

Solving Partial Differential Equations by Collocation using Radial Basis Functions

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Abstract

After a series of application papers have proven the approach to be numerically effective, this paper gives the first theoretical foundation for methods solving partial differential equations by collocation with (possibly radial) basis functions.

0 Introduction

We consider a general class of boundary or initial value problems for partial differential equations:

$$\begin{aligned} Lu = f & \quad \text{in } \Omega \subset \mathbb{R}^d & L : \mathcal{W}_\Omega & \rightarrow \mathcal{L}_\Omega \\ Bu = g & \quad \text{in } \partial\Omega & B : \mathcal{W}_\Omega & \rightarrow \mathcal{W}_{\partial\Omega}. \end{aligned} \tag{0.1}$$

Here, the operator L is a linear partial differential operator, and B is a “boundary” operator that prescribes values on (possibly only part of) the boundary $\partial\Omega$ of the underlying bounded domain $\Omega \in \mathbb{R}^d$. The domain and range spaces can be viewed as certain instances of Sobolev or L_2 spaces such that appropriate trace theorems hold. We can also allow multiple differential, integral, or boundary operators, but we do not want to introduce too much notation at this stage.

The goal of this paper is to prove the feasibility of collocation methods using radial basis functions. The solution u of the PDE is approximated by

$$u \approx u_h, \quad u_h \in \mathcal{S}_h \subset \mathcal{W}_\Omega,$$

where \mathcal{S}_h is a space of trial or “ansatz” functions that consists of linear combinations of translates of a single global *basis* function $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$ and/or of translates of its multivariate derivatives

$$\frac{\partial^\alpha}{\partial x^\alpha} \Phi(\cdot - x) \quad \text{or} \quad L\Phi(\cdot - \cdot)$$

using the differential operator L arising in the problem setting. If $\Phi(\cdot) = \phi(\|\cdot\|_2)$ holds for a univariate function $\phi : \mathbb{R} \rightarrow \mathbb{R}$, then Φ is called a *radial* basis function. The most important examples of the latter are

| | | |
|--------------------|--|--|
| Gaussians | $\exp(-c\ \cdot\ _2^2)$ | $c > 0$ |
| Multiquadrics | $(c^2 + \ \cdot\ _2^2)^{\beta/2}$ | $c > 0, \beta \in \mathbb{R}_{\neq 0} \setminus 2\mathbb{N}$ |
| thin-plate splines | $\ \cdot\ _2^\beta$ | $\beta \in \mathbb{R}_{>0} \setminus 2\mathbb{N}$ |
| | $\ \cdot\ _2^\beta \log \ \cdot\ _2$ | $\beta \in 2\mathbb{N}$ |
| Wendland functions | $(1 - \ \cdot\ _2)_+^m p(\ \cdot\ _2)$ | p polynomial, [15] |

However, we do not want to restrict ourselves to radial functions here. Furthermore, one can generalize the above setting by using $\Phi(x, y)$ instead of $\Phi(x - y)$, with Φ now defined on $\mathbb{R}^d \times \mathbb{R}^d$. To cope with nonconvex domains having inward corners, we can finally enlarge \mathcal{S}_h by adding specific functions with singular derivatives, depending on the angle of the corner. But in order to keep the paper short, we omit such details.

There is quite some literature on the practical feasibility of collocation with radial basis functions, see e.g. [8], [3], [9], [2], [14], and [5] in chronological order. However, none of the above papers provides a convergence proof or an error bound, and it will be the goal of this paper to fill that gap partially. On the positive side, these papers contain various numerical examples showing that one can get use collocation with radial basis functions to get good results at reasonably low computational cost. Therefore this paper does not contain any further numerical examples; the reader is referred to the above papers for practical test cases. These still work with globally defined functions that imply non-sparse “stiffness matrices”. But if the new compactly supported positive definite functions [15] are used, these matrices become sparse and the numerical complexity decreases dramatically, thus opening a wider range of applications.

