Meshless Collocation Method for High Accuracy Computation

Alexander Cheng

University of Mississippi

石延平講座

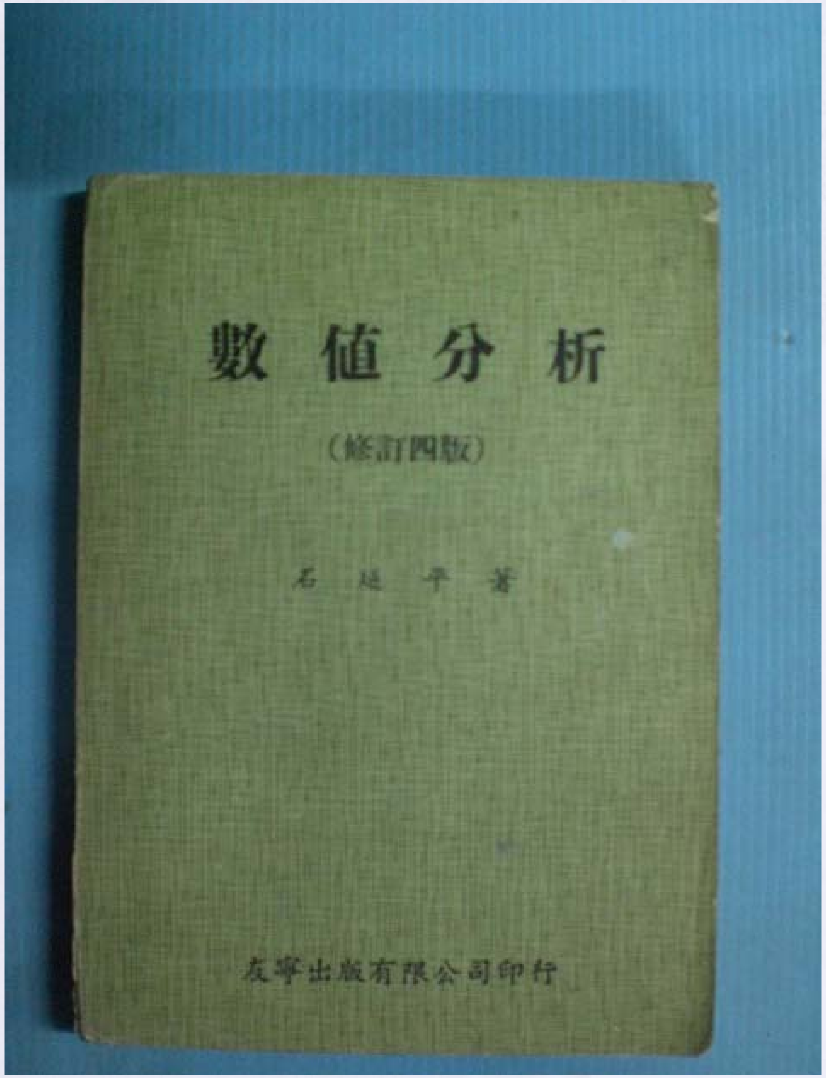
Presented at

National Taiwan Ocean University, Keelung, Taiwan

December 28, 2007

石延平 教授

(1932-1996)

