APPLICATIONS OF FMM TO MECHANICS PROBLEMS

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PRESENTATION OUTLINE

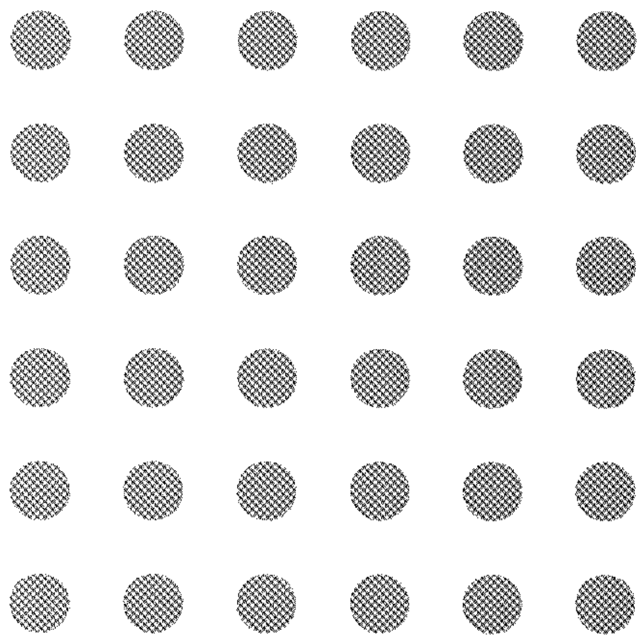
- Periodic problems (jointly with J. R. Overfelt)
- Solid composites and stokesian emulsions (jointly with Y. Fu and J. R. Overfelt)
- Boundary algebraic equations (jointly with P.-G. Martinsson)

Periodic Problems
(GJR & Overfelt, 2004)

- Motivation
- Periodic FMM
- Integral equation

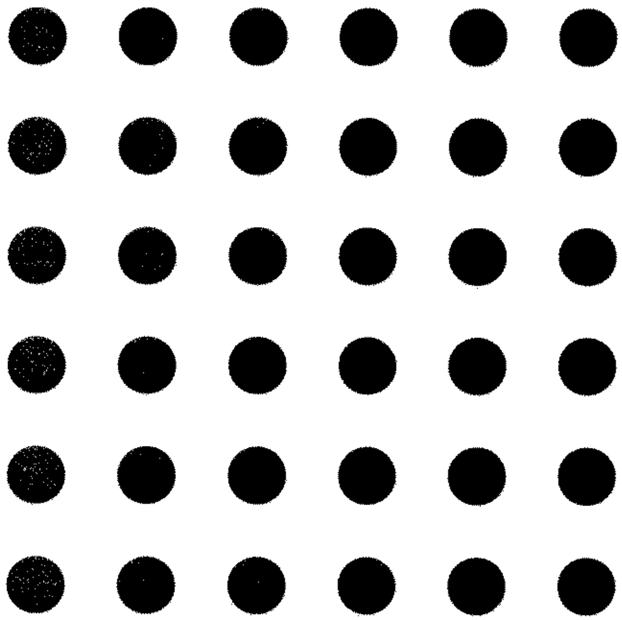
Periodic array of dipoles

(Rayleigh's Problem)



$$e = \nabla \varphi = \sum_{m \neq 0} \frac{1}{\left(m_1^2 + m_2^2 + m_3^2\right)^{\frac{3}{2}}}$$

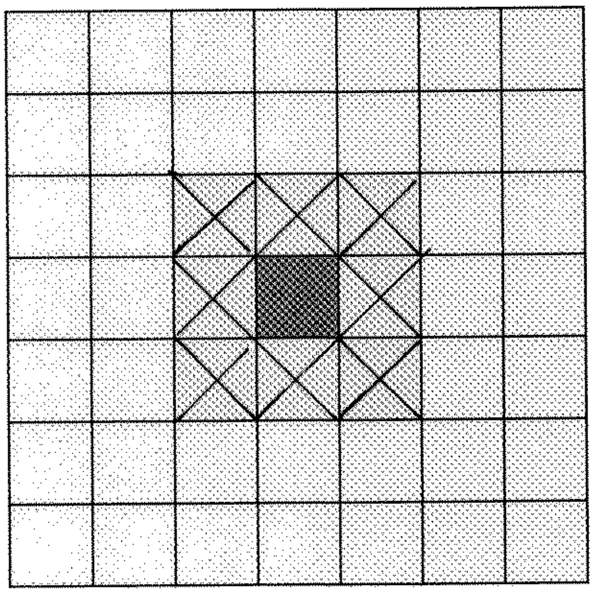
Periodic array of charges without neutrality



$$\varphi = \sum_{m \neq 0} \frac{1}{\sqrt{m_1^2 + m_2^2 + m_3^2}}$$

$$\sum_{m \neq 0} \frac{1}{\left(m_1^2 + m_2^2 + m_3^2\right)^{3/2+\varepsilon}} \sim \int_1^{\infty} r^{-3-2\varepsilon} r^2 dr \sim r^{-2\varepsilon}\Big|_1^{\infty}$$

