Fictitious Domain Approach for Spectral/hp Element Method

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Abstract: We propose a fictitious domain method combined with spectral/hp elements for the solution of second-order differential problems. This paper presents the formulation, validation and application of fictitiuos domain-spectral/hp element algorithm to one- and two-dimensional Poisson problems. Fictitious domain methods allow problems formulated on an intricate domain Ω to be solved on a simpler domain Π containing Ω. The Poisson equation, extended to the new domain Π, is expressed as an equivalent set of first-order equations by introducing the gradient as an additional indipendent variable, and spectral/hp element method is used to develop the discrete model. Convergence of relative energy norm η is verified computing smooth solutions to one- and two-dimensional Poisson equations. Thermal field calculations for heatsink profile is presented to demonstrate the predictive capability of the proposed formulation.

Keyword: fictitious domain, Lagrange multipliers, spectral/hp element method, Poisson problem.

1 Introduction

The main motivation for fictitious domain approach, alternatively called immersed boundary method, is that, defining the extended problem on a simple domain, enables the use of efficient discretization methods on simple structured grids. Literature on fictitious domain methods goes back to the sixties [Saul'ev (1963)]. In the following years there has been a crescent interest on this kind of methodologies [Babuska (1973); Pitkaranta (1979); Pitkaranta (1980); Pitkaranta (1981); Barbosa and Hughes (1991); Barbosa and Hughes (1992)]. So that several

approaches have been developed to implement immersed conditions and we can find different applications: to acoustics [Heikkola, Kuznetsov, and Lipnikov (1999); Hetmaniuk and Farhat (2002); Hetmaniuk and Farhat (2003)], fluid dynamics [Glowinski, Pan, and Periaux (1994); Glowinski, Pan, and Periaux (1995); Glowinski, Pan, and Periaux (1997); Glowinski, Pan, Hesla, Joseph, and Periaux (1999); Glowinski, Pan, Hesla, Joseph, and Periaux (2001)], biomedical problems [Arthurs, Moore, Peskin, Pitman, and Layton (1998); Roma, Peskin, and Berger (1999); Jung and Peskin (2001); de Hart, Peters, Schreurs, and Baaijens (2000); Baaijens (2001); de Hart, Peters, Schreurs, and Baaijens (2003)]. In general we have to distinguish the case of Dirichlet, Neumann or Robin conditions. Methods to implement Dirichlet conditions can be classified in *penalty methods* and *Lagrangian methods*, as illustrated by [Heikkola, Kuznetsov, Neittanmaki, and Pironneau (2003)]. There are examples of Elimination method [Zienkiewicz and Taylor (2000)], Penalty method [Zienkiewicz and Taylor (2000); Ramiere, Angot, and Belliard (2005)], Distributed Lagrangian method [Haslinger, Maitre, and Tomas (2001); Glowinski, Pan, Hesla, and Joseph (1999); Glowinski, Pan, Hesla, Joseph, and Periaux (2000)], Boundary Lagrangian method [Stenberg (1995); Joly and Rhaouti (1999)], Fat Boundary method [Maury (2001)]. Among all the possible approaches, a technique which is popular, given its efficiency, is to enforce the Dirichlet condition by Lagrange multipliers, which is the method we propose in this paper. Unfortunately, the same approach can not be adopted for Neumann immersed boundary condition because that one can not be directly enforced by Lagrange multipliers [Hetmaniuk and Farhat (2003)]. Enforcing Neumann boundary conditions within a fictitious domain framework

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is not an easy task. To treat them within a fictitious domain framework least-squares formulations have been proposed by [Dean, Dihn, Glowinski, He, Pan, and Periaux (1992)], vector dual formulations with Lagrange multipliers have been presented in [Joly and Rhaouti (1999); Quarteroni and Valli (1999)] and an algebraic fictitious domain approach in [Rossi and Toivanen (1999); Makinen, Rossi, and Toivanen (2000)]. We have chosen to impose it via Lagrange multipliers, introducing the gradient of the primal variable as an unknown and converting Neumann condition into a Dirichlet-like condition for this new variable. This technique seems to be very efficient, at the expense of an increase of computational cost as it replaces a scalar problem by a vector problem.

New approach, we present in this paper, is the coupling of fictitious domain together with an high order method. To discretize the problem under study we use the spectral/hp element method, based on higher order functions, locally defined over finite size parts of domain. The advantage of such kind of method, in comparison with traditional finite element method, is its exponential convergence property with the increasing of polynomial order p. Moreover using fictitious domain approach, where extended problem is defined on a simple domain, enables the use of efficient computational grids, in our case just simple Cartesian grids.

Good accuracy properties of the method are demonstrated by numerical experiments. These ones are performed with several mesh size and polinomyal order of modal function to better quantify the performance of the proposed solution procedure. Finally, the calculation of the thermal field for a heatsink fin illustrates the capabilities of the method in a practical engineering example.

2 Formulation of the problem: the Poisson equation

Let $\overline{\Omega}$ be the closure of an open bounded region Ω in $\Re^n$, where n represents the number of space dimensions, and let $\mathbf{x} = (x_1,...,x_n)$ be a point in $\overline{\Omega} = \Omega \bigcup \partial\Omega$, where $\partial\Omega = \Gamma$ is the boundary of Ω. We want to solve the Poisson problem stated

as follows:

find $\phi(\mathbf{x})$ such that

$$-\triangle\phi = f \qquad \text{in}\, \Omega \tag{1}$$

$$\phi = \phi^s \qquad \text{on}\, \Gamma_\phi \tag{2}$$

$$\nabla\phi \bullet \hat{\mathbf{n}} = q_n^s \qquad \text{on}\, \Gamma_q \tag{3}$$

where $\Gamma = \Gamma_\phi \bigcup \Gamma_q$ and $\Gamma_\phi \bigcap \Gamma_q = \emptyset$, f is the source term, $\hat{\mathbf{n}}$ is the outward unit normal on boundary Γ, ϕ^s is the prescribed value of ϕ on boundary Γ_ϕ and q_n^s is the prescribed normal flux on boundary Γ_q.

To enable the implementation of Neumann boundary condition via Lagrange multipliers, we proceed by replacing the Poisson problem, Eq. 1-Eq. 3, with its equivalent first-order system, at the expense of additional variables. The equivalent problem writes as:

find $\phi(\mathbf{x})$ and $\mathbf{u}(\mathbf{x})$ such that

$$\mathbf{u} - \nabla\phi = 0 \qquad \text{in}\, \Omega \tag{4}$$

$$-\nabla \bullet \mathbf{u} = f \qquad \text{in}\, \Omega \tag{5}$$

$$\phi = \phi^s \qquad \text{on}\, \Gamma_\phi \tag{6}$$

$$\mathbf{u} \bullet \hat{\mathbf{n}} = q_n^s \qquad \text{on}\, \Gamma_q \tag{7}$$

where $\mathbf{u}$ is a vector valued function whose components are the fluxes of scalar function ϕ, as defined in Eq. 4.

We can write the system Eq. 4-Eq. 5 defined on domain Ω in matrix form as:

$$\mathbf{L}\Phi = \mathbf{F} \tag{8}$$

where $\mathbf{L}$ is the matrix operator, Φ is the vector of unknowns and $\mathbf{F}$ is the vector of known terms. In two dimensions it is:

$$\begin{bmatrix} 1 & 0 & -\frac{\partial}{\partial x} \\ 0 & 1 & -\frac{\partial}{\partial y} \\ -\frac{\partial}{\partial x} & -\frac{\partial}{\partial y} & 0 \end{bmatrix} \left\{ \begin{array}{c} \phi_x \\ \phi_y \\ \phi \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ 0 \\ f \end{array} \right\} \tag{9}$$

with $\phi_x = \frac{\partial\phi}{\partial x}$ $\phi_y = \frac{\partial\phi}{\partial y}$.

