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Development of Parallel algorithm for Boundary Value Problems using Compact Local Integrated RBFN and Domain Decomposition

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Abstract

Compact Local Integrated Radial Basis Function (CLIRBF) methods based on Cartesian grids can be effective numerical methods for solving Elliptic Partial Differential Equations (EPDEs) for fluid flow problems. The combination of the domain decomposition technique and function approximation using CLIRBF methods yields an effective coarse-grained parallel processing approach. This feature has enabled not only each sub-domain in the original analysis domain to be discretised by a separate CLIRBF Network but also Compact Local stencils to be independently treated. The present algorithm, namely parallel CLIRBF, achieves higher throughput in solving large scale problems by, firstly, parallel processing of sub-regions which comprise the original domain and, secondly, accelerating the convergence rate within each sub-region using groups of CLIRBF stencils in which function approximations are carried out by parallel processes. The procedure is illustrated with several numerical examples of EPDEs using Message Passing Interface (MPI) supported by MATLAB.

Keywords: Integrated RBFs, Compact local stencils, Domain decomposition, Parallel algorithm.

1. Introduction

Radial Basis Functions (RBFs) have traditionally been used to provide a continuous interpolation of scattered data sets (Franke, 1982; Kansa, 1990). The Differential RBF (DRBF) based methods have been successfully used to solve a wide variety of differential equations. For this approach, once the field variables are known, its derivatives can be calculated through differentiation. Another approach namely the Integrated RBF (IRBF) method, which was proposed by Mai-Duy and Tran-Cong (2001, 2003), is based on the approximation of the highest-order derivatives of the ODE/PDE using RBF at the first step, and subsequently its lower-order derivatives and the dependent variable itself are obtained by integration. The IRBF based methods can outperform other approximation methods based on the DRBF technique owing to its ability to produce very accurate solutions using relatively small number of data nodes.

Although full-domain IRBF methods are highly flexible and exhibit high order convergence rates in their basic implementation, the associated fully-populated matrix systems can lead to poor numerical conditioning as the scale of a problem increases (Mai-Duy and Tran-Cong, 2008). The problem becomes critical with increasingly large data sets. Many techniques have also been developed to reduce the effect of the problem, including domain decompositions (Ingber et al., 2004; Tran et al., 2009), adaptive selection of data-centres (Ling et al., 2006), RBF preconditioners (Brown, 2005) and RBF based compact local stencil methods (Mai-Duy and Tran-Cong, 2011; Hoang-Trieu et al., 2012; Thai-Quang et al., 2012). While a reliable method of controlling numerical ill-conditioning and particularly computational cost, as problem scale increases, can be based on domain decomposition (DD) (Ingber et al., 2004; Tran et al., 2009), the use of compact local approximations facilitates the solution of differential equations without having to deal with large systems of global equations. In this work, a parallel algorithm based on Compact Local Integrated RBF (CLIRBF) and DD techniques is developed for the solution of Boundary Value Problems (BVP). A large problem is firstly decomposed into many smaller manageable problems each of which is analysed in parallel and secondly the acceleration of the convergence rate within each sub-region using groups of CLIRBF stencils is carried out by parallel processes.

This paper is organized as follows. In section 2, a brief review of a CLIRBF method and the domain decomposition technique is described. Section 3 presents a parallel algorithm with domain decomposition and local stencils. Numerical examples are then discussed in section 4 with a conclusion in section 5.

2. Review of domain decomposition technique and compact local IRBF methods

For the ease of presentation, consider a second-order ordinary differential equation (ODE) with Dirichlet boundary condition as follows.

$$\mathcal{L}u = f(x), \quad x \in \Omega \tag{1}$$

$$u = r, \quad x \in \partial\Omega \tag{2}$$

where u and $f(x)$ are continuous and prescribed functions, respectively; $\mathcal{L}$ a second order differential operator; r an known quantity; Ω and $\partial\Omega$ the domain under consideration and its boundary.

Domain decomposition

Domain decomposition is a general method for solution of systems of equations. In a BVP governed by differential equations, DD aims to split the whole domain into smaller subdomains of analysis while guaranteeing the continuity at the splitting boundary. DD algorithms can be grouped into two classes: (i) non-overlapping methods and (ii) overlapping methods (Smith et al., 1996). In this paper, the additive overlapping method is implemented on the domain under consideration.

