

# Domain Decomposition and Beyond

## A Perspective on Ideas, Methods, and Their Impact

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**Abstract** This paper is a personal perspective on a sequence of ideas in multilevel iterative methods, from my early work on iterative aggregation to multigrid, domain decomposition, and algebraic multigrid. Rather than a survey, it highlights a recurring design goal: solvers that are useful in practice should have a minimal interface, expose no parameters to tune, be fast on regular model problems, and invest additional computational work automatically only where needed.

### 1 Introduction

I am honored to be the recipient of the Olof B. Widlund Prize, awarded at DD29. The citation reads: “For the development of both primal and dual iterative substructuring classes of domain decomposition methods, in particular their convergence theory, multilevel extensions and adaptive variants.” It is a generous citation, which reflects the work of many collaborators, students, and colleagues, without whom none of this would have happened. Although we never wrote a paper together, Olof Widlund played an important role in my scientific life, has been a dear friend, and was my informal mentor in a critical period. His clarity of thought and generosity with ideas shaped the field and influenced me more than he ever realized. It is therefore especially meaningful to receive a prize named in his honor.

In my lecture, I touched on several areas I have worked in: iterative aggregation, iterative methods for high-order ( $p$ -version) finite elements, multigrid methods, domain decomposition, smoothed aggregation multigrid, early machine learning, and my later transition to wildfire modeling and data assimilation. In this paper, I provide a personal view; it is not a comprehensive or unbiased review. I try to highlight the motivations and leading ideas behind some of my papers and to trace threads of unifying ideas across these areas over time, in a roughly chronological order –

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their periods of course overlapped. By necessity, citations are incomplete, including self-citations.

My approach has always been pragmatic: I usually do not invest effort where the performance is already “good enough.” I try to build – and, if possible, analyze – useful methods rather than attempting to cover all possible variants, and to choose problems that matter to real-world users. As each field matured and the impact-to-effort ratio declined, I moved on and left the deeper specialization to others, rather than trying to “own” a part of the field.

## 2 Iterative Aggregation

My graduate advisor, Bohuslav Sekerka, was a mathematical economist. He suggested that I look into iterative aggregation in the Leontief model [29], a simplified macroeconomic model of linear relations between industries, each producing a single commodity and consuming others for intermediate use. Little did he know that he was launching me on a path of multigrid and domain decomposition!

The problem was to find the production in each industry to achieve a desired output for external use, left after the intermediate consumption. It was assumed that there was a price vector such that in each industry, more value is produced than consumed. Then it can be shown that successive iterations – repeated computing of the production of all industries as the sum of the desired final output and the intermediate use – converge to the solution.

The iterative aggregation method [16, 67] attempts to accelerate these iterations. In each cycle, it splits the industries into disjoint aggregates, and builds a smaller system of equations for the total production value for each aggregate, keeping the proportions within the aggregates. This aggregated system is solved directly, the productions of the industries in each aggregate are adjusted proportionally, and the cycle is concluded by one iteration on the original system.

These iterations converged in practice, but no proof was available. A chapter of my thesis gave a proof of local convergence of these nonlinear iterations to the solution [51], based on a remarkable theorem on orthogonal projections from [32].

Ivo Marek, who had been my professor and then informal mentor during my early research years, later continued this line of work with his students and collaborators, e.g., [59, 60], extending the analysis to the computation of stationary distributions of Markov chains, and found that global convergence fails in certain edge cases [59]. This extension continues to attract interest in theoretical physics, e.g., [17], but global convergence under the original assumptions appears to remain an open question.

### 3 Multigrid Methods

The idea of using a smaller, coarser version of the system to accelerate convergence was clearly powerful. I spent time each week reading new books and journals in the library, as I saw senior mathematicians do, and soon encountered the seminal multigrid papers by Brandt [6], Hackbusch [22], and the first multigrid proceedings [24]. It became clear that the correction in iterative aggregation is a multiplicative analog of the coarse-grid correction in multigrid.

One apparent gap in multigrid at the time was in methods for one-sided constrained problems, such as obstacle problems (variational inequalities). Since I was coming from an optimization perspective rather than PDEs, the projected multigrid method I came up with was monotone, with a guaranteed decrease in the objective function in each multigrid cycle [34], unlike the methods by Brandt and Cryer [7] and Hackbusch and Mittelmann [23]. For the obstacle problem, the method reduced in the limit to multigrid in the subregion where the constraints were not active, and a two-level convergence proof was possible in the nondegenerate case [33].