3 Fictitious domain method

Several variants of fictitious domain method exist: the basic idea is to extend the operator and the domain into a larger simple shaped domain. The

most important ways to do this are algebraic and functional analytic approaches. In algebraic fictitious domain methods the problem is extended typically at algebraic level in such a way that the solution of original problem is obtained directly as a restriction of the solution of extended problem without any additional constraint. There are several variants of such an approach [Rossi and Toivanen (1999); Makinen, Rossi, and Toivanen (2000)] and they can be rather efficient, but typically they are restricted to quite a narrow class of problems.

More flexibility and better efficiency can be obtained by using a functional analytic approach where the use of constraints ensures that the solution of extended problem coincides with the solution of original problem. In our implementation we enforce constraints by Lagrange multipliers.

For simplicity, let us consider the model problem Eq. 4-Eq. 5 with homogeneous boundary conditions. The standard approach to solve it is to search for the solution which minimizes the variational problem, in practice:

find $(\phi, \mathbf{u}) \in \mathbf{X}$ such that for all admissible weighting functions $(\varphi, \mathbf{v}) \in \mathbf{X}$

$$\langle \mathbf{v}, \mathbf{u} \rangle_\Omega - \langle \mathbf{v}, \nabla \phi \rangle_\Omega = 0 \qquad (10)$$
$$-\langle \varphi, \nabla \bullet \mathbf{u} \rangle_\Omega = (\varphi, f)_\Omega \qquad (11)$$

where $\langle \cdot, \cdot \rangle_\Omega$ and $(\cdot, \cdot)_\Omega$ denote the standard H_1 and L_2 inner products and $\mathbf{X} = \left\{ (\phi, \mathbf{u}) \in H^1(\Omega) \times \mathbf{H}^1(\Omega) : \phi|_{\Gamma_\phi} = 0, \, \mathbf{u} \bullet \hat{\mathbf{n}}|_{\Gamma_q} = 0 \right\}$.
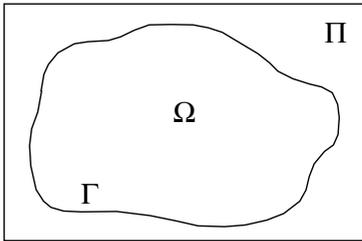

Figure 1: Example of a fictitious rectangular domain Π containing the original domain Ω

According to fictitious domain methodology the problem is extended to a simple shaped domain $\Pi \supset \Omega$ with f_Π extension of f to $L^2(\Pi)$ and immersed constraints enforced via Lagrange multipliers. The variational formulation of the new equivalent problem will be:

$$\langle \mathbf{v}, \mathbf{u} \rangle_\Pi - \langle \mathbf{v}, \nabla \phi \rangle_\Pi + \langle \mathbf{v}, \lambda_q \rangle_{\Gamma_q} = 0 \qquad (12)$$
$$-\langle \varphi, \nabla \bullet \mathbf{u} \rangle_\Pi + \langle \varphi, \lambda_\phi \rangle_{\Gamma_\phi} = (\varphi, f)_\Pi \qquad (13)$$
$$\langle \mu_q, \mathbf{u} \rangle_{\Gamma_q} = 0 \qquad (14)$$
$$\langle \mu_\phi, \phi \rangle_{\Gamma_\phi} = 0 \qquad (15)$$

where $\Gamma = \partial \Omega$ and $\Gamma = \Gamma_\phi \bigcup \Gamma_q$. The Lagrange multiplier defined on Γ_ϕ is denoted by λ_ϕ, with μ_ϕ the associated weight function, and the Lagrange multiplier defined on Γ_q is denoted by λ_q, with μ_q the associated weight function (see [Zienkiewicz and Taylor (2000)] for more details).

The solution of Poisson problem, Eq. 1-Eq. 3, will be the restriction to Ω of the solution of Eq. 12-Eq. 15, which are defined on domain Π.

4 Discretization: spectral/hp element method

The problem Eq. 12-Eq. 15 can not be solved analytically and therefore it is necessary to use a numerical method to get approximated solution. The spectral/hp element method is a numerical technique for solving partial differential equations based on variational formulation of boundary and initial value problems [Karniadakis and Sherwin (1999); Pontaza and Reddy (2003); Eskilsson and Sherwin (2005); Gerritsma and Maerschalck (2005); Wu, Liu, Scarpas, and Ge (2006); Mitra and Gopalakrishnan (2006)]. The solution is represented by a finite number of basis functions. Spectral/hp element method is based on higher order functions, which are locally defined over finite size parts of domain (elements). The advantage of such kind of method respect to traditional finite element method is its exponential convergence property with the increasing of polynomial order p.

Historically there is a distinction between hp-type FEM and spectral element method cause of the expansion which can be modal or nodal.

In hp-FEM the expansion basis is normally modal, i.e. the basis functions are of increasing

order (hierarchical) and the set of order $p-1$ is contained within the set of order p. In modal approach the expansion coefficients do not have any particular physical meaning.

In contrast in nodal spectral element methods the expansion basis are non-hierarchical and consists of $p+1$ polynomial of order p. Moreover the expansion coefficients are associated with a set of nodal points where only one basis function has non-zero value. Hence the expansion coefficients can be interpreted as the physical solution value at the nodal points.

The methods are mathematically equivalent, in numerical practice however the two approches do have different numerical properties in terms of implementation efficiency, ability to vary the polynomial order and conditioning of global sparse systems (see [Karniadakis and Sherwin (1999)] for more details). For this reason we choose a modal approach.

We proceed to define a discrete problem by choosing appropriate finite element subspaces for ϕ, each of the components of the vector valued function **u** and Lagrange multipliers λ. There are no restrictive compatibility conditions on the discrete spaces, so we choose the same finite element subspace for each of the primary variables ϕ and **u**. The only requirement on approximating spaces is that we choose continuous piecewise polynomials that are at least bi-linear in two dimensions or tri-linear in three dimensions.

Consider the two-dimensional case and let $\mathscr{P}_h$ be a family of quadrilateral finite elements $\overline{\Omega}_e$ that make up the connected model $\overline{\Omega}_h$. We map $\overline{\Omega}_e$ to a bi-unit square $\hat{\Omega}_e = [-1,1] \times [-1,1]$, where (ξ,η) is a point in $\hat{\Omega}_e$. Over a typical element $\hat{\Omega}_e$, we approximate ϕ by the expression

$$\phi(\xi,\eta) = \sum_{i=1}^{n} \Delta_i \varphi_i(\xi,\eta) \quad \text{in } \hat{\Omega}_e. \tag{16}$$

In modal expansion, φ_i are tensor products of the one-dimensional C^0 p-type hierarchical basis

$$\psi_p = \begin{cases} \dfrac{1-\xi}{2} & \text{for } p=0 \\ \dfrac{1-\xi}{2}\dfrac{1+\xi}{2}P_{p-1}^{\alpha,\beta} & \text{for } 0 < p < P, \ P \geq 1 \\ \dfrac{1+\xi}{2} & \text{for } p=P \end{cases} \tag{17}$$
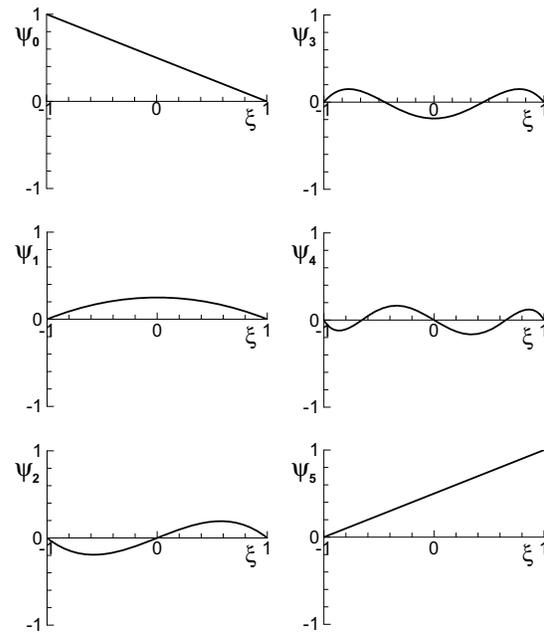