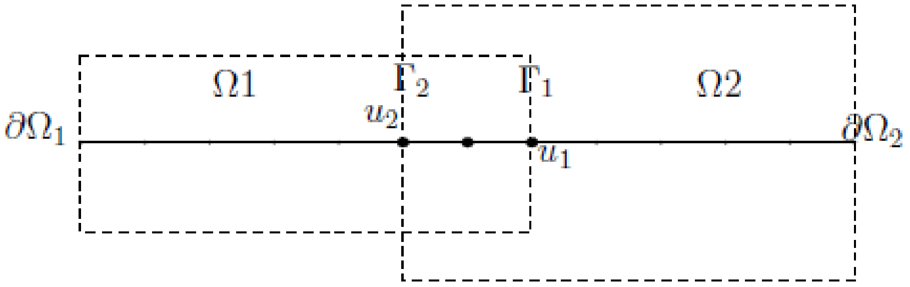

Figure 1. 1D Domain Decomposition

For illustrative purposes, the domain Ω is divided into two subdomains Ω_1 and Ω_2. Let $\partial\Omega_1$ and $\partial\Omega_1$ be boundaries of Ω_1 and Ω_2 respectively and Γ_i, $(i = \{1,2\})$ the artificial boundaries between Ω_1 and Ω_2 (Figure 1). Here the boundary condition imposed on the interface is of Dirichlet type. The DD algorithm for n-th step can be written as

$$\begin{aligned} &\mathcal{L}u_1^n = f, \quad x \in \Omega_1 \\ &u_1^n = r, \quad x \in \partial\Omega_1 \backslash \Gamma_1 \\ &u_1^n = u_{1\Omega_2}^{n-1}, x \in \Gamma_1 \end{aligned} \tag{3}$$

and

$$\begin{aligned} &\mathcal{L}u_2^n = f, \quad x \in \Omega_2 \\ &u_2^n = r, \quad x \in \partial\Omega_2 \backslash \Gamma_2 \\ &u_2^n = u_{2\Omega_1}^{n-1}, x \in \Gamma_2 \end{aligned} \tag{4}$$

where $u_{i\Omega_j}^{n-1}$ $(i,j = \{1,2\}, i \neq j)$ is the value of u in Ω_i obtained from the solution in Ω_j at a step $n-1$ (see Figure 1). The right most and left most sides of the overlapping zone are the artificial boundaries Γ_1, Γ_2 of Ω_1, Ω_2 respectively. While the middle part of it is for the purpose of continuity check. The BVPs (3) and (4) are solved separately using the CLIRBF method which is presented in the next section.

Compact local IRBF methods

The idea of using local RBF collocation approaches to solve DEs can be seen as a generalization of the compact finite difference scheme in terms of scattered nodes (Wright and Fornberg, 2006). In this work, the compact local 3–point stencil technique which described in (Hoang-Trieu et al., 2012) is employed to discretise BVPs.

Consider three consecutive points $[x_{i-1}, x_i, x_{i+1}]$ associated with grid point x_i $(2 \leq i \leq n-1)$ in a typical global 1D Cartesian grid line. $[x_1, x_2, x_3]$ is used to represent a stencil in local 1D Cartesian grid line (node $x_2 \equiv x_i$). The second-order derivative of the function u in Eq. (1) is decomposed into a set of RBFs as

$$\frac{d^2u}{dx^2} = \sum_{i=1}^{3} w_i \, I_i^{(2)}(x), \quad x_1 \leq x \leq x_3 \tag{5}$$

where $\{w_i\}_{i=1}^3$ are the set of RBF weights, and $\{I_i^{(2)}(x)\}_{i=1}^3$ the set of RBFs. The superscript (.) is used to indicate the associated derivative order. In this work, the multiquadric (MQ) RBF is used and given by

$$I_i^{(2)}(x) = \sqrt{(x - c_i)^2 + a_i^2}, \tag{6}$$

where c_i and a_i are the MQ center and width of RBFs, respectively. Integrating expression (5) over the stencil yields the expression for lower order derivatives and the function itself as

$$\frac{du}{dx} = \sum_{i=1}^{3} w_i \, I_i^{(1)}(x) + C_1, \tag{7}$$

$$u = \sum_{i=1}^{3} w_i \, I_i^{(0)}(x) + C_1 x + C_2, \tag{8}$$

where C_1 and C_2 are constants of integration. Expression (5), (7) and (8) can be rewritten into the matrix form as follows.

