Error Estimate (Accuracy) and Effective Condition Number (Stability) of Collocation Trefftz Method, Method of Fundamental Solutions, and Radial Basis Function Method

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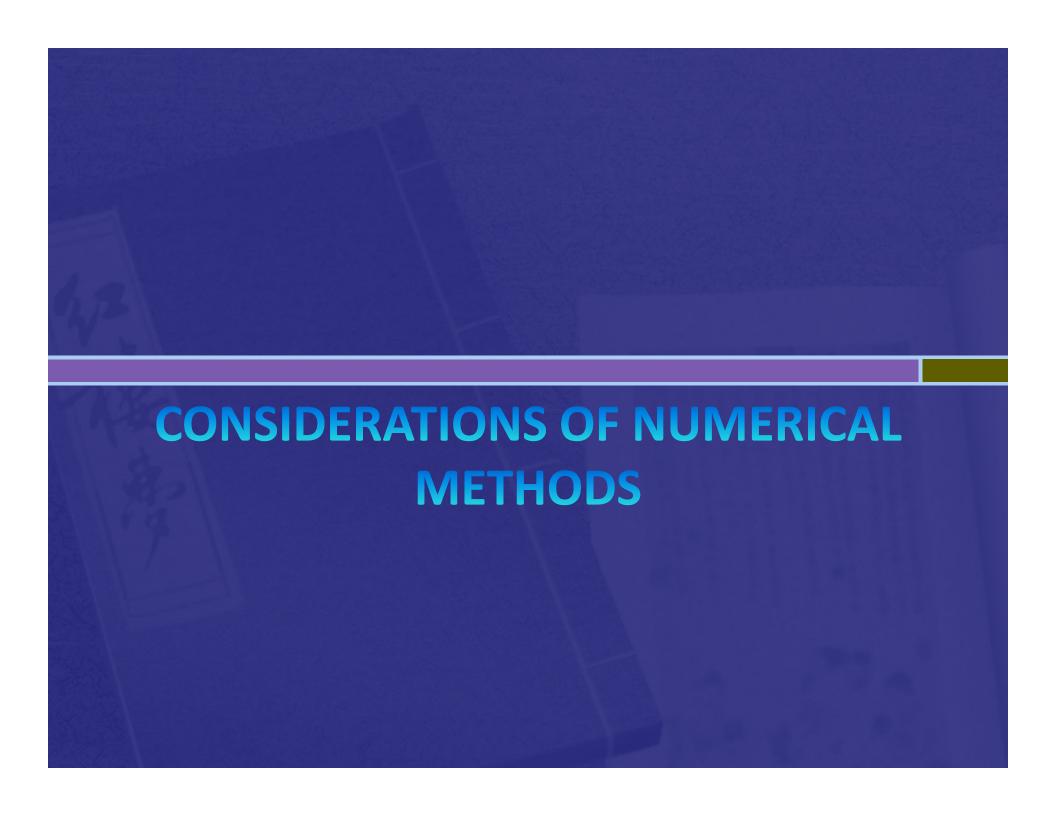
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(Point) Collocation Methods

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

Why Collocation Method?

- High accuracy (exponential error convergence)
- Simplicity in formulation
- Meshless
- Boundary method (Trefftz, MFS)
- Solve ill-posed BVP without iteration
- > Easy to adapt to *n*-dimensional problem



Considerations

- Is it suitable for engineering applications, such as arbitrary geometry?
- Is it efficient? (CPU time)
- > Is it accurate? (Coupled with efficiency)
- > Is the theory easy to understand?
- > Is it easy to write computer 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 (people are comfortable with the method they use)?



Original Trefftz Method

Solve the Dirichlet problem

$$\nabla^2 u = 0 \quad \text{in } \Omega$$

$$u = f(x)$$
 in Γ

> Utilize the Ritz method

Ritz Method

Approximate the solution using a set of trial

functions $\phi_i(x)$

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

> Minimize the functional

$$\Pi = -\iiint_{\Omega} \frac{1}{2} u \nabla^2 u \, dx - \iint_{\Gamma} \frac{\partial u}{\partial n} \left(\frac{1}{2} u - f \right) dx$$

Walter Ritz (1878-1909)

with respect to the trial functions

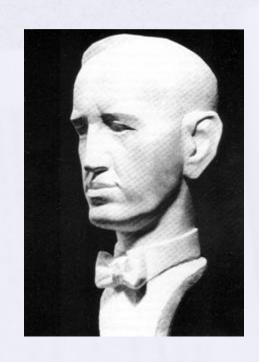
Trefftz's Contribution

 Require trial functions to satisfy the governing equation

$$\nabla^2 \phi_i = 0$$

> The functional reduces to

$$\Pi = -\iint_{\Gamma} \sum_{i=1}^{n} \alpha_{i} \frac{\partial \phi_{i}}{\partial n} \left(\frac{1}{2} \sum_{i=1}^{n} \alpha_{i} \phi_{i} - f \right) d\mathbf{x}$$



Erich Trefftz (1888-1937)

Solution System

> Use harmonic polynomials

$$\phi_i = \{1, x, y, z, x^2 - y^2, y^2 - z^2, xy, yz, xz, ...\}$$

Linear solution system

$$\sum_{i=1}^{n} a_{ij} \alpha_{i} = b_{j}; \quad j = 1, ..., n$$

$$a_{ij} = \frac{1}{2} \iint_{\Gamma} \frac{\partial \phi_{i} \phi_{j}}{\partial n} d\mathbf{x}; \quad b_{j} = \iint_{\Gamma} f \frac{\partial \phi_{j}}{\partial n} d\mathbf{x}$$

Other Formulations of Trefftz Method

- > Trefftz-Herrera formulation
- Weighted residual formulation
- > Collocation formulation
- Hybrid methods