I then left this direction and was happy to see it advanced by others [25, 26]. With Steve McCormick and others, I turned to the emerging multigrid algebraic convergence theory, e.g. [48, 49], multigrid for eigenvalue problems [10, 45], and composite meshes, a transition to domain decomposition [47].

### 4 Domain Decomposition and Substructuring

The transition from iterative aggregation to multigrid clarified a common principle: large problems should be addressed by separating global and local behavior through a hierarchy of scales. Domain decomposition extended this idea by introducing an explicit subdomain structure at the fine scale, together with a coarse component responsible for global error modes.

By the mid-1980s, additive Schwarz methods provided an abstract framework for such constructions, motivated in part by emerging parallel computers. The essential analytical tool, formalized by the P.-L. Lions lemma [31], is the existence of a stable decomposition controlling the energy norm. In nonoverlapping (substructuring) methods, this reduces to extension theorems from subdomain interfaces into interiors with bounded energy, e.g. [5, 14].

Scalability was quickly recognized to require a distinguished coarse component. Whether treated additively or through a projection step analogous to multigrid coarse correction, the coarse space coordinates subdomain solves and controls global modes.

Within this framework, there was still space for clarifying structure rather than introducing new machinery. With Petter Bjørstad, we interpreted additive Schwarz methods and the associated estimates as statements about orthogonal projections [4]. The writing process reflected its time: written over the nascent internet, the manuscript was exchanged between Colorado and Norway over several days, often arriving mangled by sendmail and incompatible text encodings.

These ideas were already well established when I entered the field. Rather than attempting to contribute to the quickly maturing classical numerical PDE framework, I took a bypass through  $p$ -version finite elements (brought to my attention by Ivo Babuška), where individual elements could naturally be viewed as subdomains, and where things did not work “well enough” yet.

## 5 $p$ -Version Finite Elements and Adaptive Solvers

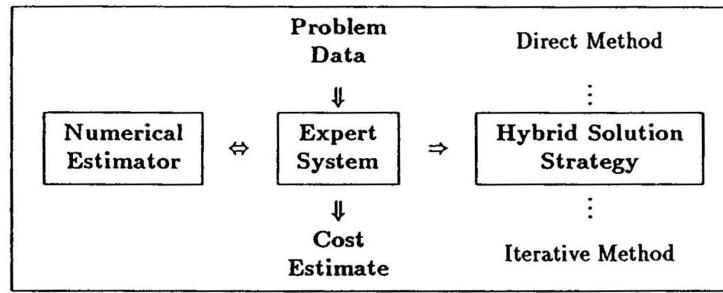
Hierarchical polynomial bases in high-order ( $p$ -version) finite elements provide excellent accuracy and good numerical stability of the approximation, but they also produce algebraic systems that become severely ill-conditioned as  $p$  increases. In three dimensions, direct solvers of the era were quickly defeated by fill-in and memory growth caused by large dense element matrices, and existing preconditioners did not provide reliable convergence of the iterations.

The key structural step was to treat each high-order element as a subdomain. This brings  $p$ -version discretizations into the additive Schwarz framework and makes the central theoretical question the same as in the P.–L. Lions lemma: the *existence* of a stable decomposition with *low-energy* components. In two dimensions, on regular element shapes, the missing ingredient was a polynomial lifting theorem, which yields the familiar  $(1 + \log p)^2$  bound [3]. Alan Craig and I worked out the method and, on a visit to Ivo Babuška, discovered that he already had the needed lifting result with Juhani Pitkäranta essentially complete—waiting, as it were, for an application. A corresponding  $(1 + \log p)^2$  result in 3D was obtained later by Pavarino and Widlund [63].

On the practical side, the hierarchical bases [2] provided linear coarse functions consistent with rigid body modes and thus scalability with the number of elements. In three dimensions, however, the obvious vertex–edge–face–interior splitting does not behave well: trilinear vertex functions have high energy, and forcing them into a low-energy role by full orthogonalization would destroy scalability. This is an early place in the story where it helps to think of the *coarse space as a control knob*: choosing a larger coarse space moves the method toward a direct solve, while a smaller one yields a more purely iterative method.

