# Thesis: Numerical Computations with Fundamental Solutions

## Respondent: Per Sundqvist

## Opponent: Alison Ramage

Dept of Mathematics
University of Strathclyde
Glasgow, Scotland

UNIVERSITY OF STRATHCLYDE

# List of papers

- **Paper I:** H. Brandén and P. Sundqvist
  Preconditioners Based on Fundamental Solutions
  submitted to *BIT*.

- **Paper II:** H. Brandén and P. Sundqvist
  An Algorithm for Computing Fundamental Solutions of Difference Operators
  Numerical Algorithms 36 (4): 331-343 (2004).

- **Paper III:** H. Brandén, S. Holmgren and P. Sundqvist
  Discrete Fundamental Solution Preconditioning for Hyperbolic Systems of PDE
  submitted to *SIAM Journal on Scientific Computing*.

# List of papers (cont.)

- **Paper IV:** P. Sundqvist
  Boundary Summation Equations
  submitted to *SIAM Journal on Scientific Computing*.

- **Paper V:** P. Sundqvist and S. Holmgren
  Navier-Stokes Equations for Low Mach Number Flows Solved by Boundary Summation
  submitted to *Numerical Methods for Partial Differential Equations*.

# Fundamental Solutions of PDEs (1)

- differential equation

$$Pu = f \tag{1}$$

differential operator $P \equiv a_0 D^p + \ldots + a_p$

- if $f$ is sufficiently well-behaved:

$$f(x) = \int_{-\infty}^{\infty} \delta(x-y) f(y)\, dy \tag{2}$$

$f(x)$ is the superposition of $\infty$-many $\delta$ functions

# Fundamental Solutions of PDEs (2)

- linear superposition:

  if $f = \alpha_1 f_1 + \alpha_2 f_2$, solution is $u = \alpha_1 u_1 + \alpha_2 u_2$

  $u_i$ solves $Pu_i = f_i$

- extend to continuous integral (2):

  expect solution to be sum (integral) of solutions of

  $$Pu(x) = \delta(x - y) \tag{3}$$

- rename solution of (3): $E(x; y)$ for parameter $y$

# Fundamental Solutions of PDEs (3)

- solution of (1) is

$$u(x) = \int_{-\infty}^{\infty} E(x;y) f(y)\, dy.$$

  where

$$PE(x;y) = \delta(x-y)$$

- $E(x;y)$ is a fundamental solution (FS) for the operator $P$
- Green's function: particular FS which satisfies linear homogeneous boundary conditions associated with the differential equation

# Paper I

Preconditioners Based on Fundamental Solutions
(Brandén and Sundqvist)

- convolution:

$$f * g = \int_{-\infty}^{\infty} f(t)g(x-t)\,dt$$

- fundamental solution: $Pu = f, \quad PE = \delta$

- $P(E * f) = PE * f = \delta * f = f \Rightarrow$

$$E * Pu = E * f = u$$

left convolution with $E \equiv$ inverting $P$

# Preconditioner

- preconditioned problem:

$$\begin{aligned} KPu &= Kf, & & \text{differential equation} \\ B_k u &= g_k, \qquad k = 1, \ldots, q & & \text{boundary conditions} \end{aligned}$$

- preconditioner:

$$Ku = \int_\Omega E(x-y)u(y)\,dy, \qquad x \in \Omega$$

approximate inverse

- assume fundamental solution $E$ is known

# Effect of operator $KP$

- Example: 1D problem

$$P \equiv D^2, \quad \Omega = [0,1]$$

- weak fundamental solution $E(x) = \begin{cases} x, & x \geq 0 \\ 0, & x < 0 \end{cases}$

- for suitable $f$, solution of $D^2 u = f$ is

$$u(x) = (E * f)(x) = \int_{-\infty}^{\infty} E(x-y) f(y)\, dy$$

- preconditioner

$$(Ku)(x) = \int_0^1 E(x-y) u(y)\, dy$$

# 1D example (cont.)

$$
\begin{aligned}
(KPu)(x) \quad - \quad & u(x) = (KD^2u)(x) - u(x) \\
= \quad & \int_0^1 \left[E(x-y)(D^2u)(y) - \delta(x-y)u(y)\right] dy \\
= \quad & \int_0^1 \left[E(x-y)(D^2u)(y) - D^2(E(x-y))u(y)\right] dy \\
= \quad & \int_{\delta\Omega} J(E(x-y), u(y))\, ds \qquad \text{Green's Theorem}
\end{aligned}
$$

$$J(u, v) = vu' - uv'$$

order $p = 1$: $KP$ is no longer a differential operator
order $p > 1$: order of $KP$ reduced to $p - 1$

RHS involves only derivatives on the boundary of $\Omega$

# First order equations

- first order operator, derivative-free boundary condition

$$P = |b|\frac{\partial}{\partial x_1} + a \qquad E(x) = (c + H(x_1)/|b|)e^{-ax_1/|b|}\delta(x_2, \ldots, x_d$$