On the other hand, there is another list of applied papers [10], [18], [17], and [6] that consider the solution of homogenized PDE problems by approximation with radial basis functions in the interior of the domain. The homogenization can in turn be done comfortably by approximation of boundary values with radial basis functions, because the latter have nicely behaving extensions to all of \mathbb{R}^d . Again, the above papers lack a theoretical foundation, but this will be supplied by the parallel paper [13].

Finally, Iske and Sonar [7] apply radial basis functions to reconstruct function values of solutions of hyperbolic conservation laws from results of ENO schemes. This is an application of radial basis functions which only very indirectly involves the underlying PDE, but it nicely shows the good approximation properties of radial basis functions.

1 Collocation as Hermite–Birkhoff interpolation

We want to specify our collocation techniques as special instances of general Hermite–Birkhoff interpolation methods. To this end, we split the given collocation problem into two interpolation problems on the domain Ω and its boundary $\partial\Omega$, respectively:

$$\begin{array}{c|c}
 \text{Domain} & \text{Boundary} \\
 \hline
 X_1 = \{x_1, \dots, x_n\} \subset \overline{\Omega} & X_2 = \{x_{n+1}, \dots, x_N\} \subset \partial\Omega \\
 Lu_h = f \text{ in } X_1 & Bu_h = g \text{ in } X_2 \\
 \lambda_j(u) := (Lu)(x_j), 1 \leq j \leq n & \lambda_j(u) := u(x_j), n+1 \leq j \leq N \\
 \lambda_j(u_h) = f(x_j), 1 \leq j \leq n & \lambda_j(u_h) = g(x_j), n+1 \leq j \leq N
 \end{array}$$

This amounts to a Hermite–Birkhoff interpolation problem of finding a function u_h such that

$$\lambda_j(u_h) = y_j \in \mathbb{R}, 1 \leq j \leq N$$

holds for N functionals $\lambda_1, \dots, \lambda_N$ of mixed type. Note that the addition of other differential or boundary operators would just add some more types of functionals and is no major complication.

We now want to define a proper space of trial functions. Due to the Mairhuber–Curtis theorem [1], a space for genuinely multivariate interpolation of functions must depend on the data functionals. This can be done in our situation by picking a fixed *basis function* $\Phi \in L_2(\mathbb{R}^d) \cap C(\mathbb{R}^d)$ which is symmetric, smooth, and positive definite in the sense that for all choices of points $x_1, \dots, x_N \in \mathbb{R}^d$ and all $N \in \mathbb{N}$ the matrix

$$(\Phi(x_m - x_\ell))_{1 \leq \ell, m \leq N} \tag{1.1}$$

is positive definite. The collocation technique of Kansa [8] then forms the space

$$\mathcal{S}_h := \left\{ s_h = \sum_j \alpha_j \Phi(\cdot - x_j) \right\}$$

for collocation with general functionals $\lambda_1, \dots, \lambda_N$. This space is quite appropriate if only point evaluation functionals are considered, but in the general situation of collocation we have to replace the symmetric and positive definite matrix (1.1) by the nonsymmetric matrix

$$\left(\lambda_j^y \Phi(y - x_\ell) \right) \quad 1 \leq j, \ell \leq N$$

whose nonsingularity is an open problem. This is due to the fact that the functionals $\lambda_1, \dots, \lambda_N$ enter the definition of the space \mathcal{S}_h only via their locations x_1, \dots, x_N . As already pointed out by Wu [16] and later in the PDE context by Fasshauer [5], a mathematically well-supported way to define the space \mathcal{S}_h is

$$\mathcal{S}_h := \left\{ s_h = \sum_j \alpha_j \lambda_j^y \Phi(\cdot - y) \right\}.$$

Here λ_j^y denotes action of the functional λ_j with respect to the variable y . This requires Φ to be sufficiently smooth as to allow the application of the functionals $\lambda_1, \dots, \lambda_N$ to *both* arguments x and y of $\Phi(x - y)$. This practical rule-of-thumb is sufficient for practical applications, but needs justification in the sequel. The resulting collocation matrix consists of applications of the functionals $\lambda_1, \dots, \lambda_N$ to *both* arguments of Φ and thus writes as

$$\left(\lambda_j^x \lambda_k^y \Phi(x - y) \right) \quad 1 \leq j, k \leq N. \quad (1.2)$$

It turns out to be symmetric and positive definite in general, if the functionals are linearly independent and if the smoothness assumption on Φ is formulated properly.