Kupradze Formulation

Solution given by

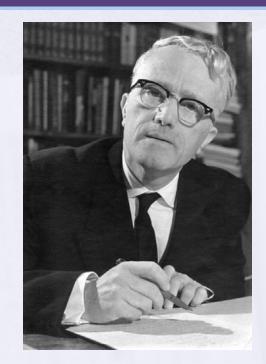
$$u(\mathbf{x}) = \frac{1}{2\pi} \iint_{\Gamma} f(\mathbf{x}') \frac{\partial G(\mathbf{x}, \mathbf{x}')}{\partial n(\mathbf{x}')} d\mathbf{x}'$$

$$+\frac{1}{\pi}\iint_{\Gamma}\sigma(x')G(x,x')\,dx';\quad x\in\Omega$$

where $\sigma(x')$ is found from

$$0 = \frac{1}{2\pi} \iint_{\Gamma} f(\mathbf{x}') \frac{\partial G(\mathbf{x}, \mathbf{x}')}{\partial n(\mathbf{x}')} d\mathbf{x}'$$

$$+\frac{1}{\pi}\iint_{\Gamma}\sigma(x')G(x,x')\,dx';\quad x\in\Gamma'$$



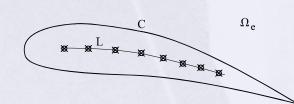
Viktor Dmitrievich Kupradze (1903-1985)

Von Karman Formulation

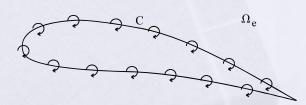
Potential flow around objects

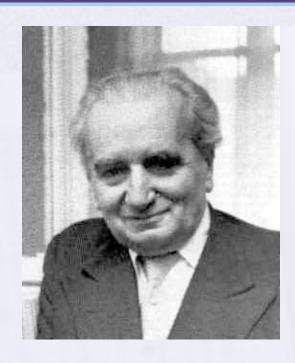
$$u(x) \approx Ux + \sum_{i=1}^{n+1} \frac{\sigma_i}{4\pi r(x, x_i)}$$

$$\sum_{i=1}^{n+1} \sigma_i = 0$$



(b)





Theodore von Karman (1881-1963)

Other Formulations

- Point collocation (Mathon & Johnson, 1997)
- Least square, optimization formulation (Fairweather)
- Boundary integral equations
- > Boundary element method.

Cheng, A.H.-D. and Cheng, D.T., "Heritage and early history of the boundary element method," Engineering Analysis with Boundary Elements, Vol. 29, No. 3, pp. 268–302, 2005.



Method of Weighted Residuals

Governing equation

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

> Essential and natural boundary conditions

$$S\{u(x)\} = g_1(x), \quad x \in \Gamma_S$$
$$\mathcal{N}\{u(x)\} = g_2(x), \quad x \in \Gamma_N$$

Minimizing Weighted Residual

Approximation by trial functions

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

Minimizing the residual

$$\iiint_{\Omega} \left[\mathcal{L}\{u(x)\} - f(x) \right] w_i \, dx + \iint_{\Gamma_s} \left[\mathcal{S}\{u(x)\} - g_1(x) \right] w_i \, dx$$
$$+ \iint_{\Gamma_N} \left[\mathcal{N}\{u(x)\} - g_2(x) \right] w_i' \, dx = 0$$

with respect to trial functions

Choosing Different Weight

Galerkin method: Trial function as weight

$$W_i = \phi_i$$

- Subdomain method: Step function
- > Collocation method: Dirac delta function

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

A Simple Example

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

$$h(0) = h_1$$
 and $h(L) = h_2$,

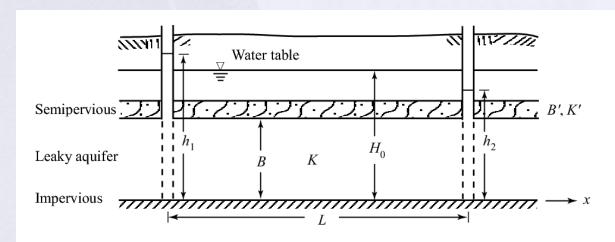


Figure 8.3.1: Flow in a leaky aquifer.

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

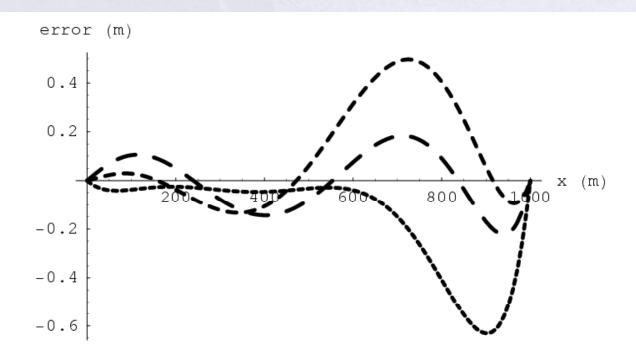


Figure 8.3.3: Comparison of error of the approximate three solutions. Short dash line: collocation method; medium dash line: subdomain method; and long dash line: Galerkin method.

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 why do we claim the point collocation has the highest accuracy?