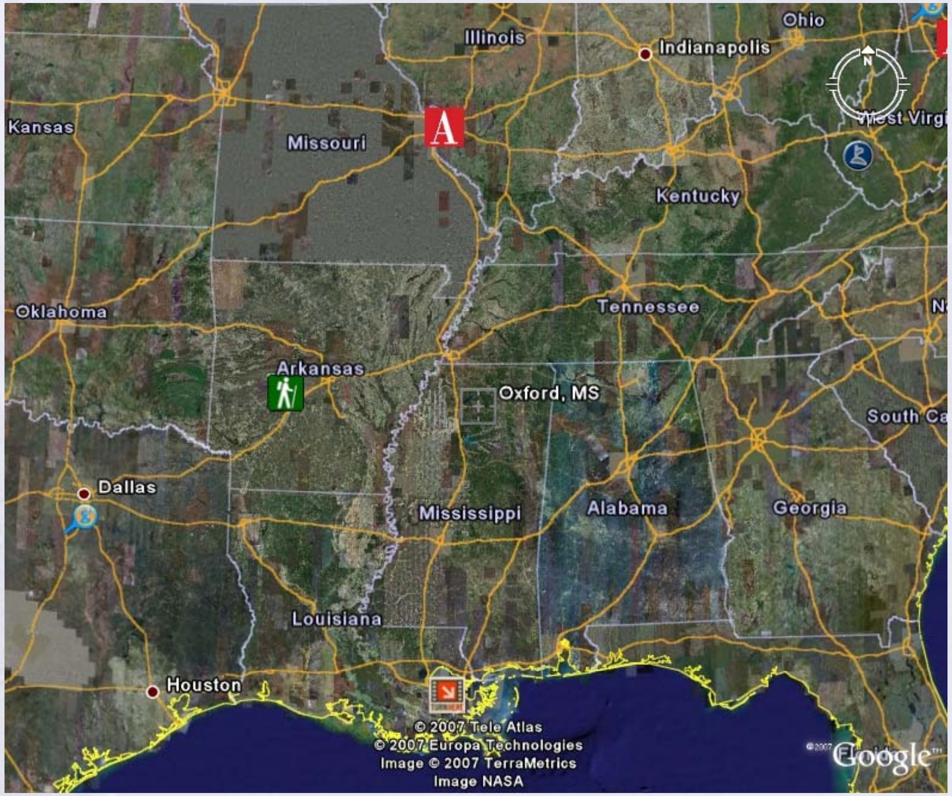

數值分析
(修訂四版)
石延平 著
友寧出版有限公司印行

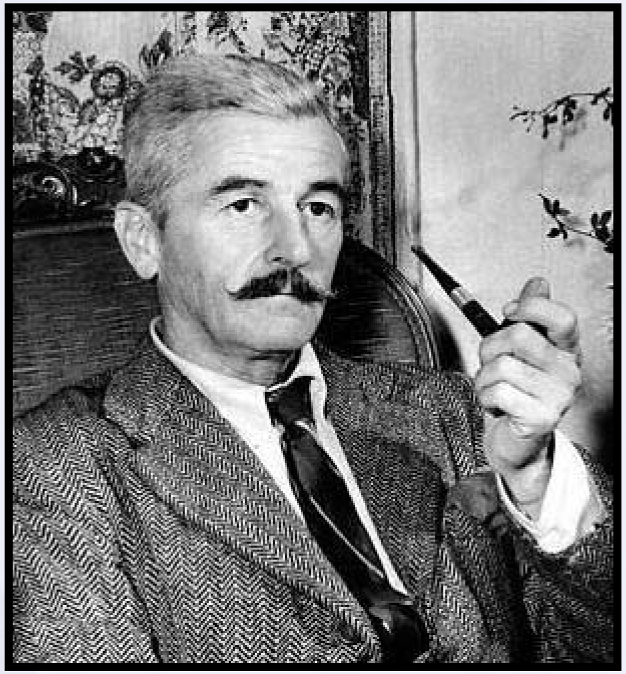
The National Ocean University Team

- Jeng-Tzong Chen 陳正宗
- Chein-Shan Liu 劉進賢
- Sung-Shan Hsiao 蕭松山
- Weichung Yeih 葉為忠
- Jiang-Ren Chang 張建仁
- Pei-Tai Chen
- Yung-Wei Chen
- Ching-Yeh Hsin

University of Mississippi

- Oxford Mississippi
- Home of William Faulkner






LIBRARY

Distinguished Alumnus
汪群從教授

- M.S. in Civil Engineering, University of Mississippi, 1966.
- Ph.D., University of Illinois, Urbana-Champaign

CONSIDERATIONS OF NUMERICAL METHODS

Considerations

- Is it suitable for engineering applications, such as arbitrary geometry?
- Is it efficient? (CPU)
- Is it accurate?
- Is the theory easy to understand?
- Is it easy to program?
- Is it general enough to solve linear or nonlinear, homogeneous or inhomogeneous, constant or variable coefficients, and all kinds of governing equations?

- Are commercial software widely available?
- Is there inertia?

Point Collocation Methods

- Radial basis function collocation
- Method of fundamental solutions
- Trefftz method

Why Collocation Method?

- Accuracy
- Simplicity
- Meshless
- Solve ill-posed BVP without iteration
- Solve *n*-dimensional problem (RBF)
- Boundary method (MFS, Trefftz)

SIMPLICITY

Intuitive Derivation

- Governing equation

$$\mathscr{L}(u) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega$$

- Boundary condition

$$\mathscr{B}(u) = g(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma$$

Approximate Solution

- Assume approximate solution is given by

$$\hat{u}(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i \, \phi_i(\boldsymbol{x})$$

where $\phi_i(\boldsymbol{x})$ are basis functions and α_i are constants to be determined.

$\phi(x)$

Choices of Basis Functions

- Monomial (X)
- Chebyshev polynomial (X)
- Fourier series (X)
- Wavelet (X)
- Fundamental solutions (MFS)
- Non-singular general solution (Trefftz)
- Radial basis function (RBF)

* “X” requires regular domain

Example: Multiquadric

- Inverse multiquadric

$$\hat{u}(\boldsymbol{x}) = \sum_{i=1}^{n} \alpha_i \frac{1}{\sqrt{r_i^2 + c^2}}$$

where

$$r_i = \sqrt{(x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2}$$

Point Collocation

- Select n_i points, $\{x_1, x_2, \cdots, x_{n_i}\} \in \Omega$, on which the governing equation is satisfied.

$$\mathscr{L}\left(\hat{u}(\boldsymbol{x}_j)\right) = \mathscr{L}\left(\sum_{i=1}^{n} \alpha_i \phi_i(\boldsymbol{x}_j)\right)$$

$$= \sum_{i=1}^{n} \alpha_i \mathscr{L}\left(\phi_i(\boldsymbol{x}_j)\right) = f(\boldsymbol{x}_j); \quad \text{for} \quad j = 1, \ldots, n_i$$

each is a linear equation in α_i

- Select n_b points, $\{x_{n_i+1}, x_{n_i+2}, \cdots, x_n\} \in \Gamma$, on which the boundary conditions are satisfied.

$$\mathscr{B}\left(\hat{u}(\boldsymbol{x}_j)\right) = \mathscr{B}\left(\sum_{i=1}^{n} \alpha_i\, \phi_i(\boldsymbol{x}_j)\right)$$

$$= \sum_{i=1}^{n} \alpha_i \mathscr{B}\left(\phi_i(\boldsymbol{x}_j)\right) = g(\boldsymbol{x}_j); \quad \text{for} \quad j = n_i + 1, \ldots, n$$

- Linear solution system

$$[\mathbf{A}]\{\boldsymbol{\alpha}\} = \{\mathbf{b}\}$$

- Once {α} is solved, the solution is a continuous function

$$u(x) = \sum \alpha_i \frac{1}{\sqrt{r_i^2 + c^2}}$$

- The function is infinitely smooth

ILL-POSED PROBLEM

Well- and Ill-Posed Boundary Value Problems

- Governing equation

$$\nabla^2 u = f(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega$$

- Boundary conditions

$$u = g_1(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma_D$$

$$\frac{\partial u}{\partial n} = g_2(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma_N$$

- Interior condition

$$u(\boldsymbol{x}_j) = \bar{u}_j, \quad j = 1, \ldots, m, \quad \boldsymbol{x}_j \in \Omega$$

Difference between well-posed and ill-posed problems

- Well-posed problem

$$\Gamma_D \cup \Gamma_N = \Gamma \qquad \Gamma_D \cap \Gamma_N = \varnothing$$

$$\Gamma_D \neq \varnothing \qquad m = 0$$

- Ill-posed problem

$$\Gamma_D \cup \Gamma_N \neq \Gamma \qquad \Gamma_D \cap \Gamma_N \neq \varnothing$$

$$m \neq 0$$

ACCURACY

How Accurate?