Figure 2: Shape of modal expansion modes for a polynomial order of $P=5$

and Δ_i are coefficients associated with each of the modes of hierarchical basis. In Eq. 17 $P_p^{\alpha,\beta}$ are the Jacobi polynomials of order p (see Appendix A: Jacobi Polynomials for more details), in particular ultraspheric polynomials corresponding to the choice $\alpha = \beta$ with $\alpha = \beta = 1$. This choice is due to the considerations about the sparsity of the matrices we obtain discretizing the problem presented by [Karniadakis and Sherwin (1999)]. In Fig. 3 it is shown the construction of a two-dimensional modal expansion basis from the product of two one-dimensional expansions of order $P=4$.
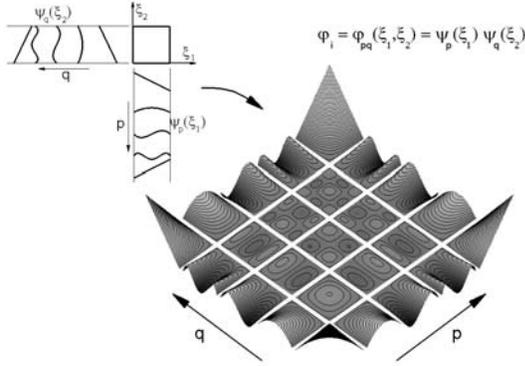
Figure 3: Construction of a two-dimensional modal expansion basis from the product of two one-dimensional expansions of order $P = 4$

We approximate the components of the vector valued function **u** on $\hat{\Omega}_e$ in similar manner as we did for ϕ in Eq. 16. The approximation of Lagrange multipliers requires the discretization of the immersed boundary Γ into curvilinear one-dimensional elements $\overline{\Gamma}_e$, which are mapped to linear unit elements $\hat{\Gamma}_e = [-1, 1]$. On these elements the function λ is approximated by the expression

$$\lambda(\xi) = \sum_{i=1}^{m} \Delta_i \psi_i(\xi) \quad \text{on } \hat{\Gamma}_e \tag{18}$$

where ψ_i are defined in Eq. 16 and Δ_i are the coefficients associated with expansion modes of function λ. In this way we proceed to generate a system of linear algebraic equations at element level using Eq. 12-Eq. 15. The integrals in these equations are evaluated using Gauss quadrature rules. In our implementation the Gauss-Legendre rules are used for the modal expansions, and full integration is used to evaluate the integrals.

The global system of equations is assembled from the element contributions using the direct summation approach. The assembled system of equations can be written as

$$\mathbf{GY} = \mathbf{F} \tag{19}$$

where Y are the modal unknown coefficients associated with ϕ, u, λ_ϕ and λ_q. The system will be solved using a direct method.

5   Validation and application

In the following we present numerical results obtained with the proposed formulation. The solved problems have been selected to assess the predictive capabilities on function and gradient using fictitious domain-spectral/hp element models. We verify the accuracy of numerical algorithm comparing the result to exact solution. Next we consider the one- and two-dimensional Poisson problem and then the one dimensional diffusion problem in a cooling fin where exact solution can be computed. In the last example we consider the diffusion problem for a two-dimensional heatsink profile where the exact solution has been computed using a finite element solver with a fine mesh.

5.1   One-dimensional stationary Poisson problem

We solve the one-dimensional boundary value Poisson problem defined on $\Omega = [-1.0, 1.0]$:

$$\frac{d^2\phi}{dx^2} = \pi^2 sin(\pi x) \tag{20}$$

with homogenous Dirichlet boundary conditions:

$$\begin{cases} \phi(-1) &= 0 \\ \phi(1) &= 0. \end{cases} \tag{21}$$

The analytical solution of the problem under study Eq. 20-Eq. 21 is $\phi(x) = sin(\pi x)$, whose derivative is $\frac{d\phi}{dx}(x) = -\pi cos(\pi x)$, as shown in Fig. 4.

To solve problem Eq. 20 we employ the fictitious domain method, so the computational domain we consider is $\Pi = [-1.2, 1.2]$, larger than the original one Ω ($\Pi \supset \Omega$), and we impose the boundary constraints Eq. 21, which are now *immersed* in the domain, via Lagrange multipliers (Appendix C: Implementation of fictitious domain for one-dimensional problems). In one-dimensional problems the Lagrange multiplier is just a constant defined on the constrained point. To get the solution
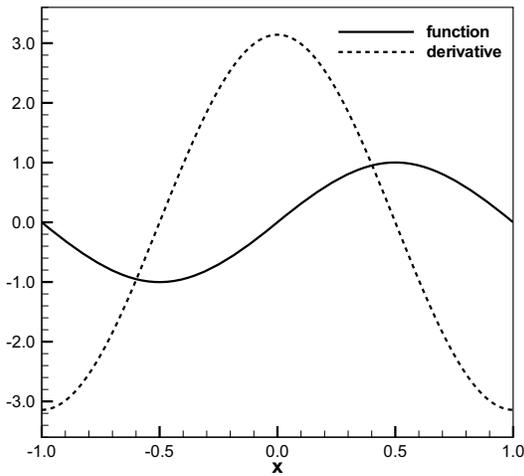
Figure 4: Analytical solution of one-dimensional stationary Poisson test problem Eq. 20-Eq. 21

of the equivalent problem spectral elements have been employed. The domain Π has been meshed uniformly. To understand how the accuracy of solution improves we have tested different grids, in particular the grid size H has been varied from 1.2 to 0.48, that means Π has been divided into 2, 3, 4 and 5 equal elements.

In Fig. 5(a) we plot the relative energy norm η of ϕ as a function of the expansion order p of spectral elements comparing different grid size.

The relative energy norm is defined as

$$\eta = \frac{[\int_\Omega (\phi_{numeric} - \phi_{analytic})^2 d\Omega]^{1/2}}{[\int_\Omega \phi_{analytic}^2 d\Omega]^{1/2}} \qquad (22)$$

In Fig. 5(b) we perform the same analysis for the gradient $\frac{d\phi}{dx}$.

During these tests we have observed that accuracy increases faster with polynomial order p than number of spectral elements, even if using a fictitiuos domain approach the spectral convergence of η is lost. For the problem under study with high numbers of p the number of elements does not influence the accuracy at all. If $p \geq 5$ the results are significantly accurate for both function ϕ
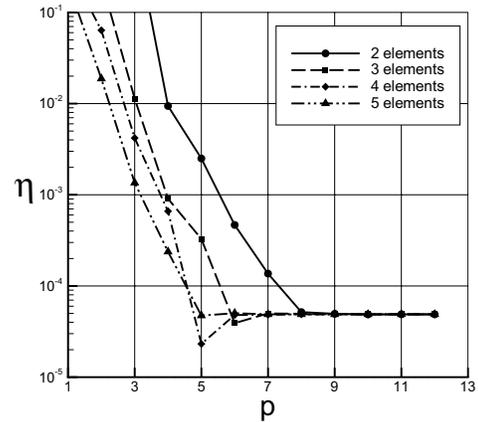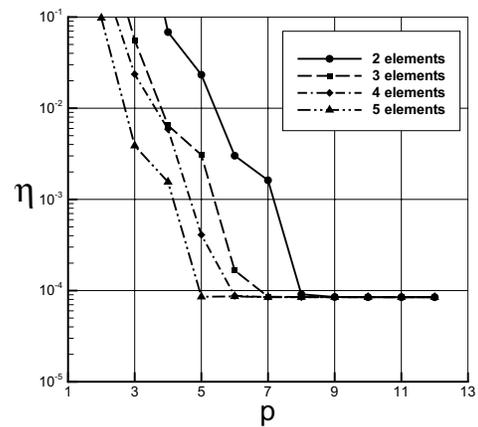
(a) function

(b) derivative

Figure 5: Relative energy norm η of function ϕ and derivative $\frac{d\phi}{dx}$ versus the expansion order p of spectral elements for Poisson test problem Eq. 20-Eq. 21

and its derivative. We have to remark that the CPU time required to solve the problem increases faster with polynomial order of trial functions, rather than with grid size of fictitious domain.