$$\frac{d^2u}{dx^2} = \left[I_1^{(2)}(x), \quad I_2^{(2)}(x), \quad I_3^{(2)}(x), \quad 0, \quad 0\right]\widehat{\boldsymbol{w}} = \mathcal{H}^{(2)}(x)\widehat{\boldsymbol{w}}, \tag{9}$$

$$\frac{du}{dx} = \left[I_1^{(1)}(x), \quad I_2^{(1)}(x), \quad I_3^{(1)}(x), \quad 1, \quad 0\right]\widehat{\boldsymbol{w}} = \mathcal{H}^{(1)}(x)\widehat{\boldsymbol{w}}, \tag{10}$$

$$u = \left[I_1^{(0)}(x), \quad I_2^{(0)}(x), \quad I_3^{(0)}(x), \quad x, \quad 1\right]\widehat{\boldsymbol{w}} = \mathcal{H}^{(0)}(x)\widehat{\boldsymbol{w}}, \tag{11}$$

where $\widehat{\boldsymbol{w}} = (w_1, w_2, w_3, c_1, c_2)^T$. The conversion matrix $\mathcal{C}$ is formed as

$$\begin{pmatrix} \widehat{\boldsymbol{u}} \\ \widehat{\boldsymbol{e}} \end{pmatrix} = \underbrace{\begin{bmatrix} \mathcal{H}^{(0)} \\ \mathcal{K} \end{bmatrix}}_{\mathcal{C}} \widehat{\boldsymbol{w}}, \tag{12}$$

where $\widehat{\boldsymbol{u}} = (u_1, u_2, u_3)^T$, $\widehat{\boldsymbol{u}} = \mathcal{H}^{(0)}\widehat{\boldsymbol{w}}$ is a set of three equations representing nodal values of u over the stencil, $\widehat{\boldsymbol{e}} = \mathcal{K}\widehat{\boldsymbol{w}}$ is employed to represent values of (1) at x_1 and x_3.

As a result, values of function u and its derivatives at an arbitrary point x on the stencil are calculated in the physical space as

$$\frac{d^2u}{dx^2} = \mathcal{H}^{(2)}(x)\mathcal{C}^{-1}\begin{pmatrix} \widehat{\boldsymbol{u}} \\ \widehat{\boldsymbol{e}} \end{pmatrix}, \tag{13}$$

$$\frac{du}{dx} = \mathcal{H}^{(1)}(x)\mathcal{C}^{-1}\begin{pmatrix} \widehat{\boldsymbol{u}} \\ \widehat{\boldsymbol{e}} \end{pmatrix}, \tag{14}$$

$$u = \mathcal{H}^{(0)}(x)\mathcal{C}^{-1}\begin{pmatrix} \widehat{\boldsymbol{u}} \\ \widehat{\boldsymbol{e}} \end{pmatrix}. \tag{15}$$

3. Implementation

The parallelization is carried out using the 3 node CLIRBF scheme and based on the domain decomposition technique as detailed in section 2 above. In this work, the overlapping DD scheme is employed. It is noted that each stencil does not needthe data from other stencils to start its calculation. This data independency allows stencils calculation to run on parallel CPU cores. The flowchart of the algorithm is shown in Figure 2. It can be seen that the algorithm is divided into three main parts. The first one is initialization, which allocates the memory and calculates initial values. The second part is the parallel part of algorithm where stencils are assigned equally to CPU cores. As all cores share the same memory, they can store the results of calculation in a predefined matrix. The final part of the algorithm is to solve the final system of equations to obtain the approximated result. Parallel implementation of the algorithm is based on the single program, multiple data (SPMD) paradigm with message passing interface (MPI) for parallel communication. In this paper, we use the MPI parallel programming within the MATLAB environment.

4. Numerical examples

Consider the following second-order ODE.

$$\frac{\partial^2 u}{\partial x^2}+\frac{\partial u}{\partial x}+u=-\exp(5x)[9979\sin(100x)+900\cos(100x)],\quad 0\leq x\leq 1, \tag{16}$$

with an analytic solution $u=\exp(-5x)\sin(100x)$. The problem is solved using the present method for two different types of boundary condition. The domain is partitioned into 2 sub-domains and a wide range of grids $(301,302,\ldots,501)$ is considered.