- fixed point iteration $\quad u_{n+1} = F(u_n), \quad n = 0, 1, \ldots$

  homogeneous: $\quad F(u) = u - \phi_\epsilon KPu - (1 - \phi_\epsilon)u$

  inhomogeneous: $\quad F(u) = u - \phi_\epsilon(KPu - Kf) - (1 - \phi_\epsilon)(u -$

- $F$ is a contraction mapping
- fixed point iteration converges

# Discretised problem

- finite differences, discretisation parameter $h$

$$\begin{aligned} P_h u_h &= f_h, \qquad i \in \Omega_h \\ B_{k,h} u_h &= g_{k,h} \end{aligned}$$

- preconditioner:

$$(K_h u_h)_i = \sum_{j \in \Omega_h} E(ih - jh)(u_h)_j h_1 \dots h_d, \quad i \in \Omega_h$$

- iteration operator:

$$F_h u_h = \begin{cases} u_h - K_h P_h u_h + K_h f_h, & i \in \Omega_h \\ u_h - B_{k,h} u_h + g_h, & i \in \Gamma_{k,h} \end{cases}$$

- is analysis of $KP$ relevant to $K_h P_h$?

# Implementation

- $E$ may be undefined at some points
- compute $\tilde{E}_h$ by sampling
  - sample $E$ away from problem points
  - solve $P_h \tilde{E}_h = \delta_h$ near singularities or discontinuities
- apply $K_h$ via fast Fourier transforms: $\widehat{E * u} = \hat{E}\hat{u}$
- application to non-uniform grids?

# Experiments

- example: 2D convection equation
  - comparison using convection and convection-diffusion fundamental solutions
  - with convection-diffusion $\tilde{E}_h$, grid-independent convergence observed
- example: 2D convection-diffusion equation
  - iteration count independent of viscosity for fixed boundary resolution
  - iteration count not grid independent for fixed viscosity

# Paper II

An Algorithm for Computing Fundamental Solutions of Difference Operators
(Brandén and Sundqvist)

- partial difference operator with constant coefficients

$$(Pu)_j = \sum_{k \in Z^d} B_k u_{j-k}, \quad j \in Z^d$$

- fundamental solution: matrix function $E$ such that

$$B * E = \delta I$$

- every partial difference operator with constant coefficients has a fundamental solution (de Boor et al. (1989))

# Fourier Symbols

$$\widehat{Pu} = \widehat{B * u} = \hat{B}\hat{u}$$

$\hat{B}$ is the Fourier symbol of $P$

- if symbol of $P$ is always nonsingular, $E$ can be computed using fast Fourier transforms
- to determine $E$ uniquely, apply periodic boundary conditions
- problems if the symbol of $P$ is not invertible everywhere: the division problem

# Reduced Fourier Transform

- solution: $(d-1)$-dimensional discrete Fourier transform

$$\sum_{l=-q_r}^{q_l} \tilde{B}_{l,k_2,\ldots,k_d} \tilde{E}_{j_1-l,k_2,\ldots,k_d} = \delta_{j_1} I, \quad j_1 = -m_1, \ldots, m_1 - 1$$

ordinary difference equations with constant coefficients

- unique solution $\Rightarrow$ nonsingular banded systems
- two approaches:
  - supply suitable boundary (initial) conditions for resulting ODE
  - solve resulting under-determined system of equations using $LQ$ decomposition

# Examples

- grid refinement study of norm of $E$ for
  - convection operator
  - Euler equations
- problem case: shows that this approach does not always work
- relation to Toeplitz matrices

$$(Pu)_j = \sum_{k \in Z} b_k u_{j-k}, \quad b_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-ij\theta} \, d\theta$$

# Paper III

Discrete Fundamental Solution Preconditioning for Hyperbolic Systems of PDE
(Brandén, Holmgren and Sundqvist)

- system of non-linear first-order $d$-dimensional PDEs

$$\sum_{\nu=1}^{d} A_\nu(\mathbf{v}) \frac{\partial \mathbf{v}}{\partial x_\nu} = \mathbf{g}$$

- steady state of time-dependent hyperbolic system

$$\frac{\partial \mathbf{v}}{\partial t} + \sum_{\nu=1}^{d} A_\nu(\mathbf{v}) \frac{\partial \mathbf{v}}{\partial x_\nu} = \mathbf{g}$$

# Iterative method

- discretisation:

$$\frac{dv}{dt} + B(v)v = g$$

- preconditioned explicit Runge-Kutta iteration: e.g. forward Euler method (RK1)

$$v^{i+1} = v^i - \Delta t K(v^i)(B(v^i)v^i - g)$$

- linearisation:
  - fixed point iteration: $K(v^i) \simeq B^{-1}(v^i)$
  - Newton's method: $K(v^i) \simeq J^{-1}(v^i)$

- multiplicative FS preconditioner: three-level block matrix with two levels of Toeplitz structure