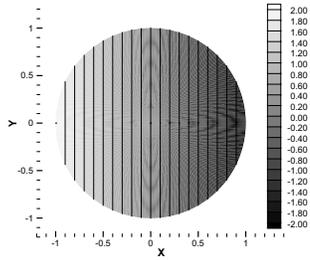## 5.2 Two-dimensional stationary Poisson problem

The Poisson problem under study is:

$$\begin{cases} -\triangle\phi = 4 & \text{on } \Omega \\ \nabla\phi \bullet \hat{n} + \phi = -2 & \text{on } \Gamma \end{cases} \qquad (23)$$
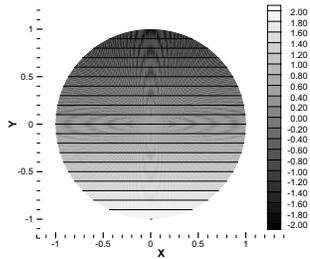
with $\Omega = \{(x,y) \in \Re^2 : x^2 + y^2 < 1\}$ and $\Gamma = \{(x,y) \in \Re^2 : x^2 + y^2 = 1\}$. The boundary condition on Γ is Robin type.
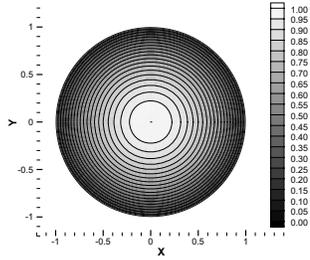
(a) function

(b) derivative in x

(c) derivative in y

Figure 6: Analytical solution of two-dimensional stationary Poisson test problem Eq. 23

The analytical solution of this problem is:

$$\phi(x,y) = 1 - x^2 - y^2 \qquad (24)$$

whose derivatives are:

$$\phi_x = \frac{\partial\phi}{\partial x}(x,y) = -2x \qquad (25)$$

$$\phi_y = \frac{\partial\phi}{\partial y}(x,y) = -2y \qquad (26)$$

as shown in Fig. 6.

We solve the problem Eq. 23 by fictitious domain method considering the square $\Pi = [-1.2, 1.2] \times [-1.2, 1.2]$ as computational domain, which include Ω.

The prescribed immersed constraints are included by means of Lagrange multiplier method which introduce an unknown function λ defined only on Γ. In the discretization process we have to use trial functions to describe both the function ϕ, its partial derivatives and Lagrange multiplier λ. Fictitious domain Π is meshed uniformly by square cells. To understand how the accuracy of solution improves we have tested different grid steps and different expansion order for modal polynomial of unknowns ϕ, $\partial\phi/\partial x$ and $\partial\phi/\partial y$. The immersed boundary Γ is meshed uniformly with one-dimensional curved elements on which the Lagrange multipliers are defined. The modal functions of Lagrange multipliers are piecewise linear. This means Lagrange multipliers are discontinuous between contiguous immersed elements. This choice is due to the analysis of the results obtained for different problems. The behaviour of the algorithm has been investigated varying the polynomial order of trial functions for Lagrange multiplier. Moreover the accuracy obtained using continuous or discontinuos functions to approximate λ has been compared. We expected to find a relationship between the polynomial order of constraint and that one of multiplier, but the accuracy of solution was not influenced in the way we thought. In general the best behaviour was obtained for functions piecewise linear to interpolate the Lagrange multiplier.

The problem under study Eq. 24 is interesting because it shows the great efficiency of the method.
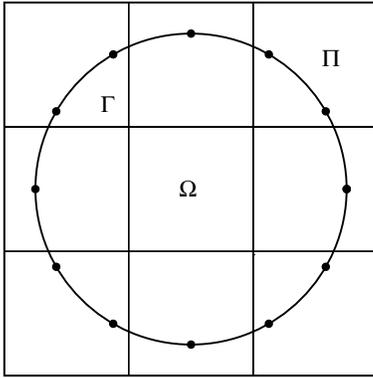
Figure 7: Computational domain for Poisson test problem Eq. 23. Domain spans the region $-1 \leq x \leq 1, -1 \leq y \leq 1$ into $N_{el} = 9$ equal quadrilateral elements

Table 1: Relative energy norm η for the two-dimensional stationary Poisson problem Eq. 23, obtained using a grid of 9 elements for domain and 12 for Lagrange multipliers, with second order polynomials to approximate the function ϕ and its derivatives and piecewise linear modal functions to approximate Lagrange multipliers

η_ϕ	$\eta_{\partial\phi/\partial x}$	$\eta_{\partial\phi/\partial y}$
4.541E-07	6.825E-07	6.895E-07

But it is not particularly attractive to illustrate the behaviour of the algorithm varying the refinement of discretization and the order of trial functions. As the solution of problem under study is a paraboloid, we expect to obtain really precise results when expansion modes of spectral elements are second order polynomials. In Tab. 1 it is shown the accuracy of solution and gradients according to definition of η in Eq. 22. To get such result we used second order polynomials for modal functions of unknowns ϕ, $\partial\phi/\partial x$ and $\partial\phi/\partial y$.

Cause of the simplicity of the problem different grid steps for fictitious domain and different ele-

ment number of immersed boundary mesh do not influence the accuracy of results. The values of relative energy norm in Tab. 1 are obtained using a grid of 9 elements for domain and 12 for Lagrange multipliers (Fig. 7). If we increase these values we do not improve the accuracy of the model, but we get the same accuracy obtained previously.

It should be suitable to consider a more complex Poisson problem to show the efficiency of fictitious domain spectral/hp element algorithm. Let us consider the new problem:

$$\begin{cases} -\triangle\phi = -2\pi^2 \, sin(\pi x) \, sin(\pi y) & \text{on } \Omega \\ \phi = sin(\pi x) \, sin(\pi y) & \text{on } \Gamma \end{cases} \quad (27)$$

with $\Omega = \{(x,y) \in \Re^2 : x^2 + y^2 < 1.2^2\}$ and $\Gamma = \{(x,y) \in \Re^2 : x^2 + y^2 = 1.2^2\}$. The boundary condition on Γ is Dirichlet type. The analytical solution of this problem is:

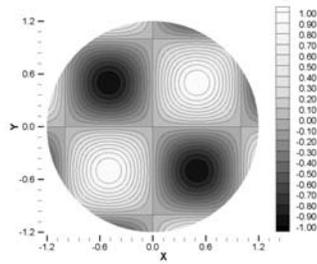$$\phi(x,y) = sin(\pi x) \, sin(\pi y) \quad (28)$$

whose partial derivatives are:

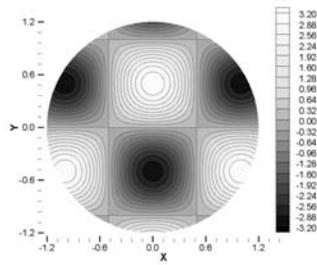$$\phi_x = \frac{\partial\phi}{\partial x}(x,y) = \pi \, cos(\pi x) \, sin(\pi y) \quad (29)$$

$$\phi_y = \frac{\partial\phi}{\partial y}(x,y) = \pi \, sin(\pi x) \, cos(\pi y). \quad (30)$$

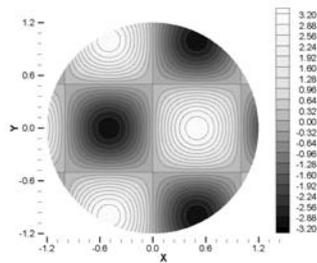The analytical solution is shown in Fig. 8.

