

Proceedings of the 6th International Conference on Numerical Analysis, pp 260-265



Contents lists available at AMCL's Digital Library
NumAn2014 Conference Proceedings



Interface Rexation Methods for the solution of Multi-Physics Problems

Digital Library Triton : http://lib.amcl.tuc.gr

Panagiota Tsompanopoulou

Dep. of Electrical and Computer Eng., University of Thessaly, Volos, Greece yota@inf.uth.gr

Abstract. Multi-physics phenomena are quite complex and it is impossible to solve them efficiently and accurately by facing them with a single complicated model. They are usually modeled as multi-domain multi-physics Partial Differential Equation (PDE) problems, initially treated with Domain Decomposition (DD) methods. Interface Relaxation (IR) methodology presented as an alternative way to overcome these problems facing most of the DD difficulties. A short review on simulation of multiphysics problems is presented. Existing IR studies for Elliptic PDEs are discussed while a first version of this methodology is proposed for parabolic multiphysics PDEs.

1 Introduction

Simulations of multiphysics phenomena is a very promising research area today [1] and in the past [2]. Computing power is increased and is offered at any level of hardware, from high speed multi-processors and clusters to multi-core GPUs. This offer the opportunity for more accurate simulations in reasonable execution times. Also the realization of computational environments [3–10] utilizing all available capabilities of both hardware and software brings us a step closer to simulate real world problems with efficiency and accuracy.

Domain Decomposition [11–17] methods are methods initially used to face such kind of problems. Their main characteristic is that they first discretize the global problem (even if it is already partitioned by its physics) and then decompose it at the linear algebra level. Several techniques, mainly iteratively, are used to solve the set of the strongly coupled systems of linear equations that arise.

Interface Relaxation (IR) methodology [18] is an alternative way to study such problems. IR methods study the global problem interpreting its own physics, in order to realize and utilize all its properties. The resulting subproblems are derived either by the original problem's physics or by computational and parallelization issues. These "small" problems are studied independently of each other and appropriate methods (FEM, FD, etc.) are used for their solution. However, these subproblems are coupled [19–21] on the common interfaces so as to satisfy the conditions resulting from the global problem's properties (e.g., continuity and smoothness of the solution of the global problem, jumps in the derivatives etc.). Initial guesses are considered on the interfaces and passed as boundary conditions to the "small" problems. These are solved concurrently and the resulting approximations are used by an IR method to relax the value and/or the derivative to get better estimates of the solution on the interfaces. These new estimates are passed again as boundary conditions to the small problems and the procedure iterates until convergence is achieved.

When studying IR methods, one should consider issues from both mathematical analysis, computational complexity and software/hardware viewpoint [1]. Mathematical analysis is often derived for model problems representatives of the original multiphysics applications since it is not possible and practical to get analysis for the realistic problems. Software reuse is of great importance when implementing IR methods. A variety of software packages for the solution of simple non-multiphysics problems exist but they have to be combined under suitable software and hardware environments.

This work is organized as follows. Examples of simulations for multiphysics applications are presented in Section 2. Section 3 contains a description of IR methods used for applications modeled with elliptic PDE and parabolic PDEs. Finally, in Section 4 conclude and propose further steps.

2 Simulations for multiphysics problems

A multiphysics problem is problem that consists of multiple parts ruled by various principles and laws. These could be equilibrium or evolution principles following conservation or constitutive laws. The components of the multiphysics problems are coupled either through a system of PDEs on common and/or overlapping domains, or through boundary conditions of interfaces (of lower dimension than the original problem) between adjacent domains. In the first class one could find problems like electricity and magnetism with hydrodynamics, while the second class contains multiphysics problems as fluid-structure dynamics (aeroelasticity) or ocean-atmosphere dynamics (geophysics) etc. All multiphysics problems are mainly described in algebraic forms before they are descritized and solved. The two most popular forms are the one for the coupled equilibrium problem

$$F(u) \equiv \begin{pmatrix} F_1(u_1, u_2) \\ F_2(u_1, u_2) \end{pmatrix} = 0,$$
(1)

and the one for the coupled evolution problem (2)

$$\frac{\partial_t u_1 = f_1(u_1, u_2)}{\partial_t u_2 = f_2(u_1, u_2)}.$$
(2)