To facilitate such a definition, we refer to Fourier transform notation as in the review article [12] and assume Φ to have a Fourier transform $\Phi^\wedge > 0$ a.e. which is in $L_1(\mathbb{R}^d) \cap L_2(\mathbb{R}^d)$. Then we define the *native* space

$$\mathcal{F}_\Phi := \left\{ u \in L_2(\mathbb{R}^d) : u^\wedge / \sqrt{\Phi^\wedge} \in L_2(\mathbb{R}^d) \right\}$$

for Φ , which is the unique Hilbert space on which Φ introduces a certain natural inner product that we do not need in this context. But our central assumption

on the relation of the functionals $\lambda_1, \dots, \lambda_N$ to Φ is that they belong to the dual of the native space for Φ , i.e. to the space

$$\mathcal{F}_\Phi^* := \left\{ \lambda : \lambda^\wedge \cdot \sqrt{\Phi^\wedge} \in L_2(\mathbb{R}^d) \right\},$$

where the Fourier transform of a functional λ is assumed to be expressible via a function λ^\wedge on \mathbb{R}^d such that

$$\lambda(u) = \int_{\mathbb{R}^d} \lambda^\wedge(\omega) u^\wedge(\omega) d\omega$$

holds at least for all tempered test functions u in the Schwartz space. We illustrate this requirement later. The crucial result due to Wu [16] for our revised collocation technique then is

Theorem 1.3 *If $\lambda_1, \dots, \lambda_N \in \mathcal{F}_\Phi^*$ are linearly independent, then the matrix (1.2) arising in Hermite-Birkhoff interpolation*

$$\lambda_j(s) = y_j, \quad 1 \leq j \leq N, \quad s \in \mathcal{S}_h$$

is positive definite.

Let us illustrate the condition $\lambda_1, \dots, \lambda_N \in \mathcal{F}_\Phi^*$ for the differential operator $L = \Delta$. The functionals $\lambda_j(u) = (\Delta u)(x_j)$ for $x_j \in \mathbb{R}^d$ have a Fourier transform $\lambda_j^\wedge(\omega) = -(2\pi)^{-d} \|\omega\|_2^2 \exp(i\omega x_j)$ for $\omega \in \mathbb{R}^d$. The usual basis functions Φ have a d -variate Fourier transform Φ^\wedge of at least algebraic decay, i.e.

$$\Phi^\wedge(\omega) = \mathcal{O}(\|\omega\|_2^{-d-\beta}), \quad \omega \rightarrow \infty$$

for some positive β . Then

$$\lambda_j^\wedge \cdot \sqrt{\Phi^\wedge}(\omega) = \mathcal{O}(\|\omega\|_2^{2-d/2-\beta/2}), \quad \omega \rightarrow \infty$$

and the conditions $\lambda_j^\wedge \cdot \sqrt{\Phi^\wedge} \in L_2(\mathbb{R}^d)$ and $\lambda_j \in \mathcal{F}_\Phi^*$ are satisfied, if $\beta > 4$ holds. This condition amounts to a smoothness requirement for Φ in terms of Fourier transforms, and it is satisfied for Gaussians, multiquadrics, and Wendland's [15] compactly supported positive definite radial functions

$$\begin{aligned} \Phi(x) &= (1 - \|x\|_2)_+^6 (35\|x\|_2^2 + 18\|x\|_2 + 3) && \in C^4(\mathbb{R}^d) \\ \Phi(x) &= (1 - \|x\|_2)_+^8 (32\|x\|_2^3 + 25\|x\|_2^2 + 8\|x\|_2 + 1) && \in C^6(\mathbb{R}^d), \end{aligned}$$

for instance. The two functions above require $d \leq 3$.