We solve the problem (Eq. 27) by fictitious domain method considering the square $\Pi = [-1.4, 1.4] \times [-1.4, 1.4]$, which include Ω, as computational domain. Fictitious domain Π is meshed uniformly by square cells. The immersed boundary Γ is meshed uniformly with one-dimensional curved elements on which the Lagrange multipliers are defined. The modal functions of Lagrange multipliers are piecewise linear. We have investigated how the accuracy of the solution is influenced by the discretization of Lagrange multipliers. In particular we have considered different values of ratio h/H, where h is the length of the immersed element and H is the diagonal lenght of domain element. Morevover
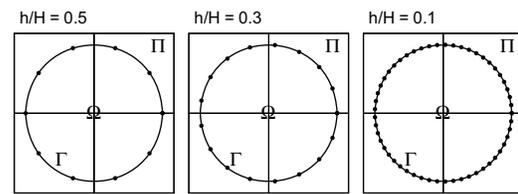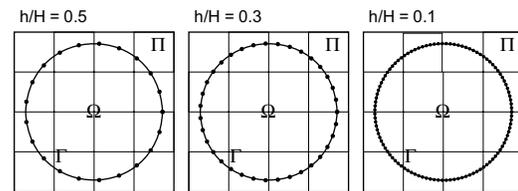
of the similarity of the derivatives. It is evident that the accuracy is influenced by the number of elements of domain, by the polynomial order p and by the ratio h/H which should be $0.3 \div 0.5$. We can notice as η reaches an asymptotic value increasing p, value that is reached faster if we refine the grid of domain. About the mesh on immersed constraint if the refinement is too excessive numerical errors are produced and the behaviour of the algorithm with high values of p is out of control. Moreover we can deduce by results that if the function under study has a low variability a coarse mesh for domain is sufficient to get good results.

(a) function

(b) derivative in x

(c) derivative in y

Figure 8: Analytical solution of two-dimensional stationary Poisson test problem Eq. 27

we have tested different grid steps and different expansion order for modal polynomial of ϕ, $\partial \phi / \partial x$ and $\partial \phi / \partial y$. Fig. 9 shows the tested computational domains. Fig. 10, Fig. 11, Fig. 12 show the accuracy of results.

Some remarks can be done observing the plots of relative energy norm η. We have obtained the same values of η for $\partial \phi / \partial x$ and $\partial \phi / \partial y$ because
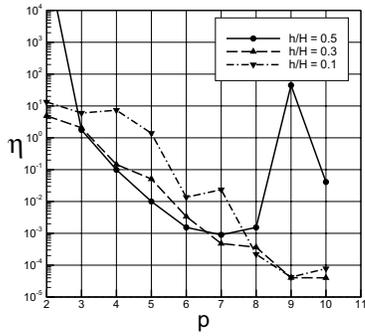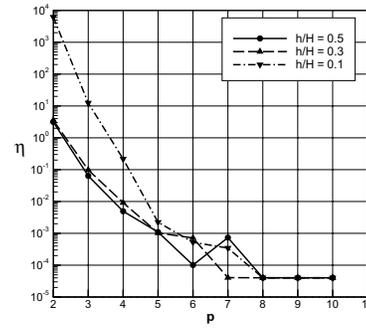
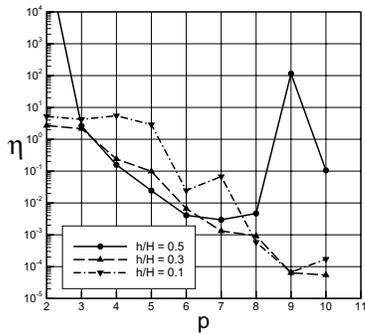

(a) $N_{el} = 4$

(b) $N_{el} = 9$

(c) $N_{el} = 16$

Figure 9: Computational domain for Poisson test problem Eq. 27. Domain spans the region $-1.4 \le x \le 1.4$, $-1.4 \le y \le 1.4$ into $N_{el} = 4, 9, 16$ equal quadrilateral elements
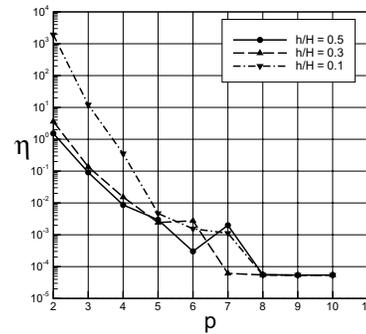
(a) function

(b) derivative in x and derivative in y

Figure 10: Relative energy norm η of function ϕ, derivative $\frac{\partial \phi}{\partial x}$ and derivative $\frac{\partial \phi}{\partial y}$ versus polynomial order p of trial functions for Poisson problem Eq. 27. The solution is obtained for $N_{el} = 4$ and different immersed boundary discretizations, as shown in Fig. 9(a)

(a) function

(b) derivative in x and derivative in y

Figure 11: Relative energy norm η of function ϕ, derivative $\frac{\partial \phi}{\partial x}$ and derivative $\frac{\partial \phi}{\partial y}$ versus polynomial order p of trial functions for Poisson problem Eq. 27. The solution is obtained for $N_{el} = 9$ and different immersed boundary discretizations, as shown in Fig. 9(b)

### 5.3 One-dimensional stationary diffusion problem in cooling fins

To verify the accuracy of our numerical algorithm based on fictitious domain method we solve the equation of thermal diffusion in heatsink profiles with negligible thickness:

$$\frac{d^2\theta}{dx^2} = \frac{2h}{s\lambda}\theta \tag{31}$$

with

$$-\lambda \frac{d\theta}{dx}\Big|_{x=0} = q_0 \quad \text{and} \quad -\lambda \frac{d\theta}{dx}\Big|_{x=l} = h\theta \tag{32}$$

where $\theta = T - T_\infty$ is the relative temperature with T_∞ the ambient temperature, s is the thickness of profile, λ the conduction coefficient, h the convection coefficient and q_0 is the inlet thermal flux. For giving generality to results it has been considered the adimensional conduction equation, introducing the Biot number. The Biot number Bi is a
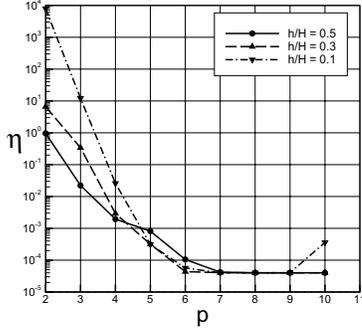
(a) function
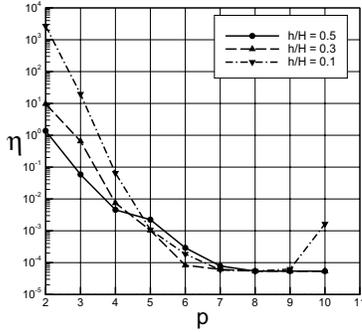
(b) derivative in x and derivative in y

Figure 12: Relative energy norm η of function ϕ, derivative $\frac{\partial \phi}{\partial x}$ and derivative $\frac{\partial \phi}{\partial y}$ versus polynomial order p of trial functions for Poisson problem Eq. 27. The solution is obtained for $N_{el} = 16$ and different immersed boundary discretizations, as shown in Fig. 9(c)

dimensionless number and relates the heat transfer resistance inside and at the surface of a body. Values of the Biot number smaller than 0.1 imply that temperature gradients are negligible inside the body.

The adimensional problem writes as:

$$\frac{d^2\Theta}{dX^2} = Bi\Theta \tag{33}$$

with

$$\frac{d\Theta}{dX}\bigg|_{X=0} = -\Phi_0 \quad \text{and} \quad \frac{d\Theta}{dX}\bigg|_{X=L} = -Bi\Theta \tag{34}$$

where we set $Bi = \frac{hL_c}{\lambda} = 10^{-5}$, $\Phi_0 = \frac{q_0 L_c}{\lambda \Theta^*} = 0.01$, $L = \frac{l}{L_c} = 100$, taken as example. The analytical solution of the problem, plotted in Fig. 13, is given by equations:

$$\Theta(X) =$$
$$\frac{\Phi_0}{\sqrt{Bi}} \frac{\left(1+\sqrt{Bi}\right)e^{\sqrt{Bi}L}e^{-\sqrt{Bi}X}+\left(1-\sqrt{Bi}\right)e^{-\sqrt{Bi}L}e^{\sqrt{Bi}X}}{\left(1+\sqrt{Bi}\right)e^{\sqrt{Bi}L}-\left(1+\sqrt{Bi}\right)e^{-\sqrt{Bi}L}} \tag{35}$$