Setting as $J = \frac{\partial(F_1, F_2)}{\partial(u_1, u_2)}$ and $u = (u_1, u_2)^T$, the algorithms for the equilibrium problems (1) can be categorized in three classes as in Table 1. These are Jacobi, Gauss-Seidel or Newton style. In the left class of algorithms each single PDE problem is solved for its corresponding unknown using all other unknowns from the previous iteration. For example, during the k iteration the first problem is solved for the first unknown u_1^{k+1} using u_2^k while the second one is solved for the second unknown u_2^{k+1} using u_1^k . Thus, this scheme corresponds to the Jacobi iterative procedure for the solution of linear equation systems. One can expand this for more PDE problems, solving the *i* problem for the *i*th unknown using the rest unknowns from the previous iteration. This scheme is

Jacobi	Gauss-Seidel	Newton
Given intial guess (u_1^0, u_2^0) for k=1,2, (until convergence)		
$ \begin{array}{c} \text{Solve for } (u_1^{k+1}, u_2^{k+1}) \\ F_1(u_1^{k+1}, u_2^k) = 0 \\ F_2(u_1^k, u_2^{k+1}) = 0 \end{array} \end{array} $	$ \begin{array}{l} \text{Solve for } (u_1^{k+1}, u_2^{k+1}) \\ F_1(u_1^{k+1}, u_2^k) = 0 \\ F_2(u_1^{k+1}, u_2^{k+1}) = 0 \end{array} $	$ \begin{array}{l} \text{Solve for } \delta u \\ J(u^k) \delta u = -F(u^k) \\ \text{Update } u^{k+1} = u^k + \delta u \end{array} $
end for		

Table 1. Algorithms for equilibrium problems.

fully parallelized.

The Gauss-Seidel algorithms work as the corresponding method for the linear systems. Considering n coupled problems, the i problem is solved for the u_i unknown using unknowns $u_1, u_2, \ldots, u_{i-1}$ just computed in this iteration, while the ones u_{i+1}, \ldots, u_n are used from the previous iteration. This procedure does not complain any parallelism but usually converge faster than the Jacobi one.

Finally, the Newton algorithms are considered tightly coupled schemes, since the involve terms of $\frac{\partial F_i}{\partial u_j}$ in the Jacobian matrix. They are used in both equilibrium and evolution problems.

Table 2. Algorithms for evolution problems.

Given initial guess $(u_1(t_0), u_2(t_0))$ for $n = 1, \dots, N_t$

Proceed one timestep for u_1 solving $\partial_t u_1 = f_1(u_1, u_2(t_{n-1}))$ at the *n* timestep (i.e., $u_1(t_n)$) Proceed one timestep for u_2 solving $\partial_t u_2 = f_2(u_1(t_n), u_2)$ at the *n* timestep (i.e., $u_2(t_n)$) end for

For the evolution type of multiphysics problems one can consider schemes as in Table 2. This scheme is the simplest one could be used for parabolic multiphysics PDE problems. Each subproblem can be faced with implicit or explicit methods, and nested iterations for convergence purposes maybe used.

3 Interface Relaxation Methodology

IR methodology considers that all multidomain-multiphysics PDE problems consist of many "single PDE on simple domain" subproblems. Also, considers that there are existing PDE solvers for these simple subproblems. Therefore, one could combine these simple PDE solvers to solve the original composite problem. The procedure is iterative as seen below is shown in [20]:

- 1. Guess solution values (and derivatives if needed) on all sub-domain interfaces.
- 2. Solve all single PDEs exactly and independently on all the sub-domains with these values as boundary conditions.
- 3. Compare and improve the values on all interfaces using a relaxer (discussed below).
- 4. Return to Step 2 until satisfactory accuracy is achieved.

