

# TOPS (Terascale Optimal PDE Simulations)

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Activities at the Courant Institute  
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Toselli, and Barbara I. Wohlmuth.

**1. Summary.** Our work has focused on the development and analysis of domain decomposition algorithms for a variety of problems arising in continuum mechanics modeling. In particular, we have extended and analyzed FETI-DP and BDDC algorithms; these iterative solvers were first introduced and studied by Charbel Farhat and his collaborators, see [11, 45, 12], and by Clark Dohrmann of SANDIA, Albuquerque, see [43, 2, 1], respectively. These two closely related families of methods are of particular interest since they are used more extensively than other iterative substructuring methods to solve very large and difficult problems. Thus, the FETI algorithms are part of the SALINAS system developed by the SANDIA National Laboratories for very large scale computations, and as already noted, BDDC was first developed by a SANDIA scientist, Dr. Clark Dohrmann. The FETI algorithms are also making inroads in commercial engineering software systems. We also note that the analysis of these algorithms poses very real mathematical challenges. The success in developing this theory has, in several instances, led to significant improvements in the performance of these algorithms.

A very desirable feature of these iterative substructuring and other domain decomposition algorithms is that they respect the memory hierarchy of modern parallel and distributed computing systems, which is essential for approaching peak floating point performance. The development of improved methods, together with more powerful computer systems, is making it possible to carry out simulations in three dimensions, with quite high resolution, relatively easily. This work is supported by high quality software systems, such as Argonne's PETSc library, which facilitates code development as well as the access to a variety of parallel and distributed computer systems. The success in finding scalable and robust domain decomposition algorithms for very large number of processors and very large finite element problems is, e.g., illustrated in [24, 25, 26]. This work is based on [29, 31].

Our work over these five and half years has, in our opinion, helped advance the knowledge of domain decomposition methods significantly. We see these methods as providing valuable alternatives to other iterative methods, in particular, those based on multi-grid. In our opinion, our accomplishments also match the goals of the TOPS project quite closely.

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**2. DOE contacts.** In addition to our TOPS colleagues, our contacts with DOE funded scientists are primarily with the PETSc group at Argonne, in particular with Dr. Barry Smith, with whom four members of our research group have spent extended periods of time. Over the last three years, there have also been fruitful contacts with Drs. Clark Dohrmann, Ulrich Hetmaniuk, Richard Lehoucq, and Kendall Pierson of SANDIA, Albuquerque, with whom we share many interests.

In particular, joint work began in Spring 2006 with Dr. Dohrmann. One archival publication [4] and two conference papers, [3, 5], have so far resulted and one additional publication is now being completed, see [6]; that paper will provide the first relevant theoretical results on overlapping Schwarz methods applied to the saddle point problems that arise when almost incompressible elasticity problems are approximated using mixed finite element methods. Our long-tem coworker Axel Klawonn and his collaborator Oliver Rheinbach are also playing important roles in this work. Our work with Dohrmann is focused on an interesting hybrid family of domain decomposition methods, which combines features, and strength, of the overlapping Schwarz algorithms with those of iterative substructuring methods which are based on the decomposition of the region of the continuum mechanics problem into non-overlapping subdomains. The coarse component of these domain decomposition preconditioner turns out to be closely related to that of a method introduced over a decade ago by Maksymilian Dryja, Barry Smith, and the P.I. in [8]; see also [46, Algorithm 5.16].

The project with Dohrmann and Klawonn has led, quite surprisingly, to an extension of some basic tools which are central in the analysis of domain decomposition methods. In particular, we have been able to extend the theory to cases when the subdomains satisfies quite minimal geometric conditions. This work, which is inspired by the fact that mesh partitioners often result in subdomains with quite irregular boundaries, is now complete for two dimensional problems. So far, two archival papers have been submitted for publication, see [4, 28]. The latter concerns FETI-DP algorithms.

**3. Other publications and completed work.** In early 2005, the Springer Verlag, published a 450 page research monograph on domain decomposition methods [46] coauthored by the PI and his former student Andrea Toselli. It appeared in the Springer Series in Computational Mathematics and brings together most of the existing theory and algorithms in the field. Older results were reexamined and the book also contains new previously unpublished results. This book was the winner of the 2005 Award for Excellence in Professional and Scholarly Publishing of the Association of American Publishers in the category maths/statistics.

Progress can also be reported on domain decomposition methods for compressible elasticity, see Klawonn, Rheinbach, and Widlund [30, 27, 31]. This work was, in part, built on earlier results reported in Klawonn, Widlund, and Dryja [32, 33] for scalar elliptic problems and addresses the important question of the minimal possible dimension of the coarse component of FETI-DP algorithms which is compatible with robustness and a rapid rate of convergence of the iteration. This issue is now quite relevant since the coarse problems have developed into bottlenecks when the number of subdomains and processors becomes very large. Our ideas have been tested extensively in large scale experiments by Klawonn and Rheinbach, see [24, 26]; Rheinbach's codes are all developed using the PETSc system.