$$\Phi(X) = -\frac{d\Theta}{dX} =$$
$$\Phi_0 \frac{-\left(1+\sqrt{Bi}\right)e^{\sqrt{Bi}L}e^{-\sqrt{Bi}X}+\left(1-\sqrt{Bi}\right)e^{-\sqrt{Bi}L}e^{\sqrt{Bi}X}}{\left(1+\sqrt{Bi}\right)e^{\sqrt{Bi}L}-\left(1+\sqrt{Bi}\right)e^{-\sqrt{Bi}L}}. \tag{36}$$
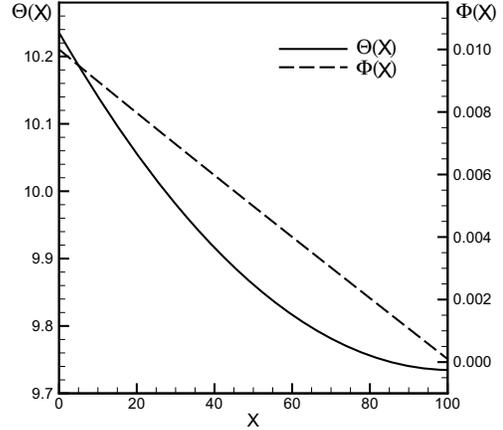

Figure 13: Analytical solution of one-dimensional stationary diffusion problem in heatsink profile for $Bi = 10^{-5}$

For more details about thermal diffusion in heatsink profiles see [Kreith (1975); Bonacina, Cavallini, and Mattarolo (1989)].

To verify the accuracy of our algorithm, the numerical solution will be compared with the analytical one. The numerical solution is obtained

considering the fictitious domain $\Pi = [-25, 125]$, which has been meshed uniformly with a grid step H varying from 30 to 75, that means it has been devided into 2, 3, 4 and 5 elements. The Neumann and Robin constraints have been imposed by Lagrange multipliers.

In Fig. 14(a) we plot the relative energy norm of function θ as function of expansion order p, for different grid steps. We perform the same analysis for the specific flux q in Fig. 14(b). We can observe that the results are significantly accurate for $p \geq 5$ for both the temperature and the flux, but in general the accuracy of the numerical function will be higher than that one of its derivative. It can be remarked that η has an asymptotic behaviour and it can not be improved, beyond its asymptotic value, increasing the number of spectral elements or the polynomial order of trial functions. The asymptotic value, corresponding to machine round-off, is reached quickly, indicating a very high accuracy of the method.

5.4 Two-dimensional stationary diffusion problem in cooling fins

Employing the fictitious domain method we solve the diffusion equation for a two-dimensional cooling fin, which writes as:

$$\begin{cases} -\triangle \Theta = 0 & \text{on } \Omega \\ -\frac{\partial \Theta}{\partial n} = \Phi_0 & \text{on } \Gamma_b \\ -\frac{\partial \Theta}{\partial n} = Bi\Theta & \text{on } \Gamma_a \end{cases} \tag{37}$$

referring to adimensional form. The unknowns are the adimensional temperature Θ and the specific adimensional fluxes $\Phi_x = -\partial\Theta/\partial X$ and $\Phi_y = -\partial\Theta/\partial Y$. $\Omega \in \Re^2$ is the domain shown in Fig. 15, Γ_b is the boundary of geometry in contact with the body to cool and Γ_a the boundary of geometry immersed in a fluid ast temperature T_∞. We set the Biot number at 10^{-4} and the inlet specific flux Φ_0 on Γ_b at 0.1 (Fig. 16).

The analytical solution of two-dimensional thermal conduction problem can be computed for simple geometries and boundary constraints, but in general the employment of numerical methods are required. For this reason we compare our
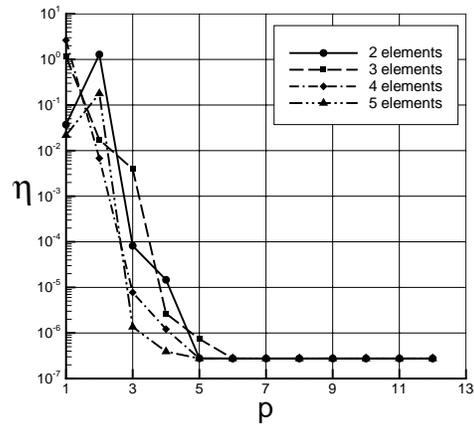
(a) function
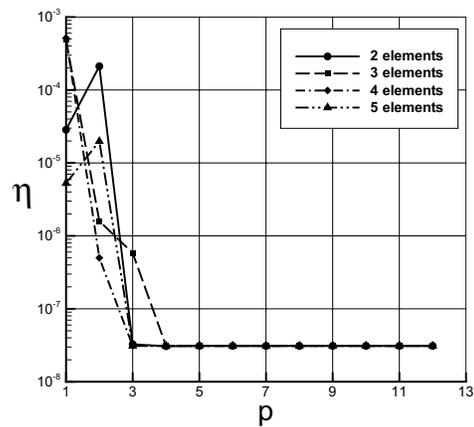
(b) derivative

Figure 14: Relative energy norm η of temperature Θ and specific flux Φ versus the expansion order p of spectral elements for thermal diffusion problem Eq. 33-Eq. 34

numerical solution to that one obtained by a finite element solver using a fine unstructured mesh of 61952 elements (Lagrange quadratic type) (Fig. 17).

The fictitious domain we consider is the rectangle $\Pi = [-2.5, 12.5] \times [-4.0, 4.0] \supset \Omega$. The domain Π is meshed by a cartesian grid with 8 rectangular cells, 4 along x and 2 along y (Fig. 18). The aspect ratio of cells is 0.94. The immersed boundary Γ on which the Lagrange multipliers
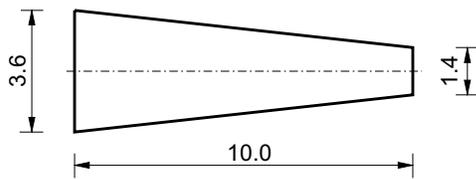
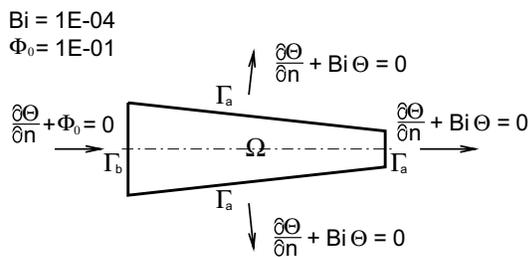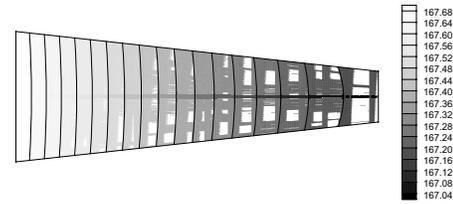Figure 15: Geometry of the two-dimensional heatsink profile under study

Figure 16: Boundary conditions for thermal diffusion problem under study

(a) adimensional temperature

(b) adimensional specific flux in x

(c) adimensional specific flux in y

Figure 17: Finite element solution of two-dimensional stationary diffusion problem in heatsink profile under study
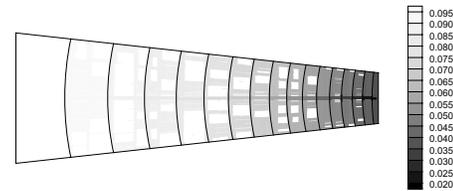
functions are defined is meshed uniformly with one-dimensional elements. The modal functions defined on the immersed elements are piecewise linear.