Dirichlet boundary condition

The Dirichlet conditions are $u(0)=0$ and $u(1)=\sin(100)\exp(-5)$. Figure 3 depicts a comparison of the results obtained by the present method, the CLIRBF and the analytic ones. The results show that the present method achieves almost the same accuracy level as the CLIRBF method. In fact, convergence rate $O(Ne)$ of the present method is 4.12, and the CLIRBF is 4.26.

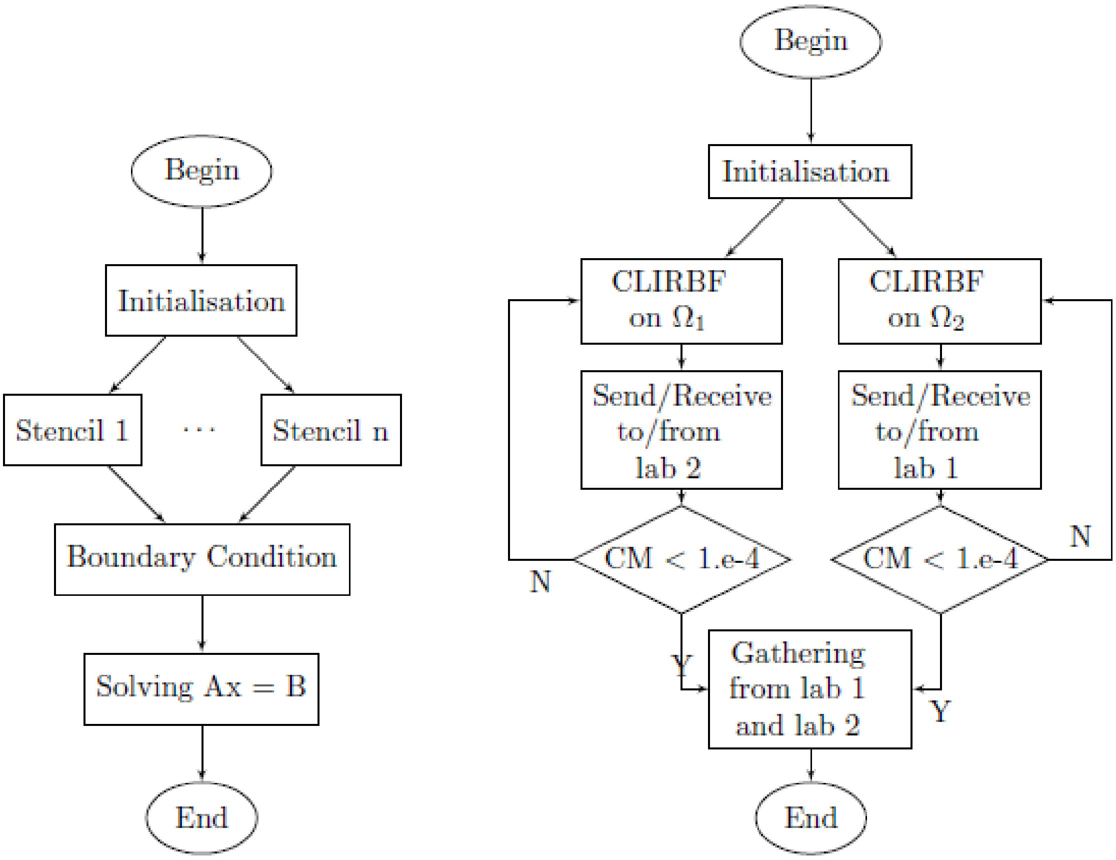

Figure 2. Parallel algorithm: Flow-chart of CLIRBF with parallel stencils (left figure); flowchart of domain decomposition with 2 sub-domains (right figure)