My solution in 3D was to enlarge the coarse space by including quadratic functions and to use a sparse change of basis (what I called *partial orthogonalization*) to decouple harmful interactions, particularly between face and edge components. The resulting element-level block-diagonal (after back-and-forth change of basis) preconditioner performed well for the polynomial orders needed in the application (up to about  $p = 7$ –8) and substantially outperformed direct solvers of the time [35, Table 5.1].

The quadratic enrichment also suggested a more general heuristic: enlarge the coarse space *when needed*, rather than committing to a fixed choice a priori. Real geometries and material models are not collections of neat cubes, and the “right” stabilization is often local. This led me to an adaptive approach in which local



**Fig. 1** Adaptive iterative solver. From [38].

#### Design principles for a solver useful in practice

1. have a minimal interface with the engineering software;
2. have no knobs to turn (called hyperparameters today);
3. be fast for model problems with regular structure;
4. handle harder cases by additional computations automatically;
5. handle asymptotic cases important in practice (e.g., in structural mechanics, not only solids but also thin solids, plates and shells).

**Fig. 2** Design principles for a solver useful in practice.

eigenvalue problems supplied numerical estimates of conditioning, combined with local cost estimates to decide what to orthogonalize to what and which variables to add to the coarse space [38]. Special treatment was needed for high aspect ratios and laminates [46, 40]. In effect, the algorithm selected a solution strategy between a direct method (coarse space enlarged aggressively) and a standard iterative method, automatically from the algebraic data and without user-tuned parameters (Fig. 1).

The “expert system” that made these decisions was trained manually on a set of benchmarking and regression problems. The resulting adaptive iterative method proved competitive in a real industrial setting (structural mechanics models for the Gripen jet fighter), while requiring only a minimal interface: essentially local stiffness matrices and adjacency information, without access to detailed model metadata, and shaped my priorities for the future (Fig. 2).

In addition, I looked for things that can be proved and, with collaborators, we proved them on the way [3, 37, 46] to increase confidence in the method. I was glad to see  $p$ -version solvers attract increasing interest and evolve into  $h - p$  solvers, e.g., [1, 62], but I did not pursue that direction further myself.

## 6 Balancing Domain Decomposition (BDD)

Balancing domain decomposition (BDD) [39] originated from adding a coarse problem to a nonoverlapping method of De Roeck and Le Tallec [12], following an inspiring conversation with Patrick Le Tallec over a glass of wine at a workshop at Schloss Meisdorf (Harz), Germany, in the early 1990s.

In the BDD method, the global stiffness matrix is assembled from subdomain matrices that are, in general, singular. The preconditioner is assembled from their inverses, which therefore do not exist on the full subdomain spaces. Consequently, residuals supplied to the preconditioner must lie in appropriate subspaces—hence be “balanced”—so that the local inverses are well defined. This requirement naturally leads to the introduction of a coarse problem. The condition number bound is obtained from a supremum of a ratio of two quadratic forms, in the spirit of the P.–L. Lions framework, and can be bounded using known properties of interface mesh spaces [14].

Closely related Neumann–Neumann and Neumann–Dirichlet ideas were developed in parallel by Dryja, Smith, and Widlund, addressing similar questions [15, 66]. However, the Neumann–Neumann methods had a regularization parameter for solving singular problems, which I preferred to avoid.

The BDD method was deliberately created in a form aimed at ease of application and impact. BDD followed the design principles set forth in Fig. 2:

1. *A minimal interface*: function calls for multiplication by local subdomain matrices and by their one-sided inverses, local to global mappings of the interface degrees of freedom, and sets of coarse vectors spanning at least the nullspace of each subdomain matrix.
2. *No additional parameters to tune*.
3. *Efficient on regular model problems*: condition number bounds of the form  $C(1 + \log(H/h))^2$  are independent of the number of subdomains.
4. *Robust for harder problems* via additional local coarse vectors added as needed, with provable insensitivity to coefficient jumps [41].
5. *Applicability to plates and shells* was achieved later with Patrick Le Tallec and Marina Vidrascu [27, 28] by enriching the coarse vectors so that the relevant interface functions have zero normal displacement at subdomain corners (crosspoints), which is a key condition for scalable convergence bounds.

A template implementation was also made available online.