Several remarks can be done on the obtained results. In Fig. 19 and Fig. 20 relative energy norms of temperature and specific flux are plotted in function of polynomial order p of expansion modes in each direction and for different refinements of immersed mesh. Fig. 21 shows the inverse of coefficient matrix condition number and Fig. 22 the CPU time required to solve the problem.
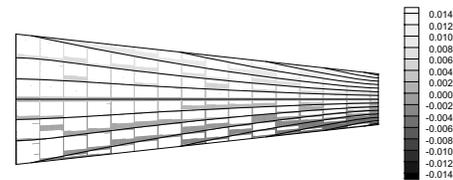
We can observe that the results are significantly accurate for $p \geq 5$. The accuracy of the solution is influenced by ratio h/H. It seems that the algorithm has a better behaviour for $h/H = 0.3 \div 0.4$, in particular for low values of p. Increasing the polynomial order p the inverse of coefficient matrix condition number decrease approximatly in

logarithmic way and the CPU time drastically grows. This implies the need of efficient matrix solvers for high values of p. The CPU time required for solving the problem with the developed code is not comparable with that required by the commercial code used to compute the reference solution. Actually in this initial phase to implement the algorithm, we have given more attention to the methodology than the time perfomance of the code. That aspect will be the object of future work, in order to reduce CPU time significantly. By the plots of relative energy norms it can be
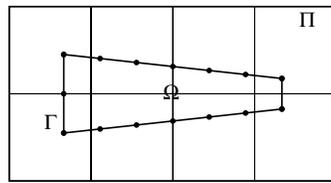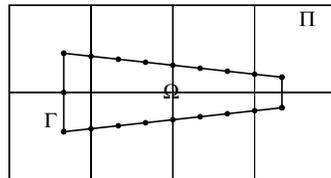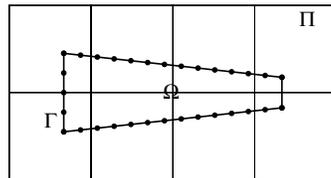
(a) $h/H = 0.4$

(b) $h/H = 0.3$

(c) $h/H = 0.2$

Figure 18: Computational domain for thermal diffusion problem under study Eq. 37. Domain spans the region $-2.5 \leq x \leq 12.5, -4.0 \leq y \leq 4.0$ into $N_{el} = 8$ quadrilateral elements with aspect ratio 0.94

Figure 19: Relative energy norm η of adimensional temperature Θ versus polynomial order p of trial functions for thermal diffusion problem under study Eq. 37. The solution is obtained for different immersed boundary discretizations, shown in Fig. 18

noticed that the algorithm is not strongly stable . Further study and additional tests are required to better understand how the stability of algorithm is influenced by dimension of fictitious domain, its grid step, immersed mesh and order of modal functions of Lagrange multipliers.

6   Conclusion

The main objective of this paper was to present a new spectral element method for the analysis of second-order differential problems with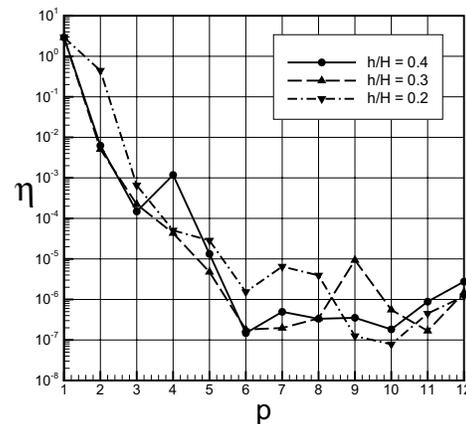 complex boundary domains.   Our algorithm employs a fictitious domain approach and for this reason its main advantage lies in the fact that only a cartesian mesh, that rapresents the enclosure, needs to be generated. The boundary constraints, immersed in the new simple shaped computational domain, are forced by means of Lagrange multipliers.   To enable all possible types of boundary constraints imposition, the scalar problem must be rewritten as a vector problem introducing as further unknowns the derivatives of the function under study.   This, at present, represent the major drowback of the method. Computational cost to solve the problem grows up in behalf of a great flexibility in studied geometries, avoiding the need of complicated mesh methodologies.

Excellent accuracy properties of method are demonstrated by numerical experiments.   We have considered the one- and two-dimensional Poisson problem and then the one-dimensional diffusion problem in a cooling fin where exact solution can be computed.   In the last example we have considered the heat conduction problem for a two-dimensional heatsink profile where the solution has been compared with that one
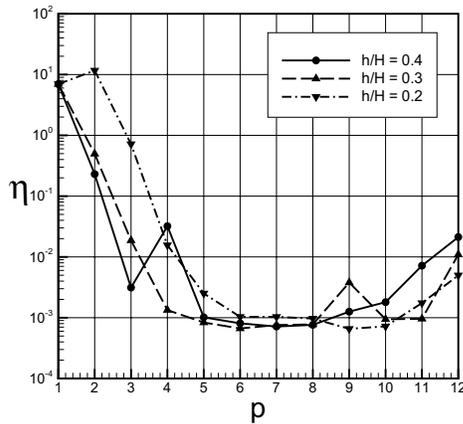
(a) adimensional specific flux in x
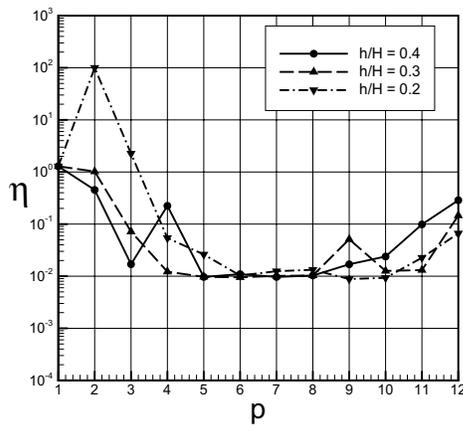
(b) adimensional specific flux in y

Figure 20: Relative energy norm η of adimensional specific flux Φ_x and adimensional specific flux Φ_y versus polynomial order p of trial functions for thermal diffusion problem under study Eq. 37. The solution is obtained for different immersed boundary discretizations, shown in Fig. 18

Figure 21: Inverse of coefficient matrix condition number versus polynomial order p of trial functions for thermal diffusion problem under study Eq. 37.
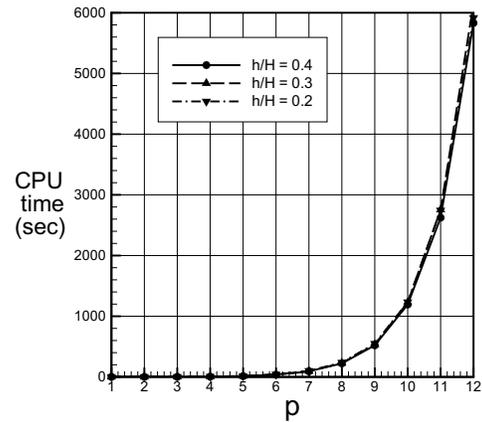
Figure 22: CPU time required to solve the thermal diffusion problem under study Eq. 37 versus polynomial order p of trial functions.

computed using a finite element solver with a fine mesh.

More tests and study are still required to understand the behaviour of the algorithm, in particular how the stability of algorithm is influenced by dimensions of fictitious domain, grid step, immersed mesh and order of Lagrange multipliers trial functions. In any case this approach should represent an advantageous alternative to standard methods for those numerical simulations which involve evolving geometries.

It is easy to understand the great advantage of such kind of approach for numerical simulations which involve changing geometries, i.e. flow with moving bodies, shape optimization problems, elastic structures, etc. The standard way to proceed in these cases is based on the

boundary variation technique which requires a lot of computational time. A new domain is constructed for each time step or optimization step. The use of a discretizing method for the numerical computation of the problem means that after any change of shape, one has to remesh the new configuration, then to recompute all data defining the discrete problem, such as stiffness matrix, load vector, etc., and then to solve a new updated problem. In this sense the formulation we propose presents a great advantage. We offer a tool for numerical resolution of unsteady problems where mesh is simple to construct and there is no need to create a different mesh for each new geometry of the problem.