FEM "Mistakes"

> FEM interpolate "physical variables"

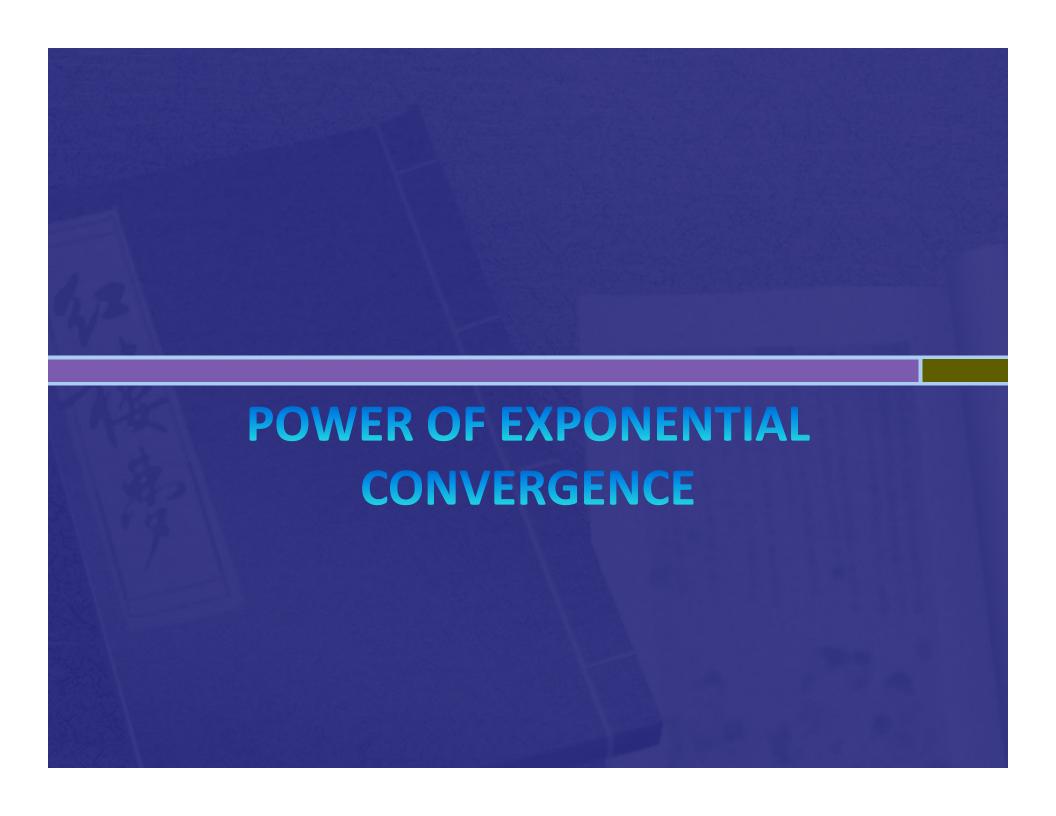
$$u(x) \approx \sum_{e=1}^{n} \sum_{i=1}^{k} u_i^e N_i$$

- > It is only feasible to interpolate physical variable locally, not globally
- > Elements are introduced
- Elements approximate geometry; hence loses accuracy

FEM Mistakes

- Low degree polynomials are used for interpolation.
- > Poor continuity between elements
- > FEM error is

$$\varepsilon \sim O(h^k)$$



What is Exponential Convergence?

$$\varepsilon \sim O(\lambda^{h^{-k}}), \quad 0 < \lambda < 1$$

$$\varepsilon \sim O(e^{-h^{-k}})$$

$$\varepsilon \sim O(\lambda^N), \quad 0 < \lambda < 1$$

Power of Exponential Convergence

- Its accuracy is impossible for FEM, FDM, or any other methods that uses local, rather than global interpolation, to match.
- Using Trefftz method, Li solved Motz problem to an accuracy of 10⁻⁸ using about 30 terms
- ➤ Using RBF collocation, a Poisson equation was solved to an accuracy of 10⁻¹⁵ using a 20x20 grid.

How Accurate is That?

- > Assume that using a modest mesh, FEM/FDM can solve a problem to an accuracy of 0.1%.
- > Using a quadratic element or central difference, the error estimate is h^2 .
- ➤ To reach an accuracy of 10⁻¹⁵, the FEM result needs to be improved 10⁻¹² fold.
- > *h* needs to be refined 10⁶ fold in linear dimension, meaning that between any two nodes, one million nodes need to be inserted.

- ➤ In a 3D problem, this means 10¹⁸ fold more degrees of freedom.
- ➤ The effort of solution will be between 10³⁶ to 10⁵⁴ fold
- > The fastest computer in the world (not yet delivered) has just reached petaflop (10¹² flops per second).
- ➤ If the original problem requires 1 floating point operation (CPU=10⁻¹² sec), the CPU time needed will be between 10¹⁷ to 10³⁵ years
- > The age of universe is 2×10^{10} years!



Intuitive Derivation

Governing equation

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

Boundary condition

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

Approximate Solution

Assume approximate solution is given by

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

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

Choices of Basis Functions

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



Continuous Solution

- > Trial functions:
 - > harmonic polynomials,
 - > translation of harmonic function
- Weighted residual formulation: Error bounded by quadrature error
- > Point collocation: Exponential error bound

$$\varepsilon \sim O(\lambda^N), \quad 0 < \lambda < 1$$

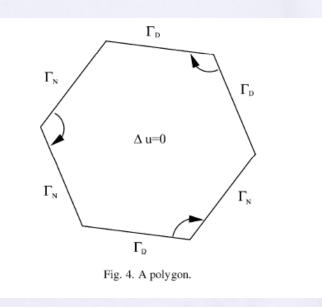
Condition number

Cond ~
$$O(\beta^N)$$
, $\beta > 1$

> Effective condition number much better

Weakly and Strongly Singular Problem

- Weakly singular problem: No treatment of singularity, using only local mesh refinement, logarithmic error convergence
- Strongly singular problem: No treatment of singularity, no convergence.



- Harmonic polynomial is not suitable when singularity is present (polygonal region).
- Should use local particular solution.