- Its accuracy is impossible to match by FEM or FDM.
- In an example solving Poisson equation, an accuracy of the order 10^{-16} is reached using a 20x20 grid.

To Make It Dramatic

- Assume that in an initial mesh, FEM/FDM can solve to an accuracy of 1%.
- Using a quadratic element or central difference, the error estimate is h^2
- To reach an accuracy of 10^{-16}, h needs to be refined 10^7 fold
- In a 3D problem, this means 10^{21} fold more degrees of freedom
- The full matrix is of the size 10^{42}
- The effort of solution could be 10^{63} fold
- If the original CPU is 0.01 sec, this requires 10^{54} years
- The age of universe is 2 x 10^{10} years

UNIFIED VIEW—METHOD OF WEIGHTED RESIDUALS

Collocation Method as Method of Weighted Residuals

- Zienkiewicz in his FEM book has discussed collocation method as a special case of method of weighted residuals. In an example, he found Galerkin method to be the most accurate.

Method of Weighted Residuals

- Governing equation

$$\mathcal{L}(u(\mathbf{x})) = f(\mathbf{x}), \quad \mathbf{x} \in \Omega,$$

- Essential and natural boundary conditions

$$\begin{aligned} \mathcal{S}(u(\mathbf{x})) &= g_1(\mathbf{x}), \quad \mathbf{x} \in \Gamma_S, \\ \mathcal{N}(u(\mathbf{x})) &= g_2(\mathbf{x}), \quad \mathbf{x} \in \Gamma_N, \end{aligned}$$

Minimizing Weighted Residual

- Approximation

$$u(\mathbf{x}) \approx \hat{u}(\mathbf{x}) = \sum_{i=1}^{n} a_i N_i(\mathbf{x}), \quad \mathbf{x} \in \Omega,$$

- Satisfying governing equation

$$\int_\Omega R(\mathbf{x})\, w_i(\mathbf{x})\; d\mathbf{x} = \int_\Omega [\mathcal{L}(\hat{u}(\mathbf{x})) - f(\mathbf{x})]\, w_i(\mathbf{x})\; d\mathbf{x} = 0,$$

- Satisfying boundary conditions

$$\int_{\Gamma_S} [\mathcal{S}(\hat{u}(\mathbf{x})) - g_1(\mathbf{x})]\, w_i(\mathbf{x})\; d\mathbf{x} + \int_{\Gamma_N} [\mathcal{N}(\hat{u}(\mathbf{x})) - g_2(\mathbf{x})]\, w_i(\mathbf{x})\; d\mathbf{x} = 0.$$

Galerkin Method

- Weight:

$$W_i = N_i$$

- Satisfying governing equation

$$\int_\Omega [\mathcal{L}(\hat{u}(\mathbf{x})) - f(\mathbf{x})]\, w_i(\mathbf{x})\, d\mathbf{x} = \int_\Omega \left[\mathcal{L}\left(\sum_{j=1}^{n} a_j N_j(\mathbf{x})\right) - f(\mathbf{x})\right] N_i(\mathbf{x})\, d\mathbf{x} = 0,$$

Collocation Method

- Weight

$$w_i(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_i)$$

- Collocate for governing equation

$$\mathcal{L}(\hat{u}(\mathbf{x}_i)) = f(\mathbf{x}_i), \quad \mathbf{x}_i \in \Omega.$$

- Collocate for boundary condition

$$\begin{aligned} \mathcal{S}(\hat{u}(\mathbf{x}_i)) &= g_1(\mathbf{x}_i), \quad \mathbf{x}_i \in \Gamma_S, \\ \mathcal{N}(\hat{u}(\mathbf{x}_i)) &= g_2(\mathbf{x}_i), \quad \mathbf{x}_i \in \Gamma_N. \end{aligned}$$

A Simple Example

$$\frac{d^2h}{dx^2} + \frac{H_o - h}{\lambda} = 0,$$

$$h(0) = h_1 \text{ and } h(L) = h_2,$$

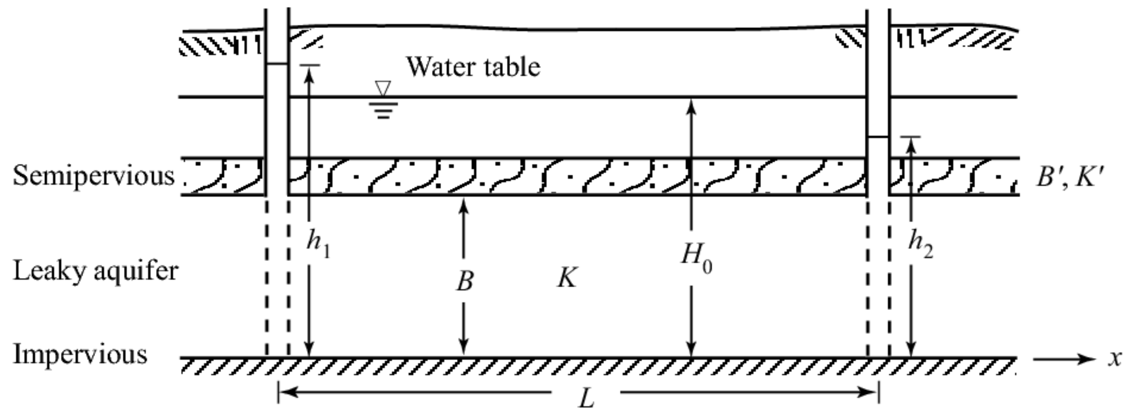


Figure 8.3.1: Flow in a leaky aquifer.