Periodic FMM



- Use regular translations within the red and blue domains
- Use lattice sums for the translations from yellow to red
- Most of the FMM machinery is preserved
- Lattice sum operators can be pre-computed

Brief History

- Rayleigh (1892): dipole-dipole interactions
- Ewald (1921): evaluation of lattice sums
- Korringa (1973), O'Brien (1979), Bonnecaze and Brady (1991): convergent integral equations
- Levine (1966) Zuzovsky & Brenner (1977), McPhedran et al. (1978): analysis of basic lattices
- Greengard and Rokhlin (1987): FMM and 2-D periodic FMM
- Schmidt and Lee (1991) 3-D periodic FMM
- Greengard and Helsing (1991): Periodic FMM for integral equations
- Sangani *et al.* and Zinchenko *et al.*: Fast methods for integral equations with periodic kernels (1990's …)

Integral Equation in Ω

$$\phi(x) = \frac{1}{4\pi k^0} \int_{\partial\Omega^* \cup \partial\Omega} n(y) \cdot \left[j(y) \frac{1}{|x-y|} + k^0 \phi(y) \nabla \frac{1}{|x-y|} \right] \mathrm{d}y$$

$$\int_{\partial\Omega^*} n(y) \cdot \left[j(y) \frac{1}{|x-y|} + k^0 \phi(y) \nabla \frac{1}{|x-y|} \right] \mathrm{d}y = \int_{\Omega} \tau(y) \cdot \nabla \frac{1}{|x-y|} \mathrm{d}y$$

$$\bar{I}(x) = \frac{1}{4\pi k^0} \int_{\partial\Omega} n(y) \cdot \left[\bar{j} \frac{1}{|x-y|} + k^0 \bar{\phi}(y) \nabla \frac{1}{|x-y|} \right] \mathrm{d}y$$

$$\tilde{I}(x) = \frac{1}{4\pi k^0} \int_{\partial\Omega} n(y) \cdot \left[\tilde{j}(y) \frac{1}{|x-y|} + k^0 \tilde{\phi}(y) \nabla \frac{1}{|x-y|} \right] \mathrm{d}y$$

Integrals $\bar{I}$ and $\tilde{I}$

$$\bar{I}(x) = \frac{1}{4\pi k^0} \int_{\partial\Omega} n(y) \cdot \left[\bar{j} \frac{1}{|x-y|} + k^0 \bar{\phi}(y) \nabla \frac{1}{|x-y|} \right] \mathrm{d}y$$

$$= \bar{\phi}(x) - \frac{1}{4\pi k^0} \int_{\Omega} \bar{\tau}(y) \cdot \nabla \frac{1}{|x-y|} \mathrm{d}y$$

$$\nabla \tilde{I}(x) \to 0 \quad \text{as} \quad D(\Omega) \to \infty$$

Convergent Integral Equation

$$\phi(x) = \bar{\phi}(x) + \tilde{I}(x) + \frac{1}{4\pi k^0} \int_{\Omega} \tilde{\tau}(y) \cdot \nabla \frac{1}{|x-y|} \mathrm{d}y$$

$$e(x) = e^0 + \underline{\nabla \tilde{I}(x)} - \frac{1}{4\pi k^0} \int_{\Omega \setminus \Omega^{\epsilon}(x)} \tilde{\tau}(y) \cdot \nabla\nabla \frac{1}{|x-y|} \mathrm{d}y - \frac{1}{3k^0} \bar{\tau}$$

