

# MATH 590: Meshfree Methods

## Chapter 1 — Part 1: Introduction and a Historical Overview

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# Outline

- 1 Introduction
- 2 Some Historical Remarks



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# Meshfree Methods

- have gained much attention in recent years
- interdisciplinary field
- many traditional numerical methods (finite differences, finite elements or finite volumes) have trouble with high-dimensional problems
- meshfree methods can often handle changes in the geometry of the domain of interest (e.g., free surfaces, moving particles and large deformations) better
- independence from a mesh is a great advantage since mesh generation is one of the most time consuming parts of any mesh-based numerical simulation
- new generation of numerical tools





# Applications

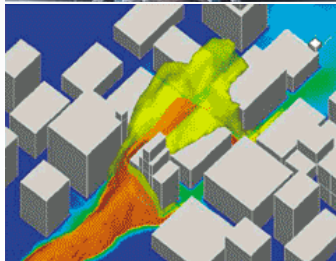
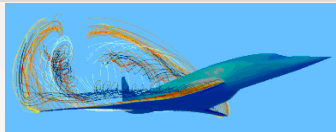
- Original applications were in geodesy, geophysics, mapping, or meteorology
- Later, many other application areas
  - numerical solution of PDEs in many engineering applications,
  - computer graphics,
  - optics,
  - artificial intelligence,
  - machine learning or statistical learning (neural networks or SVMs),
  - signal and image processing,
  - sampling theory,
  - statistics (kriging),
  - response surface or surrogate modeling,
  - finance,
  - optimization.



# Complicated Domains

Recent paradigm shift in numerical simulation of fluid flow:

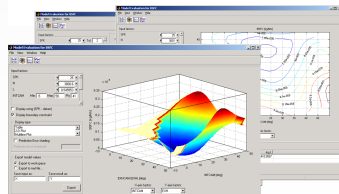
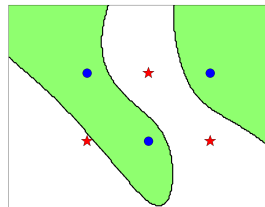
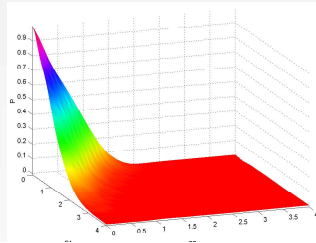
- growing demand to perform numerical simulations associated with complicated domains and geometries
  - complete aircraft configurations
  - turbo-machinery
  - urban domains



# High-Dimensional Domains

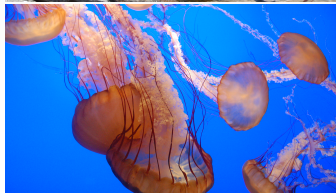
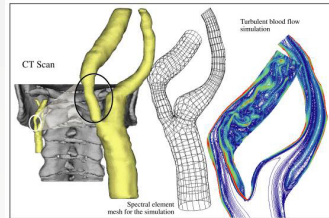
More and more applications “live” in high “space” dimensions

- pricing of basket options in finance
- classification or regression problems in machine learning
- surrogate modeling for computer experiments or other design purposes



# Life Sciences

- growing demand for flow simulation in the life sciences
  - blood flow simulations
  - flight dynamics of birds and insects (micro air-vehicles)
  - motion of fish and jellyfish



## Special Movie Effects <http://www.polhemus.com/>

Based on point cloud modeling (also look at [LotR]).



# Medical Applications <http://www.fastscan3d.com>



# Waves

- simulation of ocean waves
  - design of boats and ships in turbulent oceans
- splash dynamics
  - spacecraft and oil tankers



# Energy

- renewable energy sector
  - study of single wind turbines and whole wind farms





# A Long List of Meshfree Methods *Not* Discussed

In this class we do not plan to focus on any of the following methods, also known as **meshfree** (or **meshless**) **methods**:

- element-free Galerkin method (EFG),
- Hp-clouds,
- moving least squares (MLS),
- meshless local Petrov-Galerkin method (MLPG),
- partition of unity finite element method (PUFEM),
- reproducing kernel particle method (RKPM),
- smoothed particle hydrodynamics (SPH),
- extended finite element method (XFEM)
- and many others.