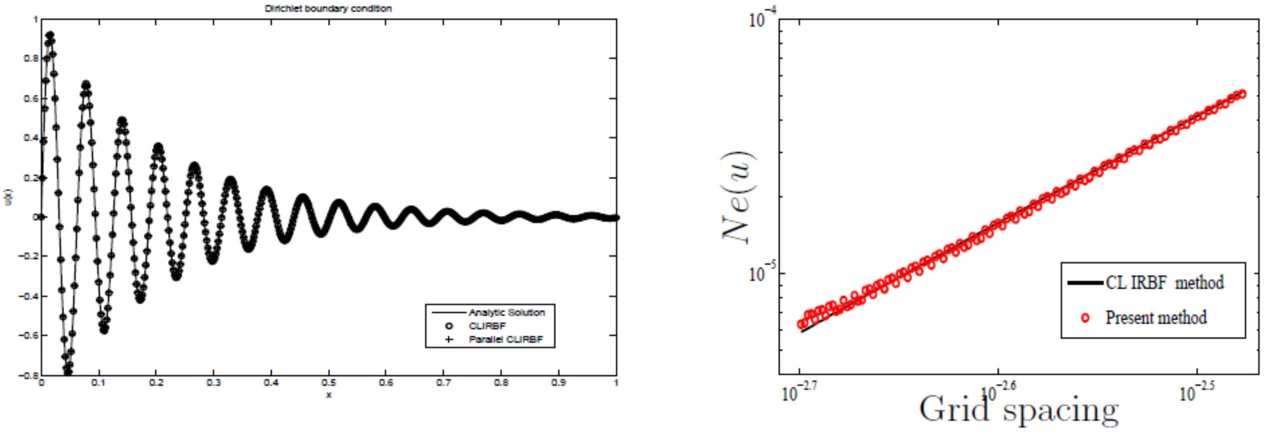

Figure 3. Second order problem with Dirichlet boundary condition: Solutions obtained by the 3×3 nodes CLIRBF method and the present method (left figure); Relative L_2 errors of the solution u against the grid size by the 3×3 nodes CLIRBF method and the present method (right figure).

Dirichlet and Neumann Boundary conditions

The Dirichlet condition is imposed on the left end $u(0) = 0$ and the Neumann condition on the right end $\frac{du(1)}{dx} = 5\exp(-5)[20\cos(100) - \sin(100)] = 0.598$.

While the result, described in the figure 4 by the present method, is in very good agreement with the analytic solution, the convergence rate displayed in the right figure shows that the present method yields a higher accuracy in comparison with the 3 node CLIRBF method.

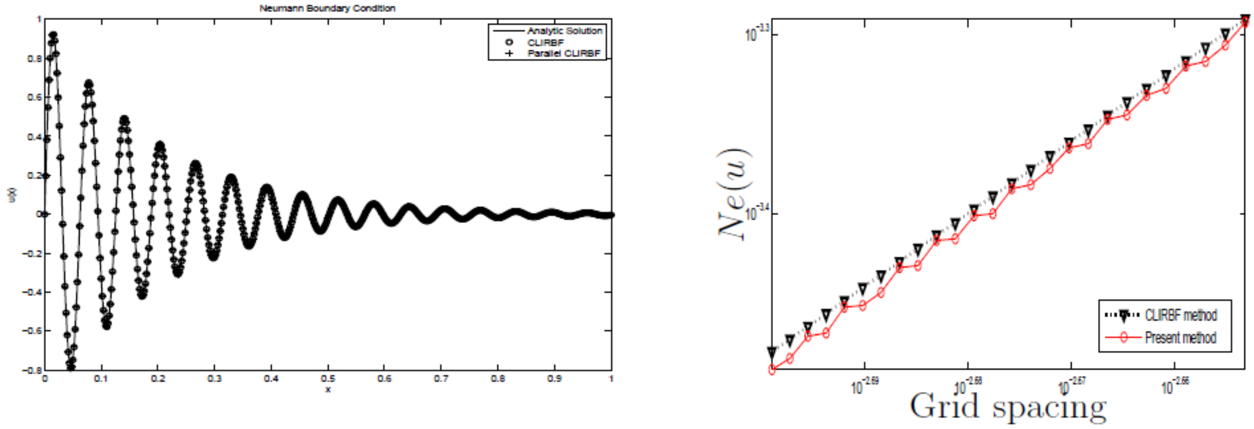

Figure 4. Second order problem with Dirichlet-Neuman boundary conditions: Solutions obtained by the 3×3 nodes CLIRBF method and the present method (left figure); Relative L_2 errors of the solution u against the grid size by the 3×3 nodes CLIRBF method and the present method (right figure).

5. Conclusion

In this paper, we have developed a parallel algorithm based on the combination of domain decomposition technique and function approximation using 3 point compact local IRBF method. The proposed algorithm allows not only a large scale problem to be discretised by parallel CLIRBF networks but also compact local stencils to be independently treated in multiple-core CPUs. Advantages of the new approach include (i) to alleviate the ill-conditioned problem associated with global IRBF methods; (ii) to avoid the reduction in convergence rate caused by differentiation and (iii) to achieve higher throughput in solving large scale problems. The method is verified with several numerical examples using MPI supported Matlab.

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