k_1, k_2)$ of error damped with symbol**

$$\begin{aligned}
\rho &= (I + hC^*C)^{-1}(I + hB^*B)^{-1}(I + hA^*A)^{-1}\cdot \\
&\quad (I - 2h(A^*B + A^*C + B^*A + B^*C + C^*A + C^*B))\cdot \\
&\quad (I + hA^*A)^{-1}(I + hB^*B)^{-1}(I + hC^*C)^{-1} \\
\widehat{\rho} &= \frac{1}{(1 + hk_1^2)^2(1 + hk_2^2)^2(1 + hs^2)^2}\begin{bmatrix} 1 & ih(s+1)bk_1 & ih(s+1)bk_2 \\ -ih(s+1)bk_1 & b^2 & 0 \\ -ih(s+1)bk_2 & 0 & b^2 \end{bmatrix}
\end{aligned}$$

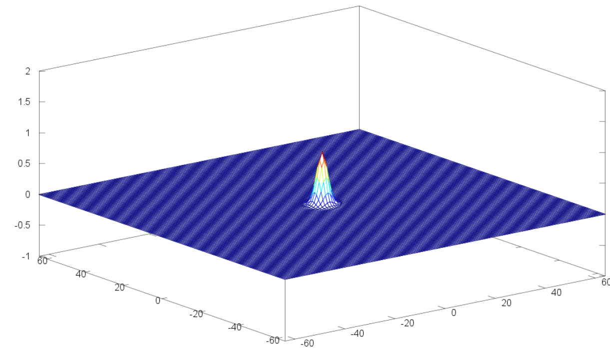
**where $b = (1 + hs^2)/(1 + h)$**

**Eigenvalues of $\widehat{\rho}$ bounded by 1 and controlled by $h$ for all real $s$**

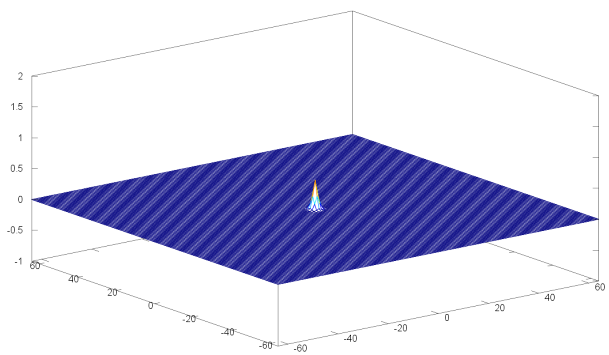
# SPECTRAL RADIUS FOR HELMHOLTZ WITH $s = 1$



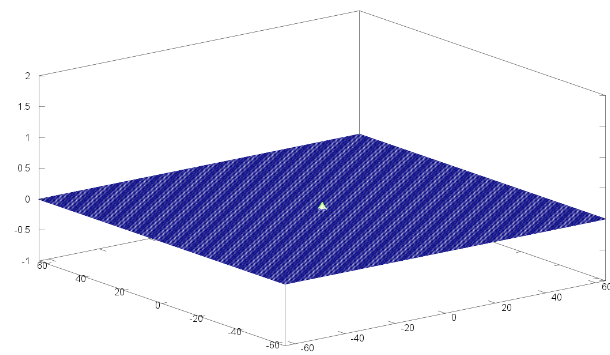

$h = 1/64$




$h = 1/16$




$h = 1/4$




$h = 1$

# PART 3. POTENTIAL THEORY

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

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

**Gauss theorem**

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

**and general jump condition $\delta_x \to \frac{1}{2}\delta_\gamma$ as $x \to \gamma \in \Gamma$**
**implies universal boundary integral equation**

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

**with normal part $A_n(\gamma) = \sum n_j(\gamma) A_j$ and volume potential**

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

## PROJECTED INTEGRAL EQUATION

**Project out boundary condition** $Bu = g$ **with** $P(\gamma) = I - B^*B$

**Solve well-conditioned 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**

$$\rho(\gamma) = P(\gamma)\Omega f(\gamma) - P(\gamma)\Gamma B^* g(\gamma)$$

**and layer potential**

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

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

$$u(x) = \Omega f(x) + \Gamma u(x) \qquad \text{in}\, \Omega$$

**Need algorithms for computing** $\rho$**,** $\mu$ **and** $u$

# PERIODIC FUNDAMENTAL SOLUTION

**Fourier series in cube $Q \supset \Gamma$ gives fundamental matrix**

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

**where $s = a^* a$ is positive definite Hermitian matrix and**

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

**Diverges badly since $s(k)^{-1} a^*(k) = O(|k|^{-1})$**

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

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

# GENERALIZED EWALD SUMMATION

**Fundamental matrix is smooth rapidly-converging series**

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

**plus local asymptotic series for correction**

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

**with local differential operators $A^*$ and $S = A^* A$**

**Implies local corrections and Ewald formulas**
**(with special function kernels) for Laplace, Stokes, . . .**

**Convergence independent of data smoothness**
**yields volume and layer potentials**

**Splits integral equation into sparse plus low-rank $A + B$**

# LOCAL CORRECTION BY GAUSS

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

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

**Geometry in second-order derivatives**

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

**Volume potential of discontinuous function $f\omega$ splits**

$$\Omega f(x) = \int_\Omega G_x(y) f(y) \,\mathsf{d}y = Q(f\omega) = Q_\tau(f\omega) + L_\tau(f\omega)$$

**Local correction $L_\tau$ satisfies product rule**

$$L_\tau(f\omega)(x) = \tau \left( (A^* f(x))\omega(x) - \sum_j A_j^* f(x) n_j(x) \delta_\Gamma(x) \right) + O(\tau^2)$$

# SPECTRAL INTEGRAL EQUATION

**Fourier series for fundamental matrix separates variables**

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

**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 filtered inverse of elliptic operator in Fourier space
– $M$ evaluates and projects Fourier series on $\Gamma$

**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**

$$(TMR)_{kq} = \int_\Gamma A_n(\sigma) P(\sigma) \mathrm{e}^{-\mathrm{i}(k-q)^T \sigma}\, \mathrm{d}\sigma\, \mathrm{e}^{-\tau s(q)} s(q)^{-1} a^*(q)$$

# NONUNIFORM FAST FOURIER TRANSFORM

Standard FFT works on uniform equidistant mesh

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

Integral operator and density $\rho$ require Fourier coefficients of **soup** of piecewise polynomials $P_j$ on simplices $T_j$ (points, segments, triangles, tetrahedra, . . . )

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

# GEOMETRIC NONUNIFORM FFT

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

Follow model of NUFFT for point sources, but
– integrate polynomials over $d$-dimensional source simplices
– and $d$-dimensional target simplices
– to apply exact transform in $D$ dimensions

Dimensional recursion evaluates Galerkin 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 $F(k, d, S, P, \alpha - e_j, \sigma)$

## CONCLUSION

**Solve general elliptic problems**
**in first-order overdetermined form**
**with**
**– fast iterations in simple domains**
**or**
**– projected boundary integral equation**
**– generalized Ewald summation**
**– geometric nonuniform fast Fourier transforms**