General Case: Boundary and Macroscopic Fluxes

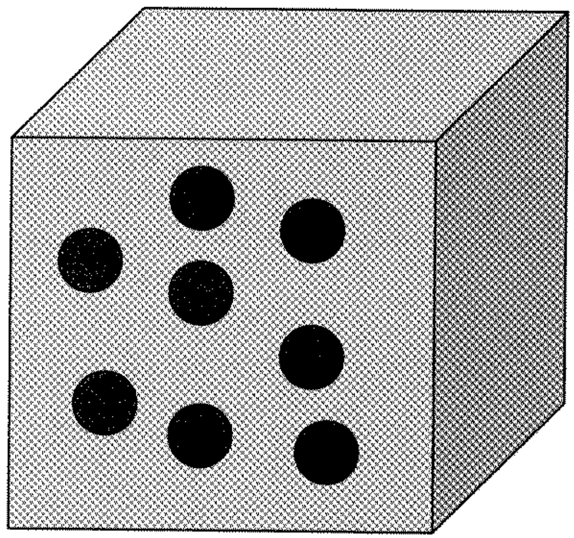
$\rho(x) = \tilde{\rho}(x) + <\rho>$

$j_0 + \frac{1}{3} <\rho> x - true\ \ macroscopic\ \ flux$

$j_0 + \frac{1}{3} <\rho> x + <\tilde{\rho} z> -\ \ apparentat\ \ macroscopic\ \ flux$

$$\int_\omega \nabla \cdot j(z) \mathrm{d}z = \int_\omega \rho(z) \mathrm{d}z$$
$$\int_\omega z \nabla \cdot j(z) \mathrm{d}z = \int_\omega z \rho(z) \mathrm{d}z$$

Model Conduction Problem



Ω^* - particle domain

Ω^0 - matrix domain

$\partial\Omega^*$ - particle boundary

$\partial\Omega$ - specimen boundary

κ^* - particle conductivity

κ^0 - matrix conductivity

Linearized Elasticity and Hydrodynamics
(with Y. Fu and J.R. Overfelt)

- Types of problems
- Connections with FMM
- Open issues

Governing Equations of Elasticity

$$(\mu + \lambda) u_{j,ij} + \mu u_{i,jj} + b_i = 0 \qquad \text{volume}$$

$$t_i = n_j \sigma_{ij} = n_j (\lambda u_{k,k} \delta_{ij} + \mu u_{i,j} + \mu u_{j,i})$$

$$[t_i] = 0 \qquad [u_i] = 0 \qquad \text{interfaces}$$

$$u_i(x) = \gamma_{ij}^0 x_j + \hat{u}_i(x) \qquad \text{boundary}$$

Stokes Equations

$$-p_{,i}+\mu u_{i,jj}+b_i=0$$

$$u_{i,i}=0$$

$$t_i=n_j(-p\delta_{ij}+\mu u_{i,j}+\mu u_{j,i})$$

$$[t_i]=\nu n_i\kappa \qquad [u_i]=0$$

$$u_i(x)=\gamma_{ij}^0 x_j+\hat{u}_i(x) \qquad p(x)=b_j^0 x_j+\hat{p}(x)$$

Connection to FMM

(Fu et al., 1998, Nishimura et al., 1998)

$$G_{ij}(x-y) = a\delta_{ij}\,|x-y|^{-1} + b\partial_i\partial_j\,|x-y|$$

$$|x-y| = \frac{(x-y)(x-y)}{|x-y|} = x^2\frac{1}{|x-y|} - 2x\frac{y}{|x-y|} + \frac{y^2}{|x-y|}$$

$$\partial_i\partial_j\,|x-y| = \frac{\partial}{\partial x_j}\frac{x_i - y_i}{|x-y|} = \frac{1}{|x-y|} - \frac{\partial}{\partial x_j}\frac{y_i}{|x-y|}$$