# Model Problem

- scalar Kreiss equation, forward Euler method
- sufficient condition for convergence: $\|I - \Delta t KB\| < 1$
- theorem:

$$\|I - KB\|_\infty < \frac{1}{2[1 - (1+h)^{-2m}]}$$

- numerical experiment shows bound is not sharp
- grid-independent convergence

| $m$ | 8 | 16 | 32 | 64 | 128 | 256 | 512 |
|---|---|---|---|---|---|---|---|
| upwind | 3 | 2 | 2 | 2 | 2 | 2 | 2 |
| central | 35 | 39 | 41 | 40 | 41 | 40 | 41 |

# Euler Equations

$$A_1(\mathbf{v})\frac{\partial \mathbf{v}}{\partial x_1} + A_2(\mathbf{v})\frac{\partial \mathbf{v}}{\partial x_2} = 0$$

- straight and narrowing channels
- comparison of fundamental solution (FS) and semicirculant (SC) preconditioners
- straight channel: FS and SC perform similarly
- narrowing channel: SC outperforms FS
- conclusion: FS needs ‘further development’

# Paper IV

Boundary Summation Equations
(Sundqvist)

- constant coefficient linear PDE, finite differences

$$Pu = f$$

$\Omega$: interior grid points
$\Gamma$: grid points with boundary modifications

- partitioning:

$$\begin{bmatrix} P_\Gamma & P_{\Gamma\Omega} \\ P_{\Omega\Gamma} & P_\Omega \end{bmatrix} \begin{bmatrix} u_\Gamma \\ u_\Omega \end{bmatrix} = \begin{bmatrix} f_\Gamma \\ f_\Omega \end{bmatrix}$$

# Reduced System

- discrete fundamental solution $E$, convolution operator $K$
- substitution:

$$\begin{bmatrix} u_\Gamma \\ u_\Omega \end{bmatrix} = \begin{bmatrix} K_\Gamma & K_{\Gamma\Omega} \\ K_{\Omega\Gamma} & K_\Omega \end{bmatrix} \begin{bmatrix} v_\Gamma \\ v_\Omega \end{bmatrix}$$

- reduced system:

$$\text{solve} \quad A v_\Gamma = f_\Gamma - C f_\Omega, \quad v_\Omega = f_\Omega$$

$$A = P_\Gamma K_\Gamma + P_{\Gamma\Omega} K_{\Omega\Gamma}, \quad C = P_\Gamma K_{\Gamma\Omega} + P_{\Gamma\Omega} K_\Omega$$

- no need to construct $A$: $K$ applied via FFT

  $O(N \log(N))$ arithmetic operations

- residual of original system easily recovered

# Examples and Experiments

- convection equation with $E^L$
  - GMRES iteration of full/reduced system
  - effect of convective field
  - grid-independent convergence observed
- convection-diffusion equation with $E^L$
  - results better for isotropic viscosity
  - mild grid dependence observed
- convergence analysis: convection equation

$$\|I - A\|_1 \leq c(n) \leq \frac{2}{3}$$

grid-independent convergence

# Further Numerical Experiments

- non-square regions
  - convection-diffusion on $L$-shaped domain
  - convection-diffusion on circular domain
  - mild grid dependence observed
- higher dimensional PDEs
  - convection equation in $d$ dimensions
  - grid-independent convergence observed
- systems of PDEs
  - linearised steady-state isentropic Euler equations
  - no dependence on grid aspect ratio

# Paper V

Navier-Stokes Equations for Low Mach Number Flows
Solved by Boundary Summation
(Sundqvist and Holmgren)

- 2D isentropic Navier-Stokes equations

$$\frac{\partial V}{\partial t} + P_0 V + P_1(V)V = P_2(V)V$$

- low Mach number flow
- Leap Frog-Backward Euler (LBFE) scheme
- second order finite differences
- driven cavity
- backward facing step

# Algorithm

1. compute fundamental solution
2. construct RHS vector $f_\Gamma - Cf_\Omega$
3. solve $Av_\Gamma = f_\Gamma - Cf_\Omega$
4. recover solution $u = Kv$

- comparison of full and reduced systems
- comparison of GMRES and direct solver
- investigation of stopping criteria
- comparison of

  $E^g$: FS from Paper II
  $E^p$: FS with full periodic boundaries
- calculation of complexities and memory needed

# Conclusions

- summary of results:
  - using $E^g$ requires fewer iterations but using $E^p$ is cheaper per time step
  - using GMRES on $A$ with $E^p$ is cheapest in terms of memory requirements
  - using GMRES on $P$ has cheapest set-up costs (i.e. none), GMRES on $A$ with $E^p$ is second
- the first of these will dominate over many time-steps

  method of choice is GMRES on $A$ with $E^p$

- performance deteriorates for large Reynolds numbers and small Mach numbers
- restriction to uniform grids

# Future Research

- approximate solvers for boundary summation equations
- further analysis of fundamental solutions
- different applications: e.g. image deblurring