The list on [Wikipedia](#) is endless.

Some references are [Atl04, AS02, BC07, LL07, Liu02, LL03].



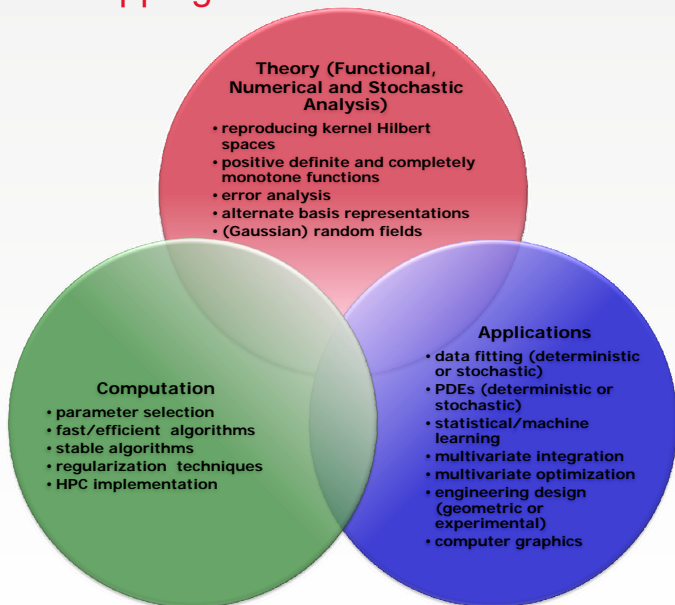
We will focus mostly on the **underlying math of kernel-based methods**. In your project you are encouraged to **work on an application**.

### Types of math involved:

- approximation theory
- numerical analysis
- linear algebra
- functional analysis
  - positive definite reproducing kernels
  - Sturm–Liouville theory and Green’s kernels
  - (generalized) Fourier series
  - Hilbert–Schmidt integral operators
- stochastic analysis and statistics
  - Gaussian random fields
  - maximum likelihood estimation
- harmonic analysis
- special functions
- measure theory
- theoretical computer science



# Three Overlapping Domains



Books that contain a significant portion on positive definite kernels:

**Analysis:** [AM02], [AG93], [Aub00], [BCR84], [Ber50], [Boc32], [Mes62], [Moo35], [RSN55], [Rit00], [Sai88, Sai97], [WW76]

**Approximation Theory:** [Buh03], [CL99], [Fas07], [FGS98], [GC98], [Isk04], [NW08], [Wen05]

**Integral Equations:** [Coc72], [Hac89], [Hoc73], [Kre99], [Pog66], [Smi58], [Sta79]

**Mathematical Physics:** [BS53], [CH53], [MF53]

**Engineering and Physics Applications:** [AAG00], [Atl04], [AS02], [BC07], [CFC14], [FSK08], [GS03], [LL07], [Liu02], [LL03], [VT01]

**Probability Theory and Statistics:** [BTA04], [Gu13], [RS05], [Wah90]

**Geostatistics:** [Cre93], [Kit97], [Mat86], [Mat65], [Ste99]

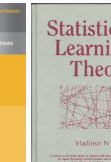
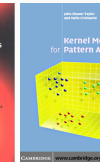
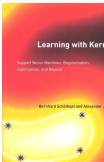
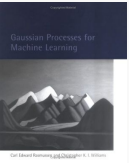
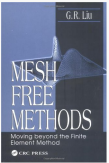
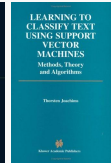
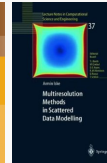
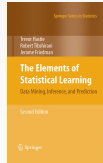
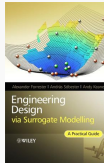
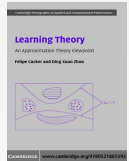
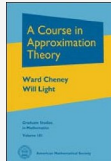
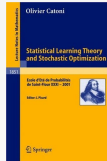
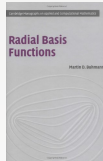
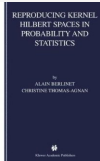
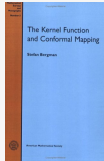
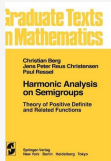
**Statistical/Machine Learning:** [Alp09], [Cat04], [CST00], [CZ07], [HTF09], [Her02], [Joa02], [RW06], [SS02], [STC04], [SC08], [SGB<sup>+</sup>02], [Vap98]