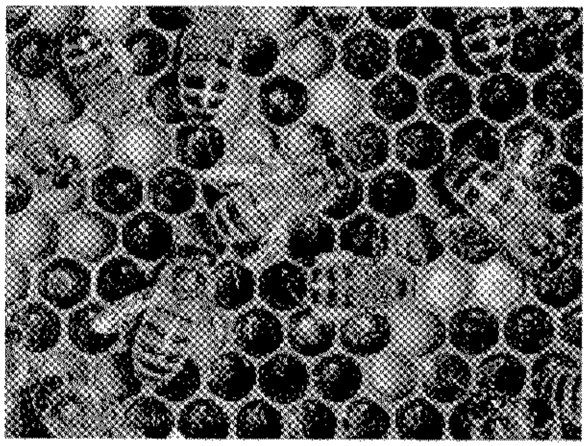
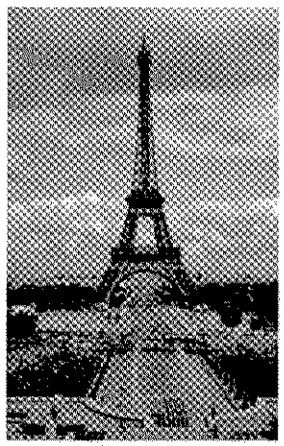
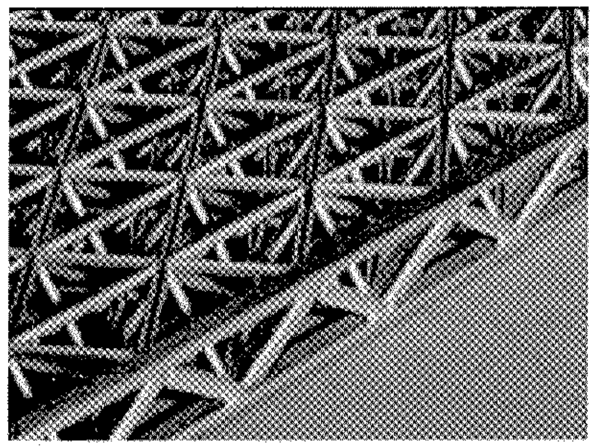
$$\sum_{\alpha=1}^{N}\partial_i\partial_j\,|x-y^\alpha|\,q_i^\alpha = x_i\frac{\partial}{\partial x_j}\sum_{\alpha=1}^{N}\frac{q_i^\alpha}{|x-y^\alpha|} - \frac{\partial}{\partial x_j}\sum_{\alpha=1}^{N}\frac{y_i q_i^\alpha}{|x-y^\alpha|}$$

Open Issues

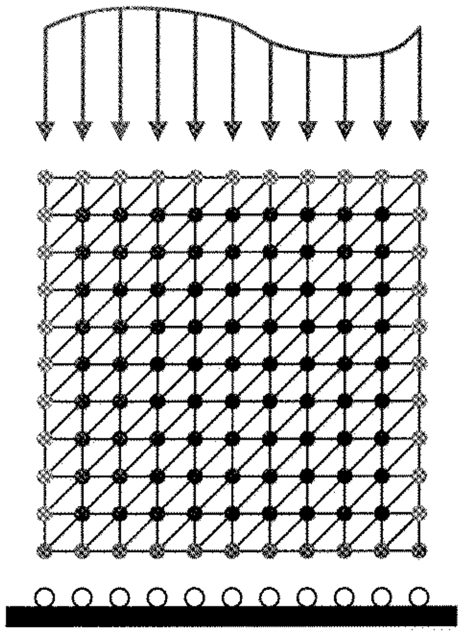
- Approximation schemes
- Interpretation of results
- Adaptivity and error control

Boundary Algebraic Equations (BAE)

joint work with Per-Gunnar Martinsson (Yale)

Model Conduction Problem



$\Omega = \Omega_{\rm i} \cup \Gamma_{\rm D} \cup \Gamma_{\rm N}$,

$\Omega_{\rm i}$ are the interior nodes,

$\Gamma_{\rm D}$ is the Dirichlet boundary,

$\Gamma_{\rm N}$ is the Neumann boundary.

$$\begin{cases} \mathfrak{A}\mathfrak{u}(m) = 0, & \text{for all } m \in \Omega_{\rm i}, \\ \mathfrak{u}(m) = \mathfrak{g}(m), & \text{for all } m \in \Gamma_{\rm D}, \\ \partial_\nu \mathfrak{u}(m) = \mathfrak{h}(m), & \text{for all } m \in \Gamma_{\rm N}, \end{cases}$$

REVIEW OF CONTINUOUS BIE

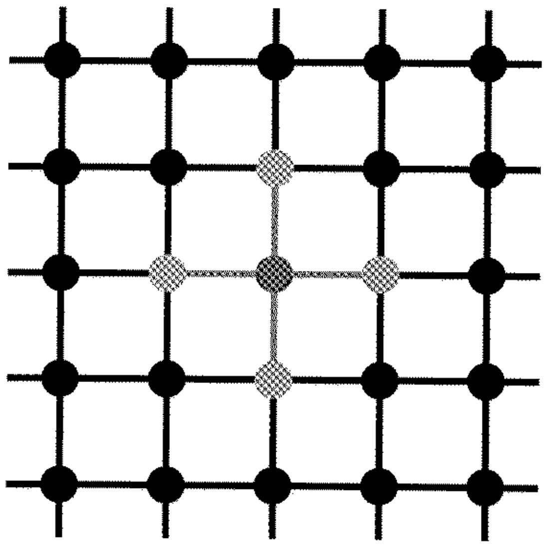
$$\begin{cases} -\Delta u = 0, & \text{on } \Omega, \\ u = g, & \text{on } \Gamma_D, \\ \partial_\nu u = h, & \text{on } \Gamma_N \end{cases}$$

Use the reciprocity theorem:

$$\frac{1}{2}u(x) + \int_\Gamma \frac{\partial G(x-y)}{\partial \nu_y} u(y)\, dy = \int_\Gamma G(x-y) \frac{\partial u(y)}{\partial \nu_y}\, dy$$

where $G(x) = -(2\pi)^{-1} \log |x|$.