Solution Strategy

- Approximate solution

$$h \approx \hat{h} = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4.$$

- Solved by collocation, subdomain, and Galerkin method
- Integration performed exactly

Solution Error

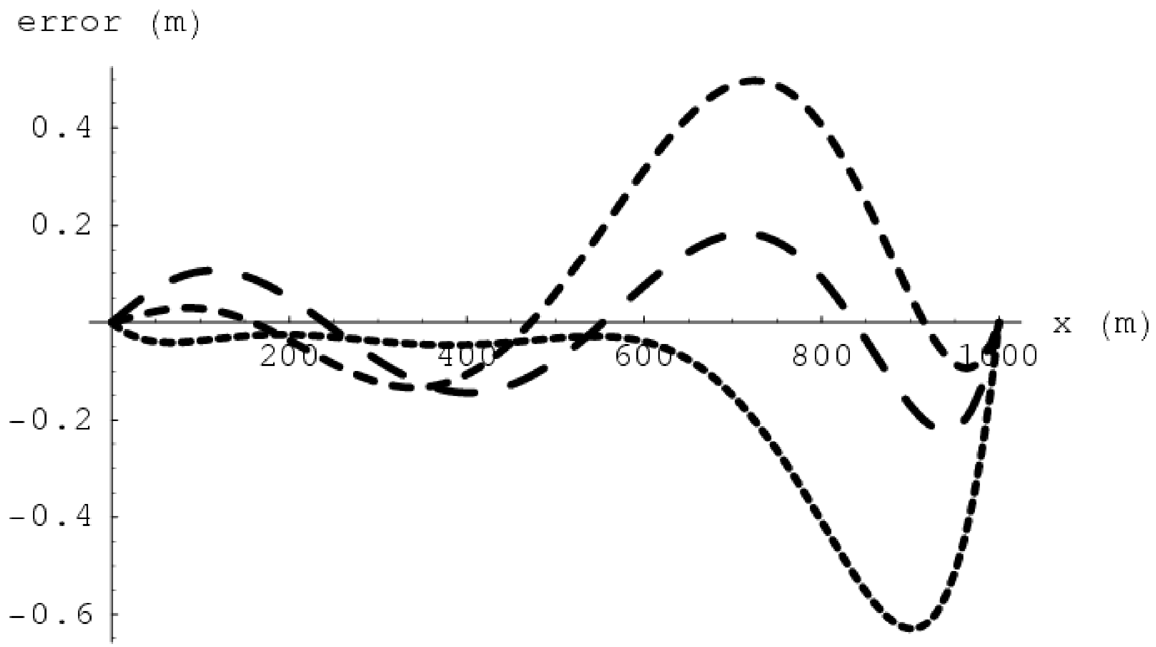


Figure 8.3.3: Comparison of error of the approximate three solutions. Short dash line: collocation method; medium dash line: subdomain method; and long dash line: Galerkin method.

Lessons Learned

- We observe that Galerkin method is the most accurate, and collocation the least.
- Integration distributes the error and point collocation concentrates the error.
- So integration using distributed weight is better.
- So why do we claim point collocation is the best?

Answer

- Because in a practical problem, Galerkin method cannot be applied as such (using global basis function and exact integration), certain approximation needs to be done.
- For a general two- or three-dimensional, irregular geometry, analytical integration cannot be performed. The domain has to be divided into integration cells (or differentiation grids).
- Local, piecewise continuous interpolation, instead of global interpolation is used.
- Both approximations are $O(h^k)$ operations. The original accuracy is lost!

Errors

- Geometric approximation error $O(h^k)$, k=1,2,... (approximating boundary by straight line segments, flat planes, quadratic curves, ...)
- Approximation (truncation) error $O(h^n)$
- Quadrature error (FEM can integrate exactly due to low degree polynomial, other weighted residual methods, such as BEM, MFS, Trefftz, cannot, depending on the weighing function)

Lessons Learned

- Do not subdivide the domain into elements, to avoid approximating the domain geometry.
- Do not integrate (or integrate analytically), to avoid quadrature error.
- Use continuous, global basis functions, not piece-wise continuous, local functions

POINT COLLOCATION

Point Collocation

- No geometric approximation error.
- No quadrature error.
- Global basis function with exponential error convergence,

$$\varepsilon \sim O\left(\lambda^{1/h^k}\right); \quad 0 < \lambda < 1$$

- Convergence is the best if we make the interpolants as flat as possible.