Relaxing on the interfaces varies form averaging the values of the adjacent subdomains to applying more complicated operators in order the global solution to satisfy all necessary conditions. This iteration scheme is defined at the mathematical-physical level of the problem, hence its convergence brings forth questions that has to be studied with mathematical analysis tools, beyond numerical analysis methods [19, 21]. The main advantages of the method are the following: i) it grants the accurate coupling of various models both for PDEs and interfaces, ii) it supports the reuse of software that treat single models, iii) it introduces a higher level parallelism in computations, iv) it is follows the geometry and physical modeling of a composite PDE problem.

Considering second order elliptic PDE problems in two dimensions, IR methodology can be written in the following way. The local PDEs problems are denoted by

$$L_i u_i = f_i \quad in \quad \Omega_i \quad for \quad i = 1, \dots, p, \tag{3}$$

assuming that Ω_i do not overlap. Also it is assumed that the interface conditions are given in the implicit form

$$G_{i,j}\left(u_i, \frac{\partial u_i}{\partial \eta_{i,j}}; u_j, \frac{\partial u_j}{\partial \eta_{j,i}}; J_1, J_2\right) = 0 \quad on \quad \Gamma_{i,j} \equiv \Omega_i \bigcap \Omega_j, \tag{4}$$

where $\eta_{i,j}$ denotes the normal direction on interface $\Gamma_{i,j}$ and J_1, J_2 the jump quantities associated with u or its derivative. We assume that $G_{i,j}$ can be a function mapping on the interface or even a functional. We also assume certain boundary conditions (not shown here) and the existence of the solution of the PDE problems. Few IR methods for elliptic problems are presented and studied in [18–21].

Parabolic multiphysics PDE problems could be treated with similar IR methods depending on the PDE terms beside the one with the time derivative, e.g., reaction-diffusion, advection-diffusion, etc. If the splitting is done operator-wise multiple algorithms are derived combining algorithms presented in Tables 1 and 2. But if the splitting is considered in the PDE domain (as in the elliptic case above), one could follow an iteration scheme like this:

- 1. Consider initial values (and derivatives if needed) on all sub-domain interfaces. These values are computed by the initial condition of global problem.
- 2. For each timestep do as:
 - (a) Evolve all single PDEs exactly and independently on all the sub-domains with the values above as boundary conditions along with the regular boundary conditions of the subproblems. Solve for the each sub-solution at the next time-step.
 - (b) Combine values and derivatives of sub-solutions on the interfaces (as in elliptic case) to be used as boundary values for the next time-step.IR method used should force the conditions that should be satisfied (continuity, smoothness, jumps etc.).

3. Nested iteration might be needed depending on the PDE problems.

This scheme is only a proposition and needs further exploitation and study.

4 Conclusions

This paper presents a short review on the multi-domain multiphysics simulations from an algorithmic viewpoint. IR methodology is described for elliptic PDE multi-physics problems, while a slightly modified methodology is proposed for parabolic PDE multidomain problems. Studies of existing or new coupling schemes from operator and domain viewpoint, for particular kinds of parabolic equations are the considered our next steps. It is clear that from applications, mathematics and computations viewpoint there are many steps to go beyond in the next years for multi-physics applications.

Acknowledgments

The present research work has been co-financed by the European Union (European Social Fund ESF) and Greek national funds through the Operational Program Education and Lifelong Learning of the National Strategic Reference Framework (NSRF) -Research Funding Program: THALIS. Investing in knowledge society through the European Social Fund (MIS 379416).