Simple Square Lattice



$$[\mathfrak{A}\mathfrak{u}](m) = -\,\mathfrak{u}(m_1-1,m_2) + 2\mathfrak{u}(m_1,m_2) - \mathfrak{u}(m_1+1,m_2)$$
$$-\,\mathfrak{u}(m_1,m_2-1) + 2\mathfrak{u}(m_1,m_2) - \mathfrak{u}(m_1,m_2+1).$$

Fundamental Solution

$$\tilde{\mathfrak{u}}(\xi) = [\mathfrak{F}\mathfrak{u}](\xi) = \sum_{m \in \mathbb{Z}^2} e^{\mathbf{i} m \cdot \xi} \mathfrak{u}(m), \qquad \xi \in (-\pi, \pi)^2.$$

$$[\mathfrak{A}\mathfrak{u}](m) = \mathfrak{f}(m) \;\; \forall\, m \in \mathbb{Z}^2, \qquad \Rightarrow \qquad \sigma(\xi)\tilde{\mathfrak{u}}(\xi) = \tilde{\mathfrak{f}}(\xi) \;\; \forall\, \xi \in (-\pi, \pi)^2,$$

$$\sigma(\xi) = 4 \sin^2 \frac{\xi_1}{2} + 4 \sin^2 \frac{\xi_2}{2}.$$

$$\mathfrak{G}(m) := \left[\mathfrak{F}^{-1} \sigma^{-1}\right](m) = \frac{1}{(2\pi)^2} \int_{(-\pi,\pi)^2} e^{-\mathbf{i} m \cdot \xi} \frac{1}{\sigma(\xi)}\, d\xi.$$

CORRECTION

$|\xi|^{-2}$ is not integrable in two dimensions

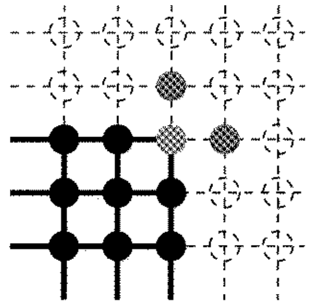
$$\sum_m \mathfrak{f}(m) = 0.$$

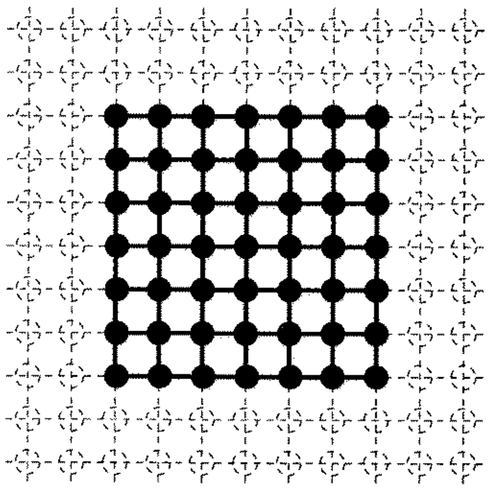
$$\mathfrak{G}(m) := \frac{1}{(2\pi)^2} \int_{(-\pi,\pi)^2} \frac{e^{-\mathbf{i}m\cdot\xi} - 1}{\sigma(\xi)} \, d\xi.$$

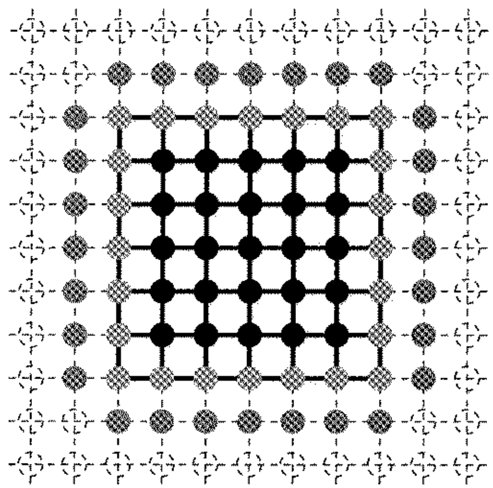
THE DISCRETE DOUBLE LAYER KERNEL $\partial_{\nu_n}\mathfrak{G}(m-n)$