ERROR ESTIMATE FOR PDE (EXPERIMENTAL)

Test Problem

$$\nabla^2 u(x,y) = -\frac{751\pi^2}{144}\sin\frac{\pi x}{6}\sin\frac{7\pi x}{4}\sin\frac{3\pi y}{4}\sin\frac{5\pi y}{4} + \frac{7\pi^2}{12}\cos\frac{\pi x}{6}\cos\frac{7\pi x}{4}\sin\frac{3\pi y}{4}\sin\frac{5\pi y}{4} + \frac{15\pi^2}{8}\sin\frac{\pi x}{6}\sin\frac{7\pi x}{4}\cos\frac{3\pi y}{4}\cos\frac{5\pi y}{4}, \quad (x,y)\in[0,1]^2, \quad (7)$$

subject to the Dirichlet type boundary conditions

$$u(0,y) = 0, \quad (8a)$$

$$u(1,y) = \sin\frac{\pi}{6}\sin\frac{7\pi}{4}\sin\frac{3\pi y}{4}\sin\frac{5\pi y}{4}, \quad (8b)$$

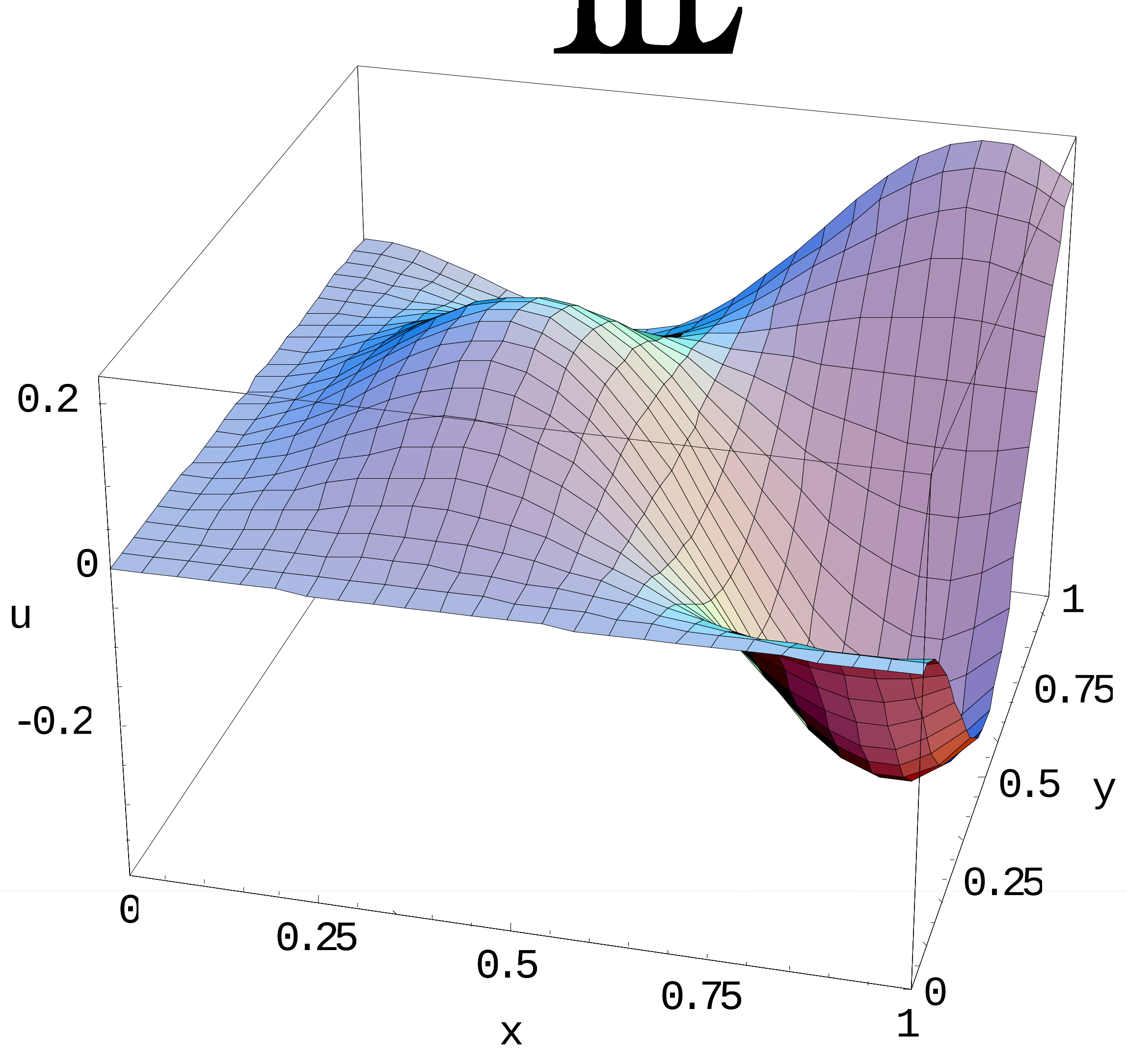
$$u(x,0) = 0, \quad (8c)$$

$$u(x,1) = \sin\frac{\pi x}{6}\sin\frac{7\pi x}{4}\sin\frac{3\pi}{4}\sin\frac{5\pi}{4}. \quad (8d)$$

The exact solution of this problem is

$$u(x,y) = \sin\frac{\pi x}{6}\sin\frac{7\pi x}{4}\sin\frac{3\pi y}{4}\sin\frac{5\pi y}{4}. \quad (9)$$