Li, Z.-C., Lu, T.-T., Hu, H.-Y. and Cheng, A.H.-D., "Particular solutions of Laplace's equations on polygons and new models involving mild singularities," Engineering Analysis WITH BOUNDARY ELEMENTS, Vol. 29, No. 1, pp. 59–75, 2005.



Comparison with Trefftz

- > As $R \to \infty$ the sources behave as harmonic polynomials.
- Error bound of MFS can only be at best as good as Trefftz method. (Bogomolny, Schabck, J.T. Chen, Zi-Cai Li)
- Condition number of MFS is much worse that Trefftz



Example: Multiquadric

> Inverse multiquadric

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

where

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

Point Collocation

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

$$\mathcal{L}(\hat{u}(\mathbf{x}_{j})) = \mathcal{L}\left(\sum_{i=1}^{n} \alpha_{i} \phi_{i}(\mathbf{x}_{j})\right)$$

$$= \sum_{i=1}^{n} \alpha_{i} \mathcal{L}(\phi_{i}(\mathbf{x}_{j})) = f(\mathbf{x}_{j}); \quad \text{for} \quad j = 1, \dots, n_{i}$$

each is a linear equation in α_i

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

$$\mathcal{B}(\hat{u}(\mathbf{x}_{j})) = \mathcal{B}\left(\sum_{i=1}^{n} \alpha_{i} \phi_{i}(\mathbf{x}_{j})\right)$$

$$= \sum_{i=1}^{n} \alpha_{i} \mathcal{B}(\phi_{i}(\mathbf{x}_{j})) = g(\mathbf{x}_{j}); \quad \text{for} \quad j = n_{i} + 1, \dots, n$$

Linear solution system

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

 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

Test Problem

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

subject to the Dirichlet type boundary conditions

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

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

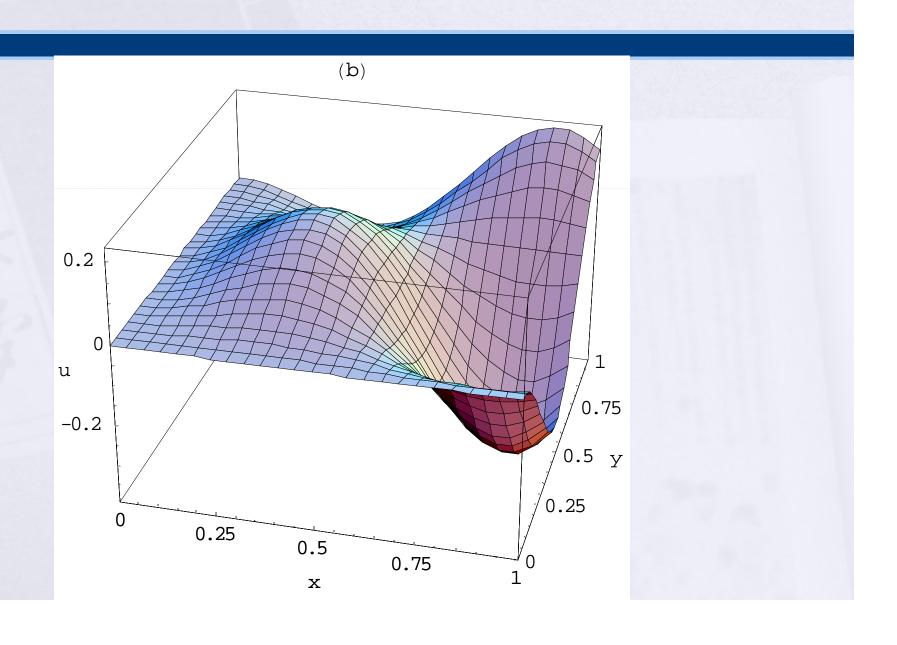
$$u(x,0) = 0, (8c)$$

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

The exact solution of this problem is

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

Exact Solution



Solution method

Approximation by inverse multiquadric

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

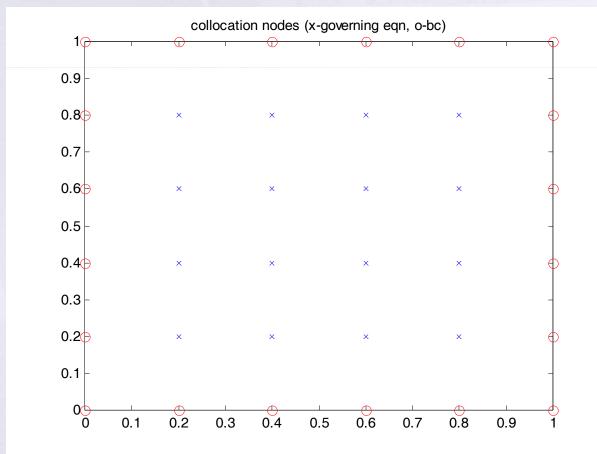
Watch out for the "c"

What Is the Role of c?

- People observe that as c increases, error decreases
- > It is generally believed that as $c \to \infty$, $\epsilon \to 0$
- 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 $c \to \infty$, ε $\to 0$?
- > (Or, is it true that for MFS, as $R \to \infty$, $\epsilon \to 0$?)
- 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	$\varepsilon_{ extbf{max}}$	$arepsilon_{ m rms}$	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	$arepsilon_{ ext{max}}$	$arepsilon_{ m rms}$	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 ^{†,*}	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

$\varepsilon_{ m max}$	$arepsilon_{ m rms}$
2.22×10^{-15}	7.86×10^{-16}
1.91×10^{-15}	9.60×10^{-16}
2.37×10^{-15}	9.26×10^{-16}
2.88×10^{-15}	8.87×10^{-16}
3.58×10^{-15}	1.06×10^{-15}
3.75×10^{-15}	41.2×10^{-15}
	2.22×10^{-15} 1.91×10^{-15} 2.37×10^{-15} 2.88×10^{-15} 3.58×10^{-15}