Note that the condition $\beta > 4$ requires a degree of smoothness of Φ that makes the functions in the trial space \mathcal{S}_h much smoother than required for weak solutions of the differential operator Δ . This fact may be startling, but it also occurs in a weaker form for classical finite-element approximations, because these usually are continuous and thus smoother than functions in Sobolev space $W_2^1(\mathbb{R}^d)$.

2 Error bounds and power functions

We now proceed to give error bounds for Hermite-Birkhoff interpolation problems. Let $f \in \mathcal{F}_\Phi$ be interpolated by the function $s_{f,\Lambda} \in \mathcal{S}_\Lambda$, where we use the notation

$$\begin{aligned}\Lambda &:= \{\lambda_1, \dots, \lambda_N\} \subset \mathcal{F}_\Phi^* \\ \mathcal{S}_\Lambda^* &:= \text{span } \Lambda \subset \mathcal{F}_\Phi^* \\ \mathcal{S}_\Lambda &:= \text{span } \{\lambda_j^y \Phi(\cdot - y), 1 \leq j \leq N\} \subset \mathcal{F}_\Phi \\ \lambda_j(s_{f,\Lambda}) &= \lambda_j(f), 1 \leq j \leq N.\end{aligned}$$

We now cite a general error bound in a specific form due to Dyn, Narcowich, and Ward [4], which can be traced back to the hypercircle inequality:

Theorem 2.1 *For all functionals $\lambda \in \mathcal{F}_\Phi^*$ we have*

$$|\lambda(f - s_{f,\Lambda})| \leq \inf_{\mu \in \mathcal{S}_\Lambda^*} \|\lambda - \mu\|_{\mathcal{F}_\Phi^*} \cdot \inf_{s \in \mathcal{S}_\Lambda} \|f - s\|_{\mathcal{F}_\Phi}.$$

This expresses the error as a product of two minimal errors of approximation problems, one concerning the given function f and the other concerning the “test functional” λ that is used for error evaluation. The second factor is

$$\inf_{s \in \mathcal{S}_\Lambda} \|f - s\|_{\mathcal{F}_\Phi} = \|f - s_{f,\Lambda}\|_{\mathcal{F}_\Phi}$$

due to one of the optimality principles [12] of interpolation by basis functions.

We now want to establish a connection to the usual error bounds for interpolation by translates of basis functions. If $\epsilon_{\lambda,\Lambda} : f \mapsto \lambda(f - s_{f,\Lambda})$ denotes the

error functional, then its norm in the dual space is expressible as a function of λ via

$$P_{\Phi, \Lambda}(\lambda) := \|\epsilon_{\lambda, \Lambda}\|_{\mathcal{F}_{\Phi}^*} = \inf_{\mu \in \mathcal{S}_{\Lambda}^*} \|\lambda - \mu\|_{\mathcal{F}_{\Phi}^*}. \quad (2.2)$$

The second equality follows from taking squares and using

$$(\lambda, \mu)_{\mathcal{F}^*} = \lambda^x \mu^y \Phi(x - y)$$

together with the usual characterization of best approximations in Hilbert spaces. Thus we get the error bound

$$|\lambda(f - s_{f, \Lambda})| \leq P_{\Phi, \Lambda}(\lambda) \|f - s_{f, \Lambda}\|_{\mathcal{F}_{\Phi}}.$$

If we specialize this to the standard case of point evaluation, i.e. setting $\lambda = \delta_x$ for the Dirac functional δ_x , then we get the usual notion of the *power function* $P_{\Phi, \Lambda}(\delta_x)$ and the pointwise error bound

$$|(f - s_{f, \Lambda})(x)| \leq P_{\Phi, \Lambda}(\delta_x) \|f - s_{f, \Lambda}\|_{\mathcal{F}_{\Phi}}. \quad (2.3)$$

Such bounds are readily available in the literature (see e.g. summaries in [12] and [11]).