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Appendix A: Jacobi Polynomials

Jacobi polynomials represent a family of polynomial solutions to the singular Sturm-Liouville problem. A significant feature of these polynomials is that they are orthogonal in the interval $[-1, 1]$ with respect to the function $(1 - x)^\alpha (1 - x)^\beta$ $(\alpha, \beta > -1)$. These polynomials can be constructed using a recursion relationship:

$$P_0^{\alpha,\beta}(x) = 1$$
$$P_1^{\alpha,\beta}(x) = \frac{1}{2}[\alpha - \beta + (\alpha + \beta + 2)x]$$
$$a_n^1 P_{n+1}^{\alpha,\beta}(x) = (a_n^2 + a_n^3 x)P_n^{\alpha,\beta}(x) - a_n^4 P_{n-1}^{\alpha,\beta}(x)$$
$$a_n^1 = 2(n+1)(n+\alpha+\beta+1)(2n+\alpha+\beta))$$
$$a_n^2 = (2n+\alpha+\beta+1)(\alpha^2 - \beta^2)$$
$$a_n^3 = (2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)$$
$$a_n^4 = 2(n+\alpha)(n+\beta)(2n+\alpha+\beta+2)$$

A class of symmetric polynomials, known as ultraspheric polynomials, corresponds to the choice $\alpha = \beta$. Well known ultraspheric polynomials are the Legendre polynomial ($\alpha = \beta = 0$) and the Chebychev polynomial ($\alpha = \beta = -1/2$).
Further formulae and properties for Jacobi polynomials can be found in [Abramowitz and Stegun (1972); Karniadakis and Sherwin (1999)].

Appendix B: Gauss-Legendre integration

To evaluate integrals of the form

$$\int_{-1}^{1} f(\xi)d\xi \tag{A:1}$$

by quadraure, the fundamental concept is the approximation of the integral by a finite summation of the form

$$\int_{-1}^{1} f(\xi)d\xi = \sum_{i=0}^{Q-1} \omega_i f(\xi_i) + \varepsilon(f) \qquad \text{(A:2)}$$

where ω_i are specified weighting coefficients, ξ_i represent an abscissa of Q distinct points in the interval $-1 \le \xi_i \le 1$ and $\varepsilon(f)$ is the approximation error.

There are many different types of numerical integration. The Gaussian quadratures provide the flexibility of choosing not only the weight factors but also the locations where the functions are evaluated, unlike the Newton-Cotes formulas, which have uniformly spaced grid points. As a result, Gaussian quadratures yield twice as many places of accuracy as that of the Newton-Cotes formulas with the same number of function evaluations. When the function is known and smooth, the Gaussian quadratures usually have decisive advantages in efficiency respect to other numerical integration formulae.

The most commonly used form of Gaussian quadratures is the Gauss-Legendre integration formula. Some numerical analysis books refer to the Gauss-Legendre formula as the Gaussian quadratures' definitive form. It is based on the Legendre polynomials $P_P^{0,0}$ (see Appendix A: Jacobi Polynomials). Introducing $\xi_{i,P}^{\alpha,\beta}$ to denote the P zeros of the Pth order Jacobi polynomial $P_P^{\alpha,\beta}$ such that

$$P_P^{\alpha,\beta}(\xi_{i,P}^{\alpha,\beta}) = 0 \quad i = 0, 1, ..., P-1$$

where

$$\xi_{0,P}^{\alpha,\beta} < \xi_{1,P}^{\alpha,\beta} < ... < \xi_{P-1,P}^{\alpha,\beta}$$

we can define abscissae and weights, which approximate the integral Eq. A:1, as :

$$\xi_i = \xi_{i,Q}^{0,0} \quad i = 0, ..., Q-1$$

$$\omega_i^{0,0} = \frac{2}{1-(\xi_i)^2} \left[\left(\frac{d}{d\xi}P_Q^{0,0} \right) \Big|_{\xi=\xi_i} \right]^{-2} \quad i = 0, ..., Q-1$$

$$\varepsilon(f) = 0 \quad \text{if } f(\xi) \in P_{2Q-1}([-1,1])$$

The zeros of the Jacobi polynomial do not have an analytic form and to evaluate the abscissa the use of a numerical algorithm is required (see [Karniadakis and Sherwin (1999)]). Having determined the zeros, the weights can be evaluated from the previous formulae.

Appendix C: Implementation of fictitious domain for one-dimensional problems

Let us consider the one-dimensional boundary value Poisson problem defined on $\Omega = [x_1, x_2] \in \Re$:

$$\frac{d^2\phi}{dx^2} = f(x) \qquad \text{(A:3)}$$

where $f(x)$ is the source term. The solution has to satisfy the boundary conditions:

$$\begin{cases} \frac{d\phi}{dx}(x_1) = u_1 \\ \phi(x_2) = \phi_2. \end{cases} \qquad \text{(A:4)}$$

The equivalent first-order system of Eq. A:3-Eq. A:4 is:

$$\begin{cases} u - \frac{d\phi}{dx} = 0 \\ \frac{du}{dx} = f(x) \\ u(x_1) = u_1 \\ \phi(x_2) = \phi_2. \end{cases} \qquad \text{(A:5)}$$

To solve the problem by classical approach, the variational formulation on Ω is:

$$\int_\Omega v_i u \, dx - \int_\Omega v_i \frac{d\phi}{dx} dx = 0 \qquad \text{(A:6)}$$

$$\int_\Omega \varphi_i \frac{du}{dx} dx = \int_\Omega \varphi_i f(x) dx \qquad \text{(A:7)}$$

for all the weighting functions $\varphi_i(x)$, $v_i(x)$, $i = 1, N_{dof}$. To find solution of the system, the domain Ω is discretized and unknowns ϕ and u approximated. The boundary conditions can be imposed by direct substitution.

If we want to solve the problem by fictitious domain method, the considered computational domain is $\Pi \supset \Omega$ and the boundary constraints, which are now *immersed* in the domain, are imposed via Lagrange multipliers. So the variational formulation according to fictitious domain

approach is:

$$\int_\Pi v_i u \, dx - \int_\Pi v_i \frac{d\phi}{dx} dx + [v_i \lambda_1]_{x_1} = 0 \qquad \text{(A:8)}$$

$$\int_\Pi \varphi_i \frac{du}{dx} dx + [\varphi_i \lambda_2]_{x_2} = \int_\Pi \varphi_i f(x) dx$$
$$\text{(A:9)}$$

$$[u]_{x_1} = u_1 \qquad \text{(A:10)}$$

$$[\phi]_{x_2} = \phi_2 \qquad \text{(A:11)}$$

for all φ_i, v_i, $i = 1, N_{dof}$, where $v_i(x)$ and $\varphi_i(x)$ are the weighting functions and $\phi(x), u(x), \lambda_1$ and λ_2 the unknowns. Notice that in one-dimensional problems the Lagrange multipliers are just a constant defined on the constrained point.

To get the solution of the equivalent problem spectral elements are employed. The computational domain Π is discretized into N_{el} elements Π_e. We map Π_e to $\Pi_e = [-1, 1]$, where (ξ) is a point in Π_e. Over a typical element Π_e, we approximate the unknowns ϕ and u by the expression

$$\phi = \sum_{p=0}^{P} \varphi_p^e(\xi) \phi_p^e \quad \text{on } \Pi_e \qquad \text{(A:12)}$$

$$u = \sum_{p=0}^{P} v_p^e(\xi) u_p^e \quad \text{on } \Pi_e \qquad \text{(A:13)}$$

where P is the polynomial order of the expansion and $\varphi_p^e(\xi)$ and $v_p^e(\xi)$ are the weighting functions in adimensional coordinate ξ (the superscript denotes the element in which the function is nonzero).

The unknowns ϕ and u on Π will be given by:

$$\phi = \sum_{j=1}^{N_{dof}} \varphi_j(x) \phi_j = \sum_{e=1}^{N_{el}} \sum_{p=0}^{P} \varphi_p^e(\xi) \phi_p^e \qquad \text{(A:14)}$$

$$u = \sum_{j=1}^{N_{dof}} v_j(x) u_j = \sum_{e=1}^{N_{el}} \sum_{p=0}^{P} v_p^e(\xi) u_p^e \qquad \text{(A:15)}$$

which are obtained solving the discretized variational problem, written in matrix form:

$$[\mathbf{G}]\{\mathbf{Y}\} = \{\mathbf{F}\}. \qquad \text{(A:16)}$$