Important (review) papers:

**Historical:** [Aro50], [Hil72], [Mer09], [Sch08], [Ste76]

**Modern:** [Buh00], [CS02], [Dyn87, Dyn89], [Fas11], [FM13], [Pow87, Pow92], [Sch99, Sch00], [SW06], [SSS13].





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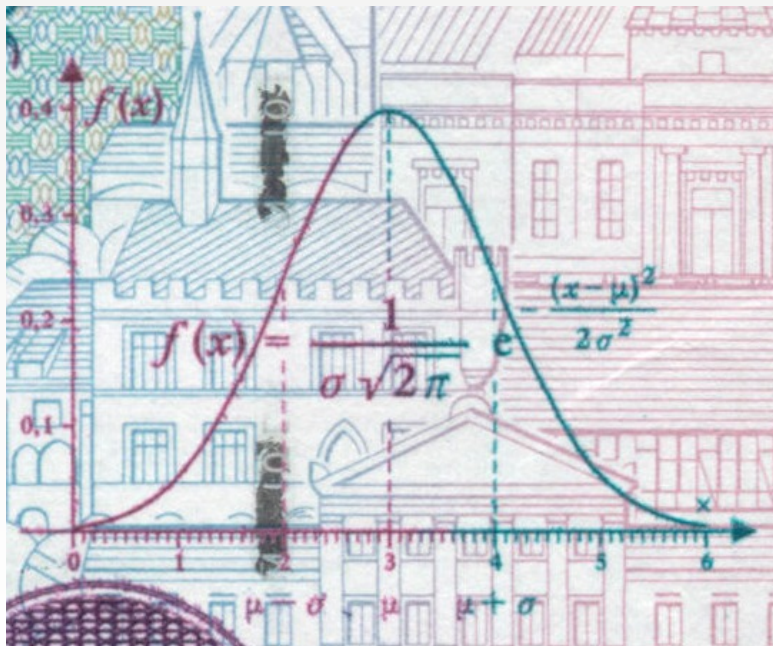




## The Gaussian kernel







THEORIA  
MOTVS CORPORVM  
COELESTIVM

IN

SECTIONIBVS CONICIS SOLEM AMBIENTIVM

AVCTORE

CAROLO FRIDERICO GAVSS

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HAMBVRGI SVMTIBVS FRID. PERTHES ET I. H. BESSER  
1809.

Venditur

PARISIIS ap. Treuttel & Würtz. LONDINI ap. R. H. EVANS.  
STOCKHOLMIAE ap. A. Wiborg. PETROFOLI ap. Klostermann.  
MADRIVI ap. Sancha. FLORENTIAE ap. Molini, Landi & C.  
AMSTELODAMI in libreria: Kunst- und Industrie-Comptoir, dicta.



Porro facile perspicitur,  $k$  necessario negativam esse debere, quo  $\Omega$  reuera fieri possit maximum, quamobrem statuemus  $\frac{1}{2}k = -hh$ ; et quum per theorema elegans primo ab ill. Laplace inuentum, integrale  $\int e^{-hh\Delta\Delta} d\Delta$ , a  $\Delta = -\infty$  vsque ad  $\Delta = +\infty$ , fiat  $= \frac{\sqrt{\pi}}{h}$ , (denotandó per  $\pi$  semicircumferentiam circuli cuius radius 1), functio nostra fiet

$$\varphi \Delta = \frac{h}{\sqrt{\pi}} e^{-hh\Delta\Delta}$$

Moreover, it is readily perceived that  $k$  must be negative, in order that  $\Omega$  may really become a maximum, for which reason we shall put

$$\frac{1}{2}k = -hh;$$

and since, by the elegant theorem first discovered by LAPLACE, the integral

$$\int e^{-hh\Delta\Delta} d\Delta$$

from  $\Delta = -\infty$  to  $\Delta = +\infty$  is  $\frac{\sqrt{\pi}}{h}$ , (denoting by  $\pi$  the semicircumference of the circle the radius of which is unity), our function becomes

$$\varphi \Delta = \frac{h}{\sqrt{\pi}} e^{-hh\Delta\Delta}.$$

[Gau09, Sect.177], Engl. translation [Gau57]