Find Error Estimate Constants by Data Fitting

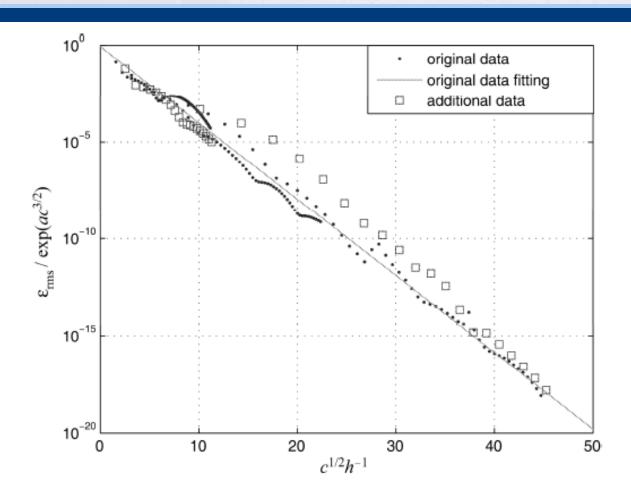


Fig. 2. Fitting for error estimate for IMQ solution of Poisson equation: composite plot of a large number of cases with different h and c values.

Error Estimate

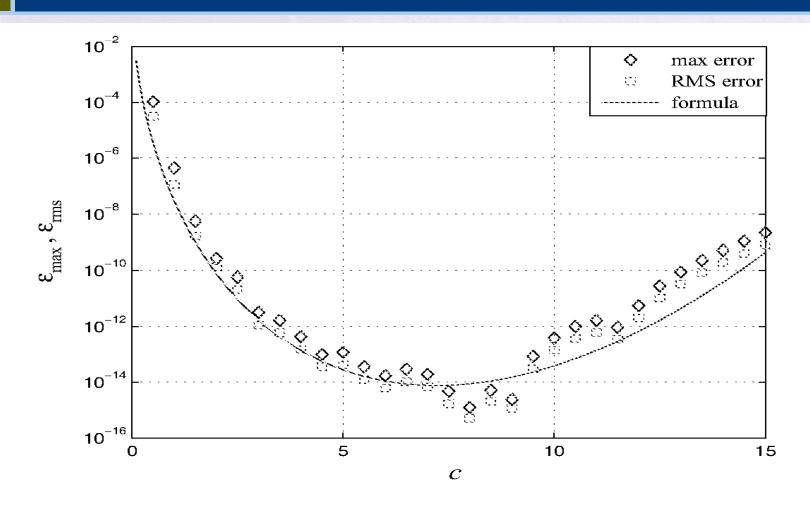


Fig. 5. Validating (15), second example.

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

>
$$h = 1/5$$
, ε ~ 10^{-2}

$$h = 1/10, \varepsilon \sim 10^{-6}$$

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



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

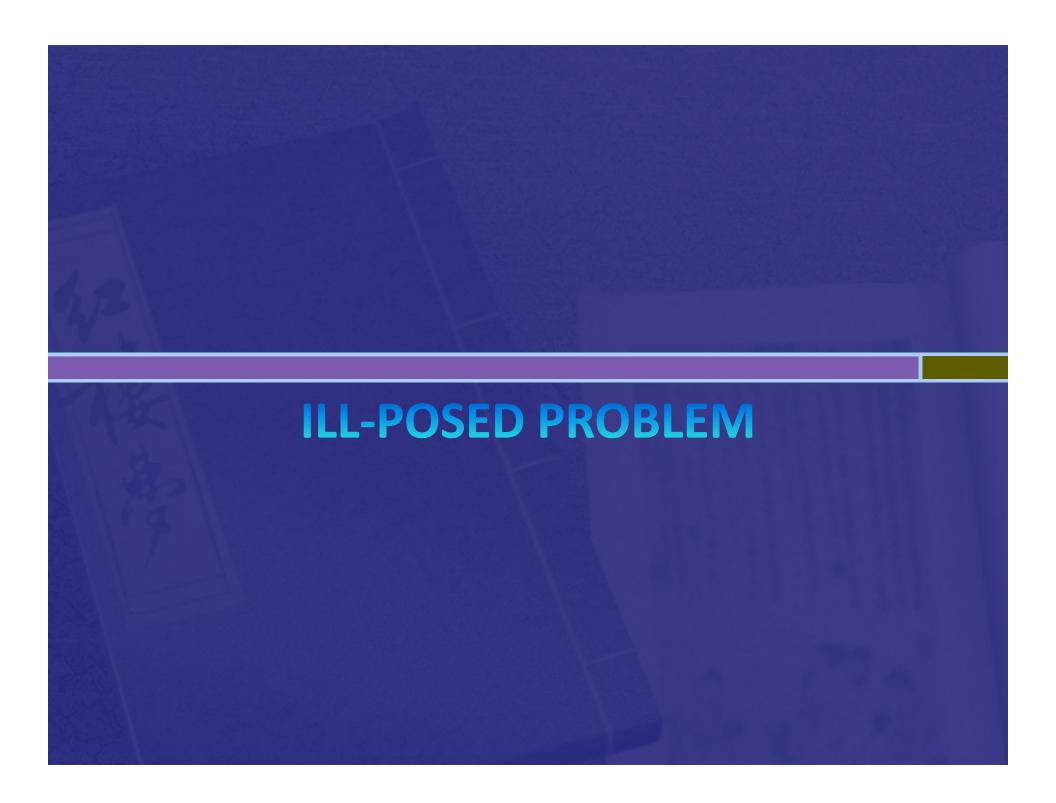
$$\varepsilon = O(e^{ac}\lambda^{c/h}); \quad 0 < \lambda < 1, \quad a > 0$$