Exact Solution



Solution method

- Approximation by inverse multiquadric

$$\hat{u} = \sum_{i=1}^{n} \alpha_i \frac{1}{\sqrt{r_i^2 + c^2}}$$

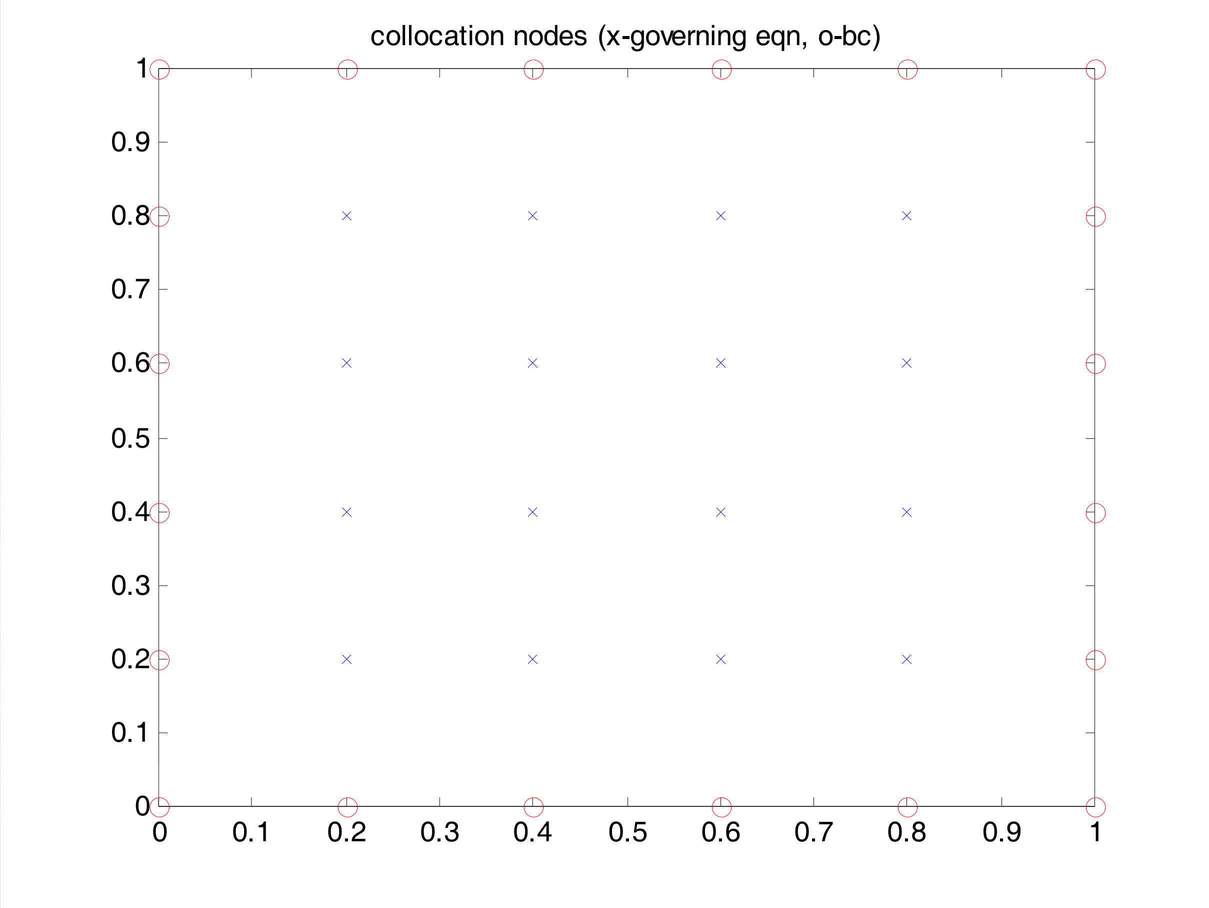
Watch out for the "c"

What Is the Role of *c*?

- People observe that as c increases, error decreases
- It is generally believed that as $c \to \infty$, $\varepsilon \to 0$
- If this is true, we have a *dream method*: higher and higher precision without paying a price
- However, matrix ill-condition gets in the way; the dream cannot be fulfilled.

- What if we can compute with infinite precision?
- Then, is it true that as $c \to \infty$, $\varepsilon \to 0$?
- (Or, is it true that for MFS, as $R \to \infty$, $\varepsilon \to 0$?)
- We can find out about these by using the infinite (arbitrary) precision computation capability of Mathematica and high precision capability of Fortran

- Use 6x6 mesh (h = 0.2, 4x4 interior collocation)



Result: h = 1/5

h	c	$\varepsilon_{\max}$	ε_{rms}	Condition Number
0.2	0.1	4.36×10^{-01}	1.40×10^{-01}	$4.95 \times 10^{+02}$
0.2	1.1	2.49×10^{-02}	9.08×10^{-03}	$8.89 \times 10^{+07}$
0.2	$1.2^{\dagger}$	1.92×10^{-02}	6.93×10^{-03}	$2.94 \times 10^{+08}$
0.2	1.3	1.94×10^{-02}	5.12×10^{-03}	$9.22 \times 10^{+08}$
0.2	$1.4^{\dagger}$	1.99×10^{-02}	4.24×10^{-03}	$2.76 \times 10^{+09}$
0.2	1.5	2.08×10^{-02}	4.94×10^{-03}	$7.92 \times 10^{+09}$
0.2	2.0^{*}	3.37×10^{-02}	1.85×10^{-02}	$8.49 \times 10^{+11}$
0.2	3.0	9.64×10^{-02}	5.84×10^{-02}	$1.09 \times 10^{+15}$
0.2	10.0	6.10×10^{-01}	4.19×10^{-01}	$6.38 \times 10^{+24}$
0.2	100.0	1.11×10^{0}	7.82×10^{-01}	$9.15 \times 10^{+42}$

Result: h = 1/10

h	c	ε_{max}	ε_{rms}	Condition Number
0.1	0.1	8.67×10^{-02}	2.89×10^{-02}	$2.19 \times 10^{+03}$
0.1	2.5	6.88×10^{-06}	1.74×10^{-06}	$2.88 \times 10^{+27}$
0.1	$4.0^{\dagger}$	1.88×10^{-06}	6.23×10^{-07}	$6.40 \times 10^{+34}$
0.1	$4.1^{\dagger,*}$	2.21×10^{-06}	6.09×10^{-07}	$1.57 \times 10^{+35}$
0.1	10.0	1.5×10^{-04}	1.11×10^{-04}	$4.82 \times 10^{+49}$
0.1	100.0	6.24×10^{0}	4.56×10^{0}	$3.49 \times 10^{+87}$