A different approach to the same issue involves the introduction of a third level. In a doctoral dissertation, prepared under the guidance of the P.I., Xuemin Tu designed and tested three level BDDC algorithms and gave a complete analysis; see [48, 50, 51]. A different approach was followed by Klawonn and Rheinbach in work on three level

FETI-DP; see [25]. Their approach is based on earlier work by Klawonn and the P.I., see [29]. Related problems have also been addressed by Jing Li and Widlund in [42].

The FETI-DP and BDDC methods turns out to be closely related. Numerical experiments with small model problems have shown that the set of eigenvalues of pairs of FETI-DP and BDDC methods are almost identical. This result was fully established by Dohrmann, Mandel, and Tezaur [44].

A greatly simplified proof of their result is provided by Li and the P.I. in [41]. The principal goal of that paper is to explain, in the simplest possible terms, the design of these algorithms in a novel framework which should be directly accessible to computational scientists and engineers. A key to all of this is a change of variables, which simplifies the description of what are called the primal constraints of the algorithms. This idea has also proven very useful in Rheinbach's implementation of FETI-DP algorithms. Our paper was recently identified by Thomson Publishing as a "Fast Breaking Paper in the field of Engineering", i.e., it is one of the most cited recent papers in the journals published by this company.

Extensive work has also been done on the stationary incompressible Stokes and the almost incompressible elasticity problems. The latest of these efforts will, as previously indicated, be reported in Dohrmann and Widlund [6]. Extensive work, based on balancing domain decomposition methods are reported in [14, 15] and in the thesis of Paulo Goldfeld [13]. The study of FETI-DP algorithms for the Stokes problem was started in the thesis of Li [36]; see also [34, 37, 35]. More recently, Li and the P.I. have returned to this problem in [39, 40] where new BDDC as well as FETI-DP algorithms are developed and analyzed.

A different type of saddle point problems arises in flow in porous media. In her dissertation [48] and in two archival papers, [47, 49], Tu developed BDDC algorithms and a full analysis of these problems. This excellent student, who now is an assistant professor at the University of California at Berkley, also wrote a paper with Dryja on parabolic problems while a graduate student, see [9]. While a postdoctoral fellow at the Courant Institute in Spring 2005, supported by the TOPS grant, she also started work on BDDC algorithms for certain nonsymmetric and symmetric, indefinite problems. This has now resulted in two papers coauthored with Li and submitted for publication; see [38, 52]. She also worked with Hyea Hyun Kim on three level BDDC algorithms for mortar finite elements.

Mortar finite element methods provide a systematic way of coupling different finite element models in different subregions. If the discretization of the subproblems is carried out independently, these techniques provide a means of dealing with the non-matching meshes that typically result. Dr. Kim spent three semesters as a postdoctoral fellow and a member of our group, supported by different DOE grants including some funding from TOPS. She received her doctoral degree from KAIST in South Korea. Already as a student, she became an expert on iterative methods for mortar finite element methods. The P.I. has also been interested in domain decomposition methods for mortar finite elements, for over a decade, but had only occasionally obtained results which led to publications; see, e.g., [10]. While Dr. Kim was in New York, she completed a joint paper with the PI on overlapping Schwarz methods for mortar finite element methods; see [23]. In joint work with Dryja and the P.I., she also developed BDDC and FETI-DP algorithms for mortar methods, see [21]. This work is important in that it provides quite general results even for what is called the geometrically nonconforming case; there were no previous results of this nature. Dr. Kim has also extended these results to the elasticity case, see [18]. Addition-

ally, several other papers were written by this very active and talented computational scientist, at least in part during her time at the Courant Institute, see [20, 19, 22].

A fourth doctoral student, Bernhard Hientzsch did extensive work on electromagnetics, [16, 17], as well as on general nonlinear elliptic problems. His thesis pioneers the use of high order spectral elements for  $H(\text{curl})$  problems. He also developed and analyzed overlapping Schwarz methods for these problems. He is now a member of Magneto-Hydro-Dynamics division of the Courant Institute, where he is using this background and his great computational skills in solving difficult problems.

The P.I. has also published a paper on multi-level methods, see [7]. This work was joint with Barbara Wohlmuth, Maksymilian Dryja, and Andreas Gantner.

The P.I. has served as an editor of the proceedings of the four most recent international conferences on domain decomposition methods. With David Keyes, he was also the main organizer of the sixteenth conference in this series, which was held at the Courant Institute January 11-15, 2005 and he also did most of the editorial work for the proceedings of that conference.

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