∂_ν is an external difference operator: given a boundary node n, let $\mathbb{D}_n \subset \Omega^c$ be the set of nodes that connect to n, then

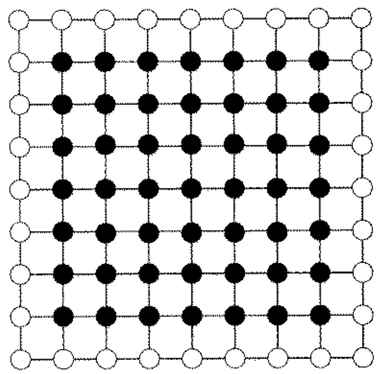
$$[\partial_\nu \psi](n) = \sum_{k\in\mathbb{D}_n} (\psi(k) - \psi(n))\,.$$







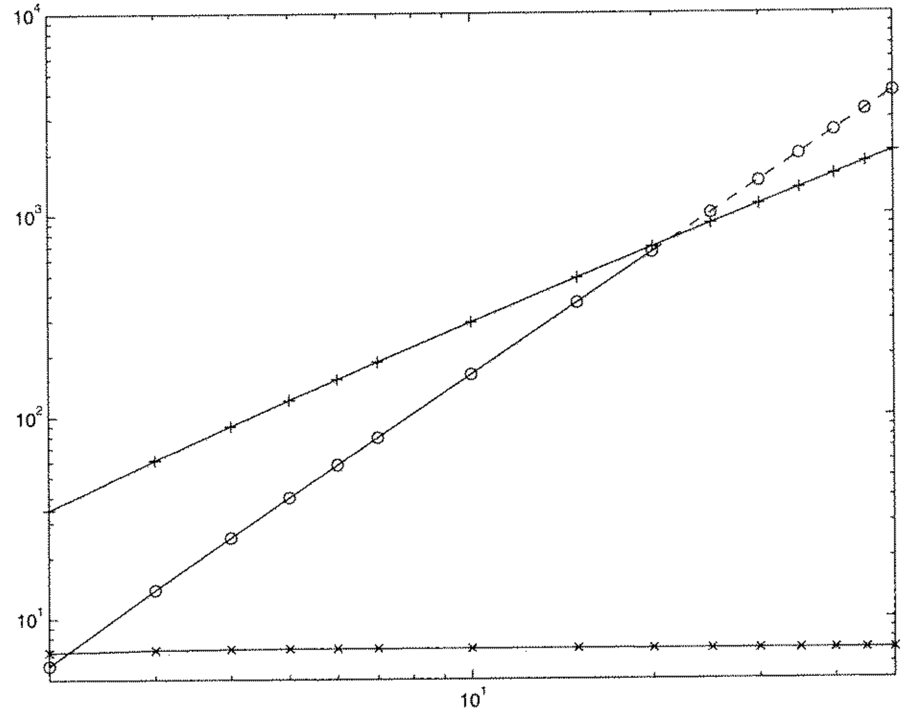
Example 1: A square domain



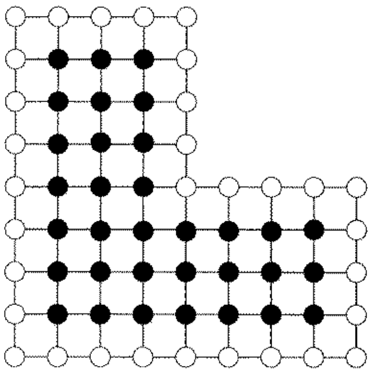
o : cond(K) $\sim$ $1.6n^2$

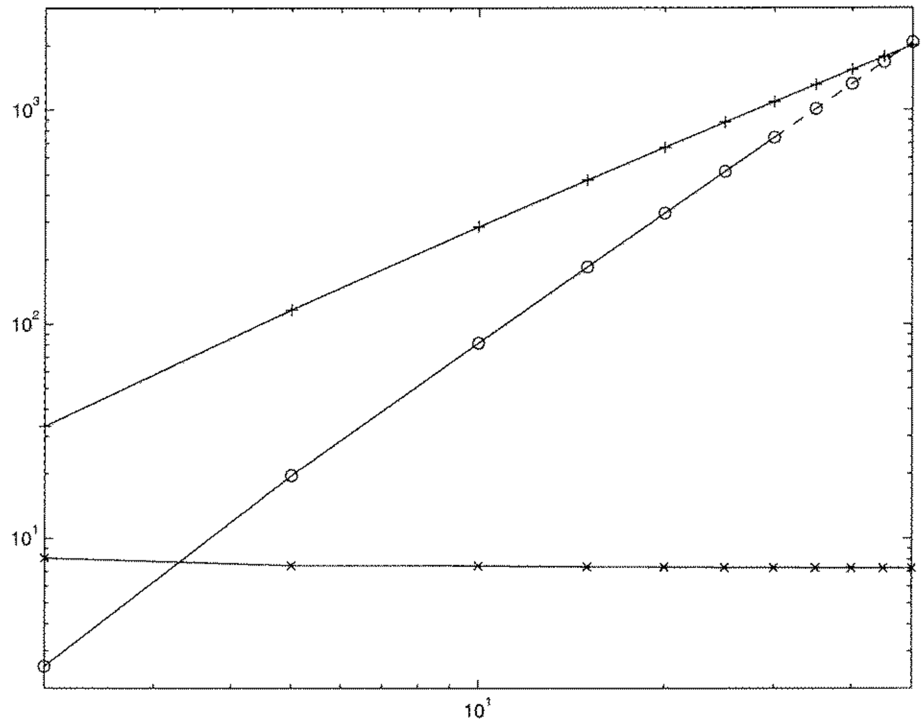
+ : cond(K_{S}) $\sim$ $40n$

x : cond(K_{D}) $\sim$ 7.0



Example 2: An L-shaped domain



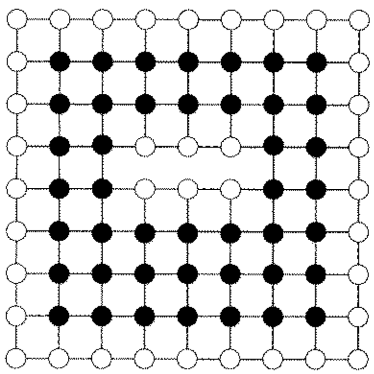


o : $\text{cond}(K) \sim 0.83n^2$

+ : $\text{cond}(K_\text{S}) \sim 40n$

x : $\text{cond}(K_\text{D}) \sim 7.3$ (!)