Result: $h = 1/20$

c	$\varepsilon_{\max}$	ε_{rms}
7.0	2.22×10^{-15}	7.86×10^{-16}
7.5	1.91×10^{-15}	9.60×10^{-16}
7.7	2.37×10^{-15}	9.26×10^{-16}
8.0	2.88×10^{-15}	8.87×10^{-16}
8.5	3.58×10^{-15}	1.06×10^{-15}
9.0	3.75×10^{-15}	41.2×10^{-15}

Find Error Estimate Constants by Data Fitting

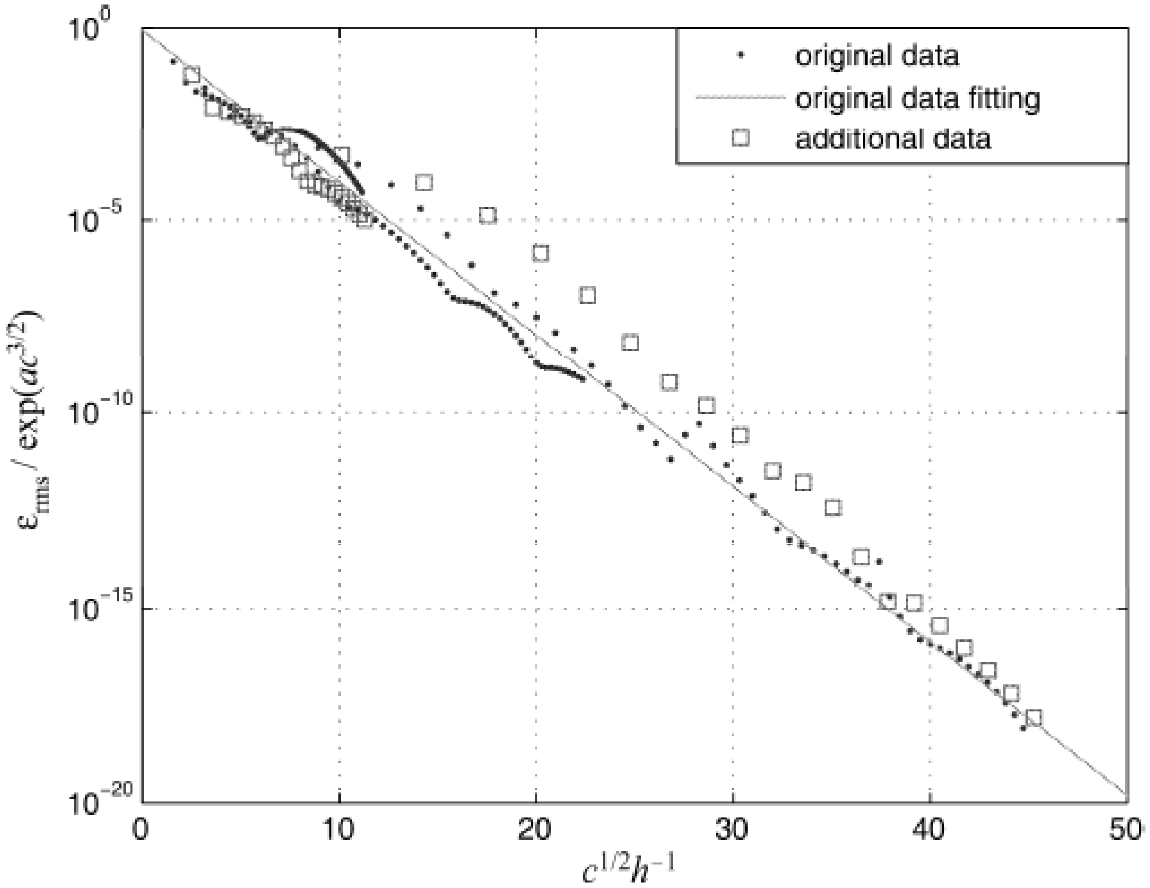


Fig. 2. Fitting for error estimate for IMQ solution of Poisson equation: composite plot of a large number of cases with different h and c values.