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## Nachman Aronszajn (1907-1980) and Stefan Bergman (1895-1977)

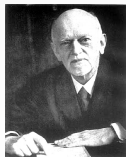
- Aronszajn was at the University of Kansas, Bergman was at Harvard and later Stanford.
- They are credited with independently introducing **reproducing kernels** [Aro50, Ber50]. Aronszajn had some earlier work in [Aro43]. Bergman already had some bits in his Ph.D. thesis [Ber21].
- The kernel  $K$  is a **symmetric function of two variables**

$$K : \Omega \times \Omega \rightarrow \mathbb{R} \quad \text{s.t.} \quad K(\mathbf{x}, \mathbf{z}) = K(\mathbf{z}, \mathbf{x}), \quad \text{where } \Omega \subseteq \mathbb{R}^d.$$

- The kernel is **reproducing** in the following sense:

$$\langle K(\mathbf{x}, \cdot), f \rangle_{\mathcal{H}_K(\Omega)} = f(\mathbf{x}),$$

where  $\mathcal{H}_K(\Omega)$  is a **Hilbert space** of functions on  $\Omega$ .



[http://en.wikipedia.org/wiki/Nachman\\_Aronszajn](http://en.wikipedia.org/wiki/Nachman_Aronszajn)

[http://en.wikipedia.org/wiki/Stefan\\_Bergman](http://en.wikipedia.org/wiki/Stefan_Bergman)



## James Mercer (1883-1932) and Erhard Schmidt (1876-1959)

- Mercer was at Cambridge University, Schmidt (a student of Hilbert's) was at the University of Berlin (now called Humboldt U.).
- Prompted by Hilbert's ground-breaking [Hil04], they independently introduced **series expansions of positive definite kernels** in [Mer09, Sch07, Sch08]:
  - Mercer's theorem (used heavily in machine learning)
  - Hilbert-Schmidt theory (also Gram-Schmidt orthogonalization)



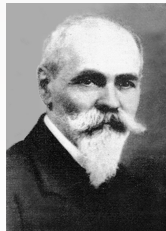
[http://en.wikipedia.org/wiki/James\\_Mercer\\_\(mathematician\)](http://en.wikipedia.org/wiki/James_Mercer_(mathematician))

[http://en.wikipedia.org/wiki/Erhard\\_Schmidt](http://en.wikipedia.org/wiki/Erhard_Schmidt)



## E.H. Moore (1862-1932), Stanislaw Zaremba (1863-1942), Maximilian Mathias (1895-?)

- Moore and Zaremba were professors of mathematics at Chicago, and Jagiellonian University in Kraków, respectively. Mathias was a PhD student of Erhard Schmidt in Berlin.
- Moore called his version of reproducing kernels **positive Hermitian matrices** [Moo16, Moo35].
- Zaremba introduced the **reproducing property** in [Zar07, Zar09].
- Mathias wrote his thesis [Mat23] on **positive definite functions**.



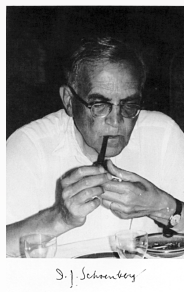
[http://en.wikipedia.org/wiki/E\\_H\\_Moore](http://en.wikipedia.org/wiki/E_H_Moore)

[http://en.wikipedia.org/wiki/Stanislaw\\_Zaremba\\_\(mathematician\)](http://en.wikipedia.org/wiki/Stanislaw_Zaremba_(mathematician))



## Salomon Bochner (1899-1982) and Iso Schoenberg (1903-1990)

- Bochner (also a student of Schmidt's) was at Princeton and then at Rice University, Schoenberg was at the University of Wisconsin-Madison.
- One of Bochner's fundamental results is **Bochner's theorem**, which characterizes positive definite functions in terms of Fourier transforms [Boc32, Boc33].
- Schoenberg is known as the father of **splines**. He also characterized positive definite functions, especially radial ones [Sch37, Sch38a, Sch38b].