> This means, as $c \to \infty$, $\varepsilon \to 0$

 Madych also stated that for a "non-bandlimited" function,

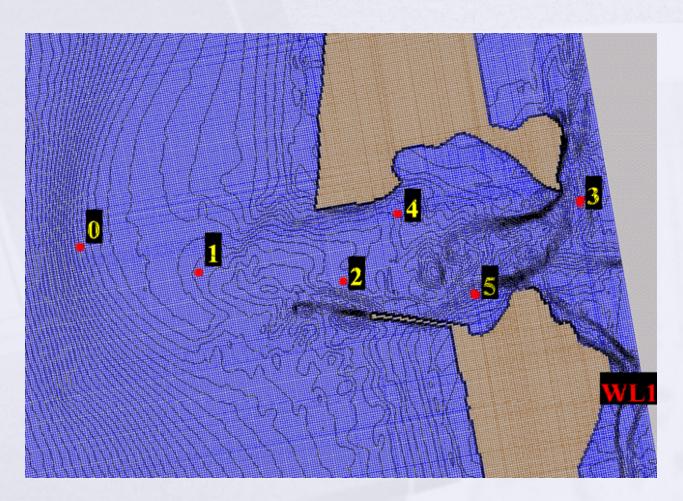
$$\varepsilon = O\left(e^{ac^2}\lambda^{c/h}\right); \quad 0 < \lambda < 1, \quad a > 0$$

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

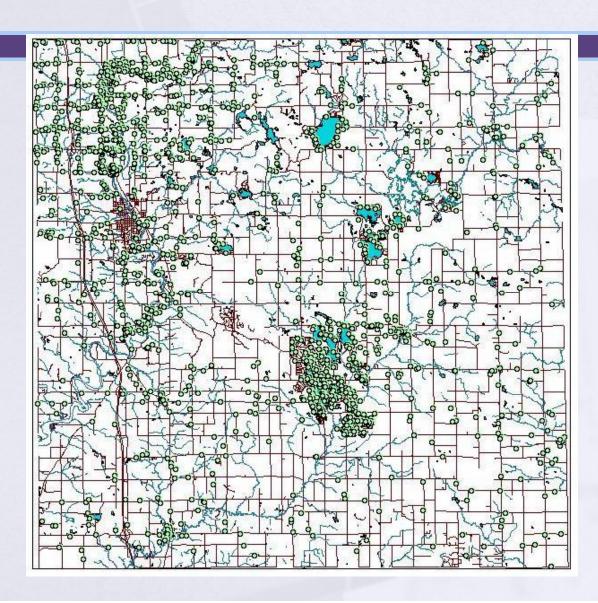


Examples of Ill-Posed Problems

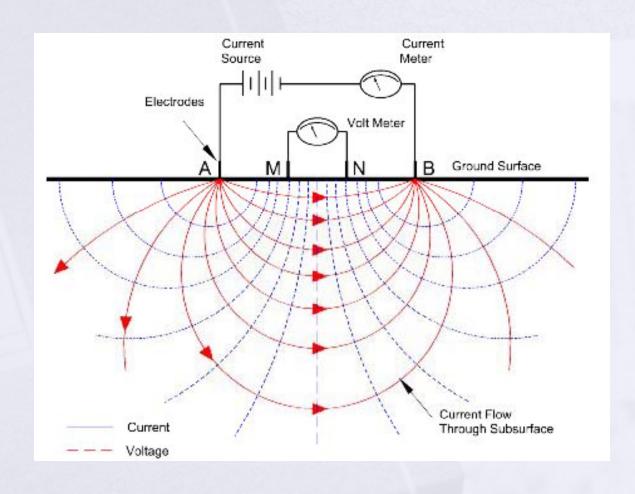
Harbor wave field



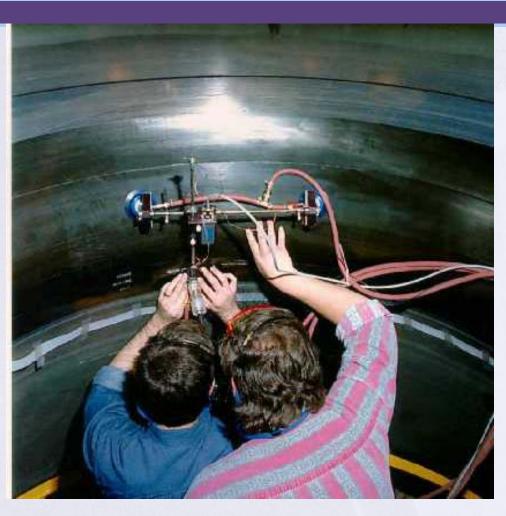
> Groundwater field



Geoprospecting



Non-Destructive Testing



Well- and Ill-Posed Boundary Value Problems

Governing equation

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

Boundary conditions

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

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

> Interior condition

$$u(\boldsymbol{x}_{j}) = \overline{u}_{j}, \quad j = 1, \dots, m, \quad \boldsymbol{x}_{j} \in \Omega$$