We now generalize such bounds to the Hermite–Birkhoff case, but we still have to identify the type of the test functional λ with the type of the data functionals λ_j . We assume that both functionals are point evaluation functionals applied after some operator L which usually will be a differential or boundary operator.

Theorem 2.4 (*Transformation Theorem for Power Functions*) *Let $\delta_x \circ L$ be in \mathcal{F}_{Φ}^* for all $x \in \mathbb{R}^d$, and let $L\Phi L$ denote the function $L^x L^y \Phi(x - y)$. Then*

$$P_{\Phi, \Lambda \circ L}(\delta_x \circ L) = P_{L\Phi L, \Lambda}(\delta_x).$$

Proof: Using the appropriate norms in the dual spaces and the Fourier transform

$$(L\Phi L)^\wedge = |L^\wedge|^2 \Phi^\wedge,$$

we get

$$\|\mu \circ L\|_{\mathcal{F}_{\Phi}^*} = \|(\mu \circ L)^\wedge \sqrt{\Phi^\wedge}\|_{L_2(\mathbb{R}^d)} = \|\mu^\wedge \sqrt{|L^\wedge|^2 \Phi^\wedge}\|_{L_2(\mathbb{R}^d)} = \|\mu\|_{\mathcal{F}_{L\Phi L}^*}.$$

This identity, when applied formally for $\mu = \delta_x$, proves that our assumptions make sure that $L\Phi L$ generates a feasible native space $\mathcal{F}_{L\Phi L}^*$. The rest follows from (2.2). \square

A generalized version of the above transformation theorem is

$$P_{\Phi, \Lambda \circ L}(\lambda \circ L) = P_{L\Phi L, \Lambda}(\lambda)$$

under suitable assumptions on the functionals, L , and Φ . It simply shifts the operator L from the functionals to the function Φ , such that the power function involving $\delta \circ L$ and Φ is reduced to the usual point–evaluation power function involving $L\Phi L$ instead of Φ . By construction, the Fourier transform of the function $L\Phi L$ will be nonnegative a.e., if the same holds for the Fourier transform of L . Thus the new basis function $L\Phi L$ will then be positive definite again. For instance, in case of $L = \Delta$ the Fourier transform of $\Phi(\omega)$ just multiplies by $\|\omega\|_2^4$ when going over to $L\Phi L$. The usual theory of pointwise bounds for power functions can then be applied to yield handy and often asymptotically optimal bounds.

But note that the transformation theorem 2.4 still has a serious drawback, because it does not apply for sets Λ of functionals of *mixed* type. We solve this problem in the next section.

3 Splitting technique

We now assume the set $\Lambda := \{\lambda_1, \dots, \lambda_N\} \subset \mathcal{F}_\Phi^*$ of given Hermite–Birkhoff interpolation functionals to be decomposable into sets Λ_j that contain only functionals of a fixed type as covered by the transformation theorem 2.4 for power functions. Then we use

Theorem 3.1 (*Splitting Theorem for power functions*) *If*

$$\Lambda = \bigcup_j \Lambda_j,$$

then

$$P_{\Phi, \Lambda}(\lambda) \leq P_{\Phi, \Lambda_j}(\lambda)$$

for all j .

Proof: We use the definition (2.2) to get

$$\begin{aligned} P_{\Phi, \Lambda}(\lambda) &= \inf_{\mu \in \mathcal{S}_\Lambda^*} \|\lambda - \mu\|_{\mathcal{F}_\Phi^*} \\ &\leq \inf_{\mu \in \mathcal{S}_{\Lambda_j}^*} \|\lambda - \mu\|_{\mathcal{F}_\Phi^*} \\ &= P_{\Phi, \Lambda_j}(\lambda). \end{aligned}$$

□

Now we can handle $P_{\Phi, \Lambda_j}(\lambda)$ with the techniques of the previous section, picking j such that the type of the test functional λ coincides with the type of functionals in Λ_j . At the beginning of section 1 we introduced such a split of the set of functionals, and in the slightly more general situation (0.1) the above splitting technique yields two error bounds: one for the error $(Lu - Lu_h)(x)$ inside Ω and one for the error $(Bu - Bu_h)(x)$ on the boundary $\partial\Omega$. By the transformation theorem 2.4 they take the general form (2.3) with Φ replaced by functions $L\Phi L$ and $B\Phi B$, respectively.