[http://en.wikipedia.org/wiki/Salomon\\_Bochner](http://en.wikipedia.org/wiki/Salomon_Bochner)

[http://en.wikipedia.org/wiki/Isaac\\_Jacob\\_Schoenberg](http://en.wikipedia.org/wiki/Isaac_Jacob_Schoenberg)





## Marc Atteia

- Was at the Université Joseph Fourier in Grenoble in the 60s, later at the Université Paul Sabatier in Toulouse.
- Possibly the first to use the term **spline** in the general multivariate setting.
- Established the foundations of a **variational theory via Green's kernels interpreted as reproducing kernels** in the sense of Aronszajn and Bergman in [Att66].



## Aleksandr Khinchin (1894-1959), Kari Karhunen (1915-1992), Michel Loève (1907-1979)

- Khinchin was a professor of mathematics at Moscow State University, Karhunen was in Helsinki and Loève at Berkeley.
- Khinchin established the foundation for **stationary stochastic processes** in [Khi34] using Bochner's theorem.
- Karhunen and Loève established the **Karhunen–Loève theorem**, a series representation for stochastic processes [Kar47, Loè77].



[http://en.wikipedia.org/wiki/Aleksandr\\_Khinchin](http://en.wikipedia.org/wiki/Aleksandr_Khinchin)

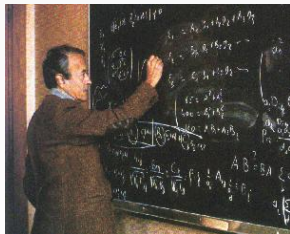
[http://en.wikipedia.org/wiki/Kari\\_Karhunen](http://en.wikipedia.org/wiki/Kari_Karhunen)

[http://en.wikipedia.org/wiki/Michel\\_Loeve](http://en.wikipedia.org/wiki/Michel_Loeve)



## Danie Krige (1919-2013) and Georges Matheron (1930-2000)

- Krige was a professor of geostatistics at the University of Witwatersrand.
- Invented the so-called **kriging method** in [Kri51].
- Matheron was a professor of mathematics and geostatistics at the Paris School of Mines in Fontainebleau.
- One of the founders of geostatistics who established the **mathematical theory for kriging** in his Ph.D. thesis [Mat65].



[http://en.wikipedia.org/wiki/Danie\\_Krige](http://en.wikipedia.org/wiki/Danie_Krige)

[http://en.wikipedia.org/wiki/Georges\\_Matheron](http://en.wikipedia.org/wiki/Georges_Matheron)



## Rolland L. Hardy (1920-2009) and Richard Franke

- Hardy was a professor of civil and construction engineering at Iowa State University (retired 1988). Franke was a mathematician at the Naval Postgraduate School in Monterey, California (retired 2001).
- Hardy introduced **multiquadrics** (MQs) in the early 1970s (see, e.g., [Har71]).
- His work was primarily concerned with applications in geodesy and mapping.
- Franke compared various scattered data interpolation methods [Fra79, Fra82], and concluded MQs and TPSs were the best. Conjectured that the interpolation matrix for MQs is invertible.



## Robert L. Harder and Robert N. Desmarais (1930-2008)

- Aerospace engineers at MacNeal-Schwendler Corporation (MSC Software), and NASA's Langley Research Center.
- Introduced **thin plate splines** (TPSs) in 1972 [HD72].
- Work was concerned mostly with aircraft design.



[http://en.wikipedia.org/wiki/Thin\\_plate\\_spline](http://en.wikipedia.org/wiki/Thin_plate_spline)



## Jean Duchon and Jean Meinguet

- Duchon is a senior researcher in mathematics at the Université Joseph Fourier in Grenoble, France. Meinguet was a mathematics professor at Université Catholique de Louvain, Belgium (retired 1996).
- Duchon provided the foundation for a **variational approach** minimizing the integral of  $\nabla^2 f$  in  $\mathbb{R}^2$  [Duc76, Duc77, Duc78, Duc80]. This also leads to **thin plate splines**.
- Meinguet introduced **surface splines** in the late 1970s [Mei79c, Mei79b, Mei79a, Mei84].
- Surface splines and thin plate splines are both considered as **polyharmonic splines**.