Error Estimate

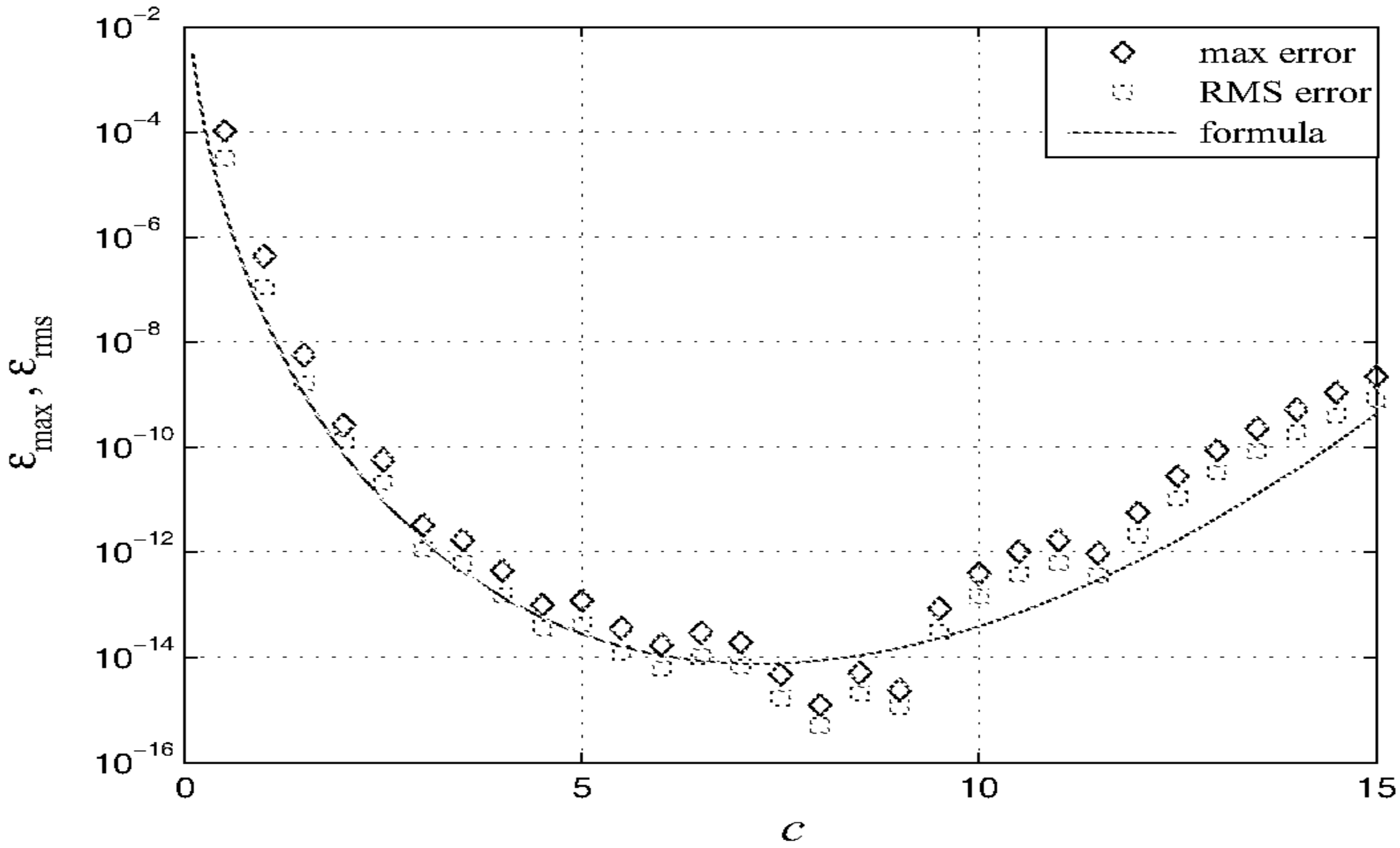


Fig. 5. Validating (15), second example.

Our Findings: Error Estimate

$$\varepsilon \sim \mathcal{O}(e^{ac^{3/2}} \lambda^{c^{1/2}h^{-1}}).$$

- $0 < \lambda < 1$, $a > 0$

Optimal *c*

- If the error estimate

$$\varepsilon \sim \mathcal{O}(e^{ac^{3/2}} \lambda^{c^{1/2} h^{-1}}).$$

is true, then there exists an optimal *c* where error is minimum

$$c_{\max} = -\frac{\ln \lambda}{3ah},$$

Revised Error Estimate

- If we can always use optimal *c* with a given mesh, what is the new error estimate?

$$\varepsilon \sim \mathcal{O}(\gamma^{h^{-3/2}}),$$

$$\gamma = \left(\lambda\, e^{-\ln\lambda/3}\right)^{\sqrt{-\ln\lambda/3a}}$$

$$0 < \gamma < 1$$

Effective Error Estimate If c_{max} Is Used

- $h = 1/5$, $\varepsilon \sim 10^{-2}$
- $h = 1/10$, $\varepsilon \sim 10^{-6}$
- $h = 1/20$, $\varepsilon \sim 10^{-15}$

THEORETICAL RESULT

Madych

- Madych (1992): For the interpolation of a class of "essentially analytic functions", which are "band limited", *using a class of interpolants that include the multiquadric, Gaussian, …, he proved*

$$\varepsilon = O\left(e^{ac}\lambda^{c/h}\right); \quad 0<\lambda<1, \quad a>0$$

- *This means, as* $c \to \infty, \quad \varepsilon \to 0$

- Is this possible?
- What is such function?
- If we are given one such function, and we use infinite precision computation, can be demonstrate that $c \to \infty, \quad \varepsilon \to 0$?
- Or, do we anticipate that $c \to \infty, \quad \varepsilon \neq 0$ and there exists $c_{opt} = c_{opt}(h)$ where $\varepsilon = \varepsilon_{\min}$?

- Madych also stated that for a "non-band-limited" function,

$$\varepsilon = O\left(e^{ac^2} \lambda^{c/h}\right); \quad 0 < \lambda < 1, \quad a > 0$$

- In this case, there exist a $c_{opt} = -\frac{\ln \lambda}{2ah}$ where $\varepsilon = \varepsilon_{\min}$
- If we can use the c_{opt} then $\varepsilon \sim O(\lambda^{1/h^2})$

- Is this true for all smooth functions?
- Can we test this by high precision computation?

RESEARCH DIRECTION

Methods

- Radial basis function collocation
- MFS
- Trefftz

Issues

- Error estimate
- Stability (condition number)
- High precision computation

MFS: Theoretical Result

- Bogomolny
- Schaback
- Jeng-Tzong Chen
- Zi-Cai Li, et al.

Trefftz Error Analysis

- Harmonic polynomials in Cartesian form
- Harmonic polynomials in polar form
- Real part of any analytic function with translation

Discontinuity and Singularity

- Particular solution

Join EMI as a Charter Member

ENGINEERING MECHANICS INSTITUTE

1687

American Society of Civil Engineers