Difference between well-posed and ill-posed problems

> Well-posed problem

$$\Gamma_D \cup \Gamma_N = \Gamma$$
 $\Gamma_D \cap \Gamma_N = \emptyset$

$$\Gamma_D \neq \emptyset$$
 $m = 0$

Ill-posed problem

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

$$m \neq 0$$

Problem 1: Onishi (1995) FEM

Governing equation

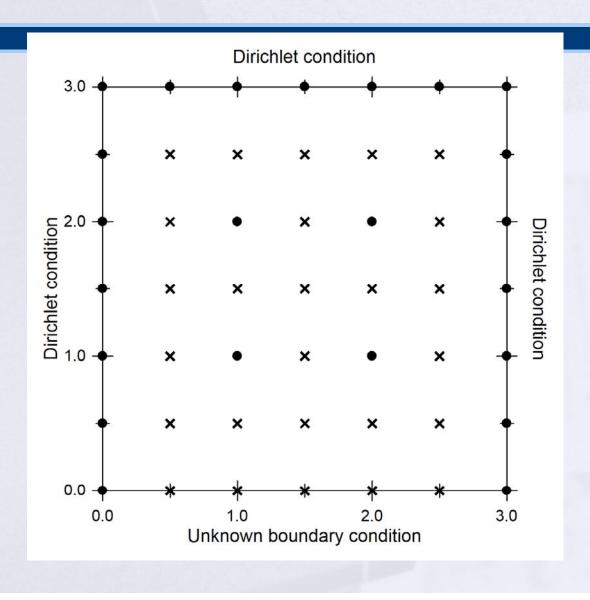
$$\nabla^2 u(x,y) = 0; \quad y \ge 0$$

> BC

$$u(x,3) = x^2 - 9;$$
 $u(0,y) = -y^2;$ $u(3,y) = 9 - y^2$

> Internal values: u(1,1) = 0, u(2,1) = 3, u(1,2) = -3, u(2,2) = 0

Collocation Nodes



Result

Method	Potential value	Percent error	
		(%)	
Exact solution	2.250	0	
Onishi, FEM 36 elements	2.323	3.2	
Onishi, FEM 144 elements	2.341	4.0	
RBF, 49 collocation nodes ($c = 3$)	2.296	2.0	
RBF, 49 collocation nodes ($c = 4$)	2.251	0.04	

Table 1: Comparison of error of potential at the point (1.5, 0).

Problem 2: Lesnic (1998) BEM

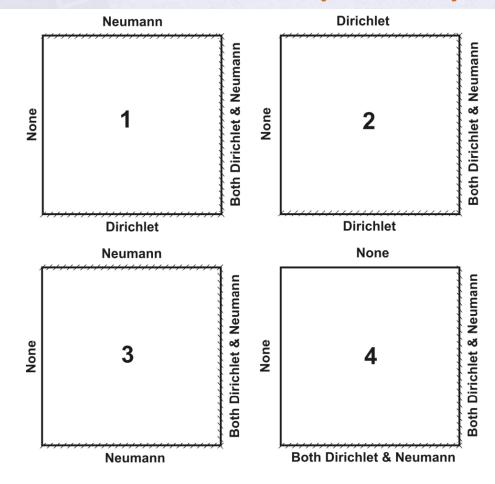


Figure 4: Four cases of Cauchy problems for steady state heat conduction with different boundary conditions (refer to Table 2 for boundary values).

Lesnic Result

	Case 1	Case 2	Case 3	Case 4
Number of elements	40	160	160	160
Number of iterations	100	1000	1000	10000
Error in temperature (%)	0.4	0.5	0.3	13
Error in heat flux (%)	2	6	1.5	50

Table 3: Percentage error of Lesnic's iterative BEM solution at the middle point of left side boundary, (0, 0.5).

RBF Result

Grid	С	Case 1	Case 2	Case 3	Case 4
		(%)	(%)	(%)	(%)
6×6	3	0.04	0.1	1.0	0.5
6×6	4	0.5	0.6	1.7	0.4
8×8	3	0.2	0.02	0.03	0.1
8×8	4	0.1	0.009	0.009	0.06
10×10	3	0.05	0.009	0.009	0.02
10×10	4	0.009	0.000	0.009	0.02

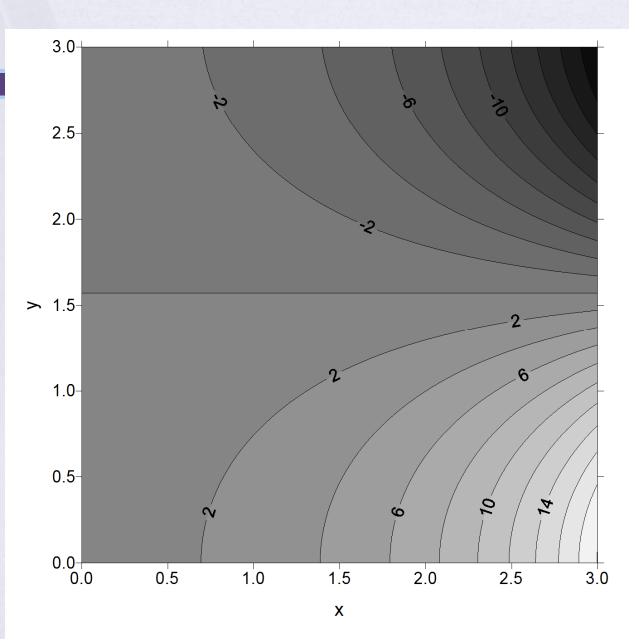
Table 4: Percentage error of RBF collocation solution for temperature at the middle point of left side boundary, (0, 0.5), for different grids and c values.