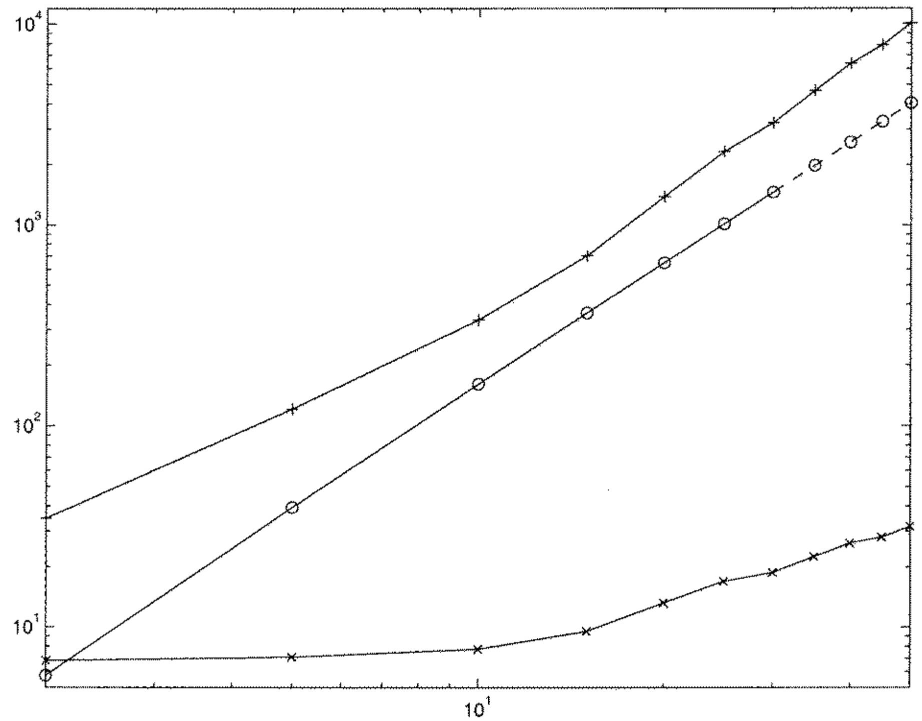
EXAMPLE 3: A DOMAIN WITH A CUT



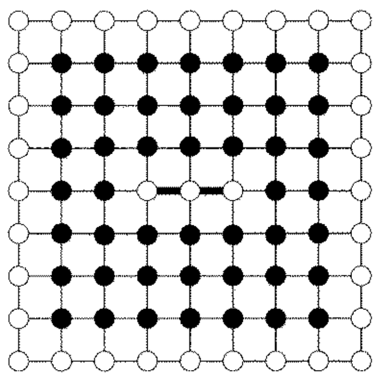
o : $\mathrm{cond}(K) \sim 1.6n^2$

$+$: $\mathrm{cond}(K_{\mathrm{S}}) \sim 4n^2$

x : $\mathrm{cond}(K_{\mathrm{D}}) \sim 0.63n$



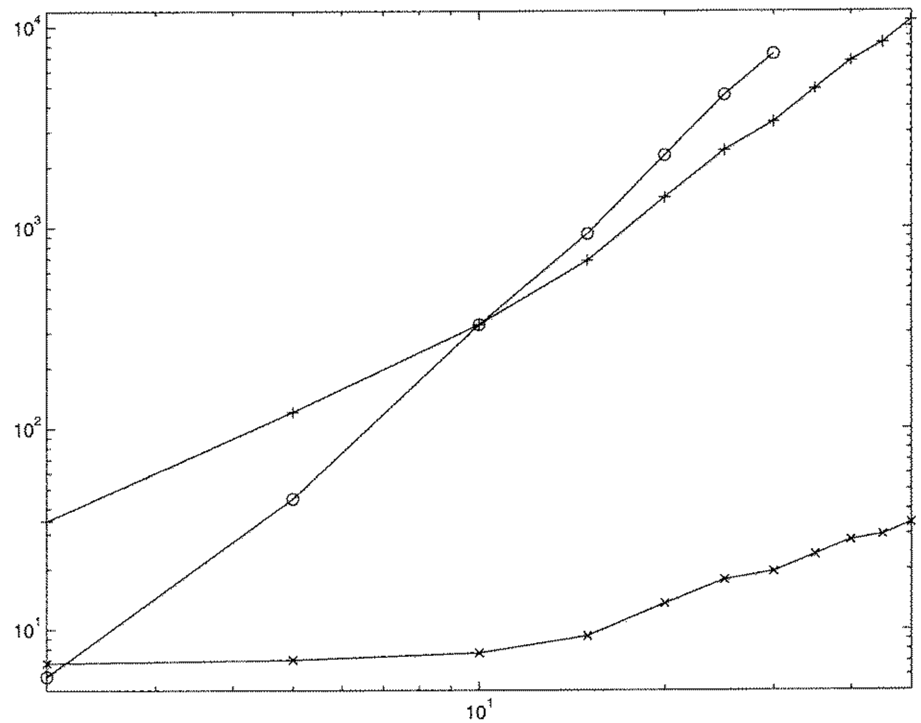
Example 4: A domain with a super-conductor



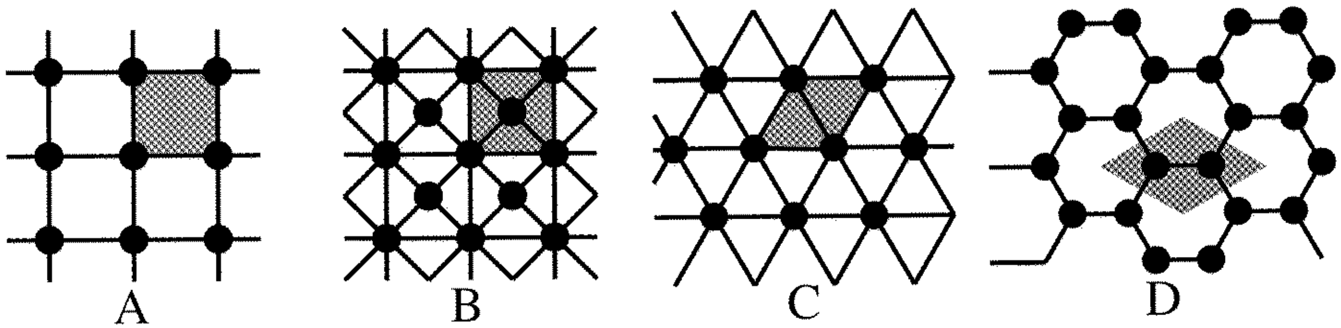
o : $\text{cond}(K) \sim 0.28n^3$

+ : $\text{cond}(K_{\text{S}}) \sim 4.2n^2$

x : $\text{cond}(K_{\text{D}}) \sim 0.68n$



GENERAL LATTICE GEOMETRIES



Any non-degenerate lattice geometry can be handled.

The treatment of **multi-atomic** lattices (such as B and D) is significantly more difficult than mono-atomic lattices.

- The symbol $\sigma(\xi)$ is a matrix.
- The governing equations may be poorly conditioned.
- The lattice equations may be degenerate.