But note that this still does not yield a bound for $u - u_h$ on $\overline{\Omega}$, as finally required for a solid foundation of the collocation technique. We solve this problem in the next section.

4 Final error bounds

The above splitting and transformation techniques allow to derive separate error bounds for the different types of operators involved in the original PDE problem. To assemble these into a final result, we invoke

Theorem 4.1 (*Composition principle for error bounds*) *If the given PDE problem is Lipschitz dependent on the data (measured in the L_∞ norm on the various parts of the domain Ω and the boundary $\partial\Omega$), then the separate error bounds of the previous section can be combined into a final error bound for the collocation technique.*

This somewhat sloppily formulated “generic” theorem is a simple consequence of the fact that the usual error bounds of the form (2.3) are L_∞ error bounds for the data of the PDE problem on the bounded subdomains of $\overline{\Omega}$ on which the (possible various) differential and boundary operators act.

To be more specific, let us illustrate Theorem 4.1 at work for the Dirichlet problem of the form (0.1) with $L = \Delta$ and a point–evaluation boundary operator $B = Id$ on $\partial\Omega$. The Lipschitz continuous dependence of the solution on the data requires two ingredients. First, for all functions $u \in W_2^2(\Omega)$ there is a coercivity inequality

$$(Lu, u)_{L_2} \geq \gamma_1 \|u\|_{W_2^2}^2 \geq \|u\|_{L_2}^2$$

which implies

$$\|Lu\|_{L_2} \geq \gamma_2 \|u\|_\infty$$

via Jensen's inequality. This in turn leads to

$$\|u - v_h\|_{\infty, \Omega} \leq C \cdot \|Lu - Lv_h\|_{2, \Omega} = C \cdot \|f - Lv_h\|_{2, \Omega}$$

for all functions $v_h \in W_2^2(\Omega)$ that also satisfy the boundary condition $Bu = Bv_h$. If we assume f and Lv_h to be continuous on Ω , we can rewrite this as an L_∞ bound

$$\|u - v_h\|_{\infty, \Omega} \leq C \cdot \sqrt{\text{vol}(\Omega)} \|f - Lv_h\|_{\infty, \Omega}$$

that describes the Lipschitz continuous dependence of the solution u on the values of Lu in Ω in case of homogeneous boundary data.

Second, the maximum principle tells us that

$$\|u - w_h\|_{\infty, \Omega} \leq \|u - w_h\|_{\infty, \partial\Omega}$$

for all functions $w_h \in W_2^2(\Omega)$ satisfying $Lu = Lw_h$ inside Ω .

We now assemble these two separate inequalities into our final error bound by picking w_h such that $Lu = Lw_h$ and $Bw_h = Bu_h$ for our collocation function u_h . Then

$$\begin{aligned} \|u - u_h\|_{\infty, \Omega} &\leq \|u - w_h\|_{\infty, \Omega} + \|w_h - u_h\|_{\infty, \Omega} \\ &\leq \|g - u_h\|_{\infty, \partial\Omega} + C \cdot \sqrt{\text{vol}(\Omega)} \|f - Lu_h\|_{\infty, \Omega} \end{aligned}$$

is the required inequality in which we can use our technique for bounding the two terms separately.

Note that this technique does not work for approximation of genuinely weak solutions of the problem, because the space $W_2^1(\mathbb{R}^d)$ does not allow continuous point evaluation functionals. So far, these are an essential ingredient of our approach, because the usual error bounds are pointwise. Thus our method implicitly assumes some higher regularity of the solution. This drawback is somewhat equalized by the fact that the resulting bounds will improve with increasing regularity [11]. Altogether, the proposed technique should not be used for cases with weak regularity and just two variables, because the power of radial basis function techniques lies in smooth cases with many variables, a situation which in turn is increasingly difficult when using finite elements.

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