Grid	c	Case 1	Case 2	Case 3	Case 4
		(%)	(%)	(%)	(%)
6×6	3	0.02	0.8	2.8	6.2
6×6	4	3.2	0.2	3.4	4.0
8×8	3	1.5	0.06	0.1	0.6
8×8	4	0.6	0.06	0.06	0.06
10×10	3	0.6	0.04	0.02	0.1
10×10	4	0.1	0.02	0.2	0.2

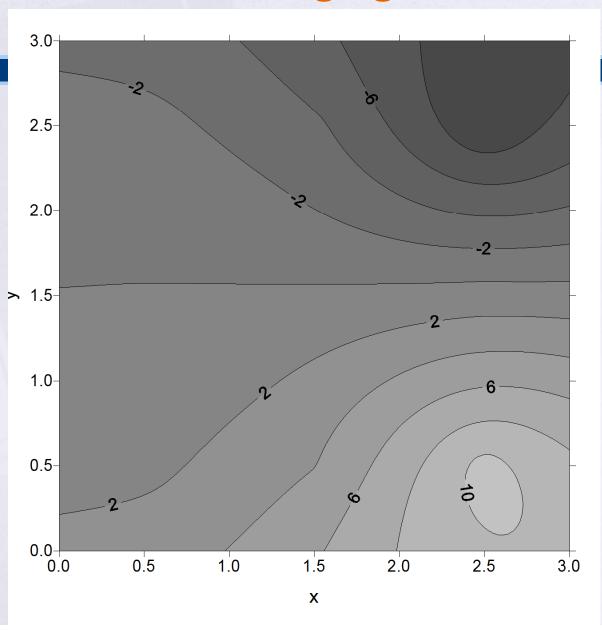
Table 5: Heat flux percentage error of RBF collocation solution at the middle point of left side boundary, (0, 0.5), for different grids and c values.

Problem 3: "Groundwater"

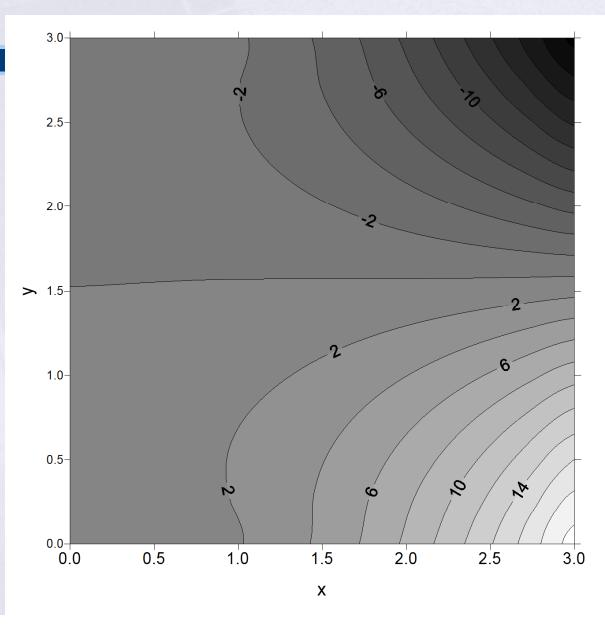
Exact
potential
9 data given

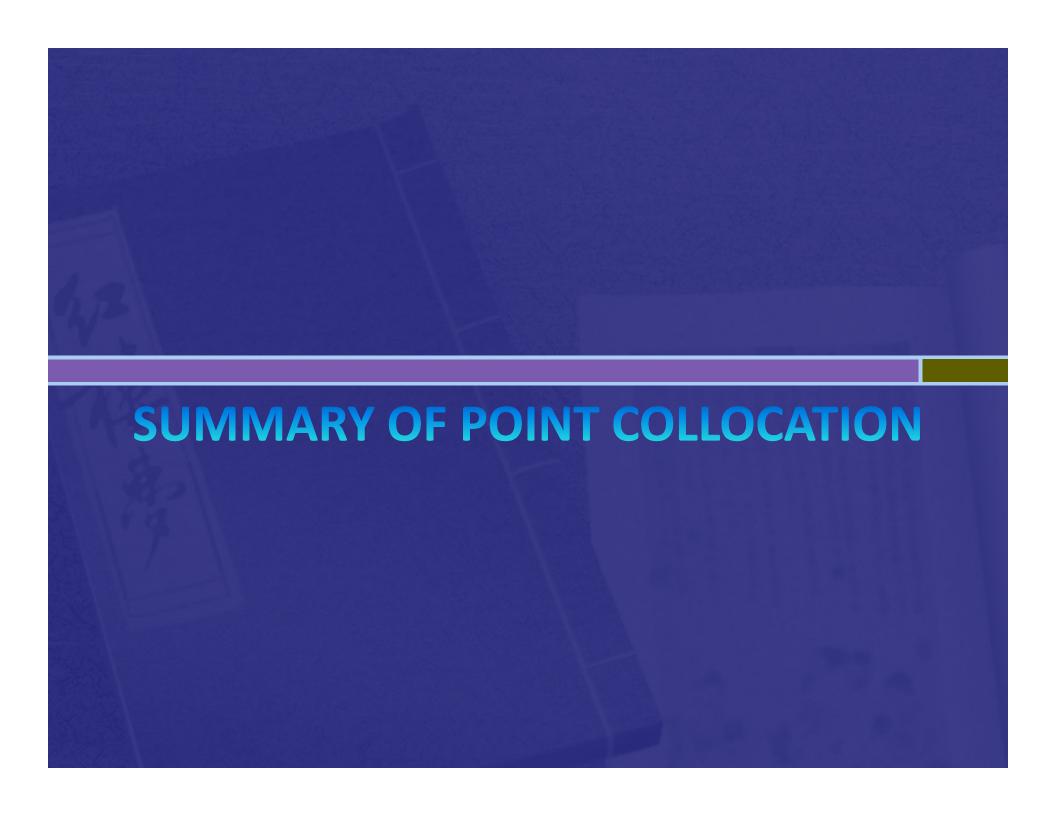


Kriging



Solving III-Posed Problem





Point Collocation

- No geometric approximation error.
- No quadrature error.
- Exponential error convergence,

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

- Convergence is the best if we make the interpolants as flat as possible.
- Meshless
- Solve ill-posed problem without iteration
- > Solve n-D problem