[http://en.wikipedia.org/wiki/Polyharmonic\\_spline](http://en.wikipedia.org/wiki/Polyharmonic_spline)



# Wolodymyr (Wally) Madych and Stuart Alan Nelson

- Both professors of mathematics. Madych at the University of Connecticut, and Nelson at Iowa State University (now retired).
- **Proved Franke's conjecture** (and much more) based on a variational approach in [MN83]. This manuscript was never published.



## Charles Micchelli

- Used to be a mathematician at IBM Watson Research Center. Now a professor at the State University of New York, Albany.
- Published [Mic86] in which he **also proved Franke's conjecture**. His proofs are rooted in the work of Bochner and Schoenberg on positive definite and completely monotone functions.
- His approach is followed throughout much of [Fas07].





## Grace Wahba

- I. J. Schoenberg Professor of statistics at the University of Wisconsin-Madison.
- Studied the use of thin plate splines for statistical purposes in the context of smoothing splines for **noisy data** and data on spheres.
- Introduced ANOVA and cross validation approaches to the radial basis function setting (e.g., [Wah79, Wah81, Wah82, WW80]).
- One of the first monographs on the subject is [Wah90].



[http://en.wikipedia.org/wiki/Grace\\_Wahba](http://en.wikipedia.org/wiki/Grace_Wahba)



## Nira Dyn and David Levin

- Professors of applied mathematics at Tel-Aviv University.
- They first used the term **radial basis function** in [DL83], and were one of the first proponents of radial basis function methods in approximation theory (see, e.g., the surveys [Dyn87, Dyn89]).
- Dyn collaborated early with Grace Wahba on connections between numerical analysis and statistics via smoothing splines (see [DWW79, DW82]).
- Both have also contributed to many other areas of approximation theory (including subdivision, MLS and computer graphics).



## Robert Schaback and Holger Wendland

- Professor of mathematics at University of Göttingen (retired 2011).
- Introduced **compactly supported RBFs** [Sch95].
- Another popular family of CSRBFs was presented by Holger Wendland (professor of mathematics at University of Bayreuth) in his Ph.D. thesis at Göttingen (see also [Wen95]).
- Both have contributed extensively to the field of radial basis functions (see, e.g., the many surveys [Sch99, Sch00, SW06, SSS13] and the book [Wen05]).



## Ed Kansa

- Physicist at Lawrence Livermore National Laboratory, California (retired).
- First proposed the use of radial basis functions for the solution of PDEs [Kan86].
- Later papers [Kan90a, Kan90b] proposed “Kansa’s method” (or non-symmetric collocation).



[http://en.wikipedia.org/wiki/Kansa\\_method](http://en.wikipedia.org/wiki/Kansa_method)



# Bengt Fornberg

- Professor of applied mathematics at the University of Colorado at Boulder.
- Has done lots of seminal work (together with a number of co-workers) on **stable evaluation of RBFs** and **RBF solution of PDEs**.
- Has also written an important book on (polynomial) pseudospectral methods [For98].



## Vladimir Vapnik

- Professor of computer science at Columbia University.
- First used reproducing kernels in machine learning as **support vector machines** in [BGV92] while at Bell Labs. This was based on [VL63].
- Author of the first book of statistical learning theory [Vap98].



[http://en.wikipedia.org/wiki/Vladimir\\_Vapnik](http://en.wikipedia.org/wiki/Vladimir_Vapnik)



# References I

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- [AM02] J. Agler and J. E. McCarthy, *Pick Interpolation and Hilbert Function Spaces*, American Mathematical Soc., 2002 (en).
- [Aro43] N. Aronszajn, *La théorie des noyaux reproduisants et ses applications, Première Partie*, Mathematical Proceedings of the Cambridge Philosophical Society **39** (1943), no. 03, 133–153.
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