References

- Keyes, D., et. all, Multiphysics simulations: Challenges and Opportunities, Intr. J. of High Performance Computing Applications, 27(4), 1–83, (2013)
- 2. Rice, J.R., Modeling with collaborating PDE solving modules. In 7th Int. Conf. Math. and Comp. Modeling, 1989
- 3. Drashansky T.: An Agent-Based Approach to Building Multidisciplinary Problem Solving Environments. PhD Thesis, Purdue University, Computer Science Department, (1996)
- Rice, J.R., Tsompanopoulou, P., Vavalis, E.A.: SciAgents Tool: User's Guide. Tech. Rpt. TR-98-043, Dept. Computer Sciences, Purdue Univ., (1998)
- Bölöni, L., Marinescu, D.C., Rice, J.R., Tsompanopoulou, P., Vavalis, E.A.: Agent Based Scientific Simulation and Modelling. Concurancy: Practice and Experience, 12, 845–861 (2000)
- Markus, S., Houstis, E., Catlin, A., Rice, J., Tsompanopoulou, P., Vavalis, E., Gottfried, D., Su K., Balakrishnan, G.: An Agent-Based Netcentric Framework for Multidisciplinary Problem Solving Environments. International Journal of Computational Engineering Science, 1, 33–60 (2000)
- Houstis, E.N., Catlin, A.C., Tsompanopoulou, P., Gottfried, D., Balakrishnan, G., Su, K., Rice, J.R.: GASTURBNLAB: A Multidisciplinary Problem Solving Environment for Gas Turbine Engine Design on a Network of Non-Homogeneous Machines. J. of Comp. and Applied Mathematics, 149(1), 83-100 (2002)
- Michopoulos, J., Tsompanopoulou, P., Houstis, E., Farhat, C., Lesoinne, M., Rice, J., Joshi, A., On a Data-Driven Environment for Multiphysics Applications, Future Generation Computer Systems, 21(6), (Apr. 2005)

- Chalkias, C.:Implementation of a Distributed System for the Solution of MultiDomain / MultiPhysics Problems, Diploma Thesis, (2013), Dep. of Electrical and Computer Eng., Univ. of Thessaly. Online. Available: http:://www.inf.uth.gr/wp content/uploads/formidable/Chalkias_konstantinos.pdf
- Wang, W., Insights from developing a multidisciplinary design and analysis environment, Computers in Industry, 65, 786–795 (2014)
- Keyes, D., Gropp, W., A comparison of domain decomposition techniques for elliptic partial differential equations and their parallel implementation, SIAM, J. Sci. Stat. Comput., 8:s166– s202, 1987
- Le-Tallec, P., De-Roecl, Y., Vidrascu, M., Domain decomposition methods for large linearly elliptic 3-dimensional problems, J. Comput. Appl. Math., 34(1):93–117, 1991
- Lions, P.L., On the Schwarz alternating method III: A variant for nonoverlapping subdomains, In Glowinski, R., Golub, G.H., Meurant, G.A., Periaux, J., editors, Domain Decomposition Methods for Partial Differential Equations, pages 202–223. SIAM, 1990
- Chan, T.F., Mathew, T.P.: Domain decomposition algorithms, in: Acta Numerica 1994, Cambridge University Press, Cambridge, 61-143 (1994)
- Natarajan, R., Domain decomposition using spectral expansions of Steklov–Poincare operators, SIAM, J. Sci. Comput., 16(2):470–485, 1995
- Rice,J.R., Vavalis, E.A., Yang, D., Convergence analysis of a non-overlapping domain decomposition method for elliptic pdes, Technical Report CSD-TR-93-048, Purdue University, W. Lafayette. IN, 1993
- Heinrichs., W., Domain decomposition for fourth–order problems, SIAM, J. Numer. Anal., 30(2):435–453, 1993
- Rice, J. R., Tsompanopoulou, P., Vavalis, E.: Interface relaxation methods for elliptic differential equations. Applied Numerical Mathematics 32 2, 219–245 (2000)
- 19. Rice, J.R., Tsompanopoulou, P. Vavalis, E.A.: Fine Tunning Interface Relaxation Methods for Elliptic Differential Equations. Applied Numerical Mathematics, 43(4), 459–481 (2002)
- Tsompanopoulou, P., Vavalis, E.: An Experimental Study of Interface Relaxation Methods for Composite Elliptic Differential Equations. Applied Mathematical Modelling, 32 1620– 1641 (2008)
- Tsompanopoulou, P., Vavalis, E.: Analysis of an interface relaxation method for composite elliptic differential equations. Journal of Computational and Applied Mathematics 226 2, 370– 387 (2009)