BDD and FETI (discussed next) became widely used methods for large-scale engineering simulation on parallel supercomputers for more than a decade. As two representative applications, BDD has long been used in oil reservoir simulation by Mary Wheeler’s group, e.g., [21]; with her student Lawrence Cowsar, we extended BDD to mixed problems [11]. In a 2015 SIAM CSE plenary lecture [71], Shinobu Yoshimura demonstrated the use of BDD for petascale structural analysis of nuclear reactors in the 2011 Tōhoku earthquake and the Fukushima disaster, performed on the K computer. His group in Tokyo has been developing massively parallel BDD-

based methods and software on leading-edge supercomputers for over two decades, e.g., [61, 65].

## 7 FETI

In the finite element tearing and interconnecting (FETI) method by Farhat and Roux [20], nonoverlapping subdomains are coupled by Lagrange multipliers that enforce continuity across interfaces. Evaluating the dual operator requires solving Neumann substructure problems which are singular, so the conjugate gradient method was projected on a subspace constructed from the substructure nullspaces. The method was successfully applied to large realistic aircraft structures.

With Charbel Farhat and François-Xavier Roux, we analyzed FETI on simplified model problems to understand its asymptotic behavior [19]. For the lumped (diagonal) preconditioner, we obtained condition number bounds of the form  $\kappa \leq CH/h$ , independent of the number  $N$  of subdomains. In practice, however, conjugate gradients converge much faster than suggested by this bound. A useful heuristic model is that the eigenvalues of the dual operator decay rapidly,  $\lambda_n \searrow 0$  as illustrated in [19, Fig. 10]. Early CG iterations therefore damp a small number of large-eigenvalue components, after which convergence is governed by a much smaller “effective” condition number  $\lambda_k/\lambda_{\min}$  rather than  $\lambda_{\max}/\lambda_{\min}$ . But as the number of subdomains increases, many similar interface modes appear and the spectrum fills in, weakening this effect and motivating stronger preconditioning based on Dirichlet subdomain solves.

For second-order elliptic problems and the Dirichlet preconditioner, with my then student Radek Tezaur, we have proved a condition number bound  $C(1 + \log(H/h))^2$  with the Dirichlet preconditioner [56]. Unlike most domain decomposition analyses, which rely on spectral equivalence of quadratic forms via the P.–L. Lions framework, the FETI preconditioner is not naturally expressed as a variational form. Instead, the analysis was done by bounding custom norms of the product of the system operator and the preconditioner, as well as their inverses, by duality pairing.

For fourth-order problems (plate bending), condition number of FETI grows quickly with the number of elements per subdomain. In [58], we have added to the coarse space the Lagrange multipliers enforcing continuity at crosspoints, which recovers fast convergence, with the  $C(1 + \log(H/h))^2$  condition number bound.

## 8 Smoothed Aggregation Algebraic Multigrid

In parallel with FETI and BDD focus, Algebraic multigrid (AMG) was another natural direction. Algebraic multigrid (AMG) builds coarse spaces automatically based on the data. One type of AMG, the *Smoothed Aggregation* (SA AMG), originated by Petr Vaněk, e.g., [68], provided a particularly effective mechanism for building

coarse spaces by smoothing piecewise constant functions. With Petr Vaněk and my past student Marian Brezina, we developed the method further into a robust tool by using the design principles in Fig. 2:

1. *Minimal interface*: A block sparse system matrix and optionally nodal coordinates.
2. *No knobs to turn*: The choice of algorithms and their parameters was governed by a GMDH neural network. The features were obtained by scanning the input data for several statistics of the problem, such as the number of degrees of freedom per node, connectivity, and estimates of anisotropy. The network was trained on a set of benchmark problems [64].
3. For *model problems with regular structure*, SA AMG worked similarly like the standard multigrid, with convergence estimates available [69].
4. *Harder problems* were handled by *additional computations automatically*: the growth of node aggregates and smoothing decisions were directed by numerical estimators including local eigenvalue problems.
5. For scalability, the coarse space needs to be able to reproduce the nullspace of the problem [36]. We have added linear functions with support on aggregates for *plates and shells* [70]. Smoothing preserves the ability of the coarse functions to generate the nullspace of the operator – constants, rigid body motions, or linear functions – and it can be interpreted as the first iteration towards coarse space basis functions with minimal energy, which are beneficial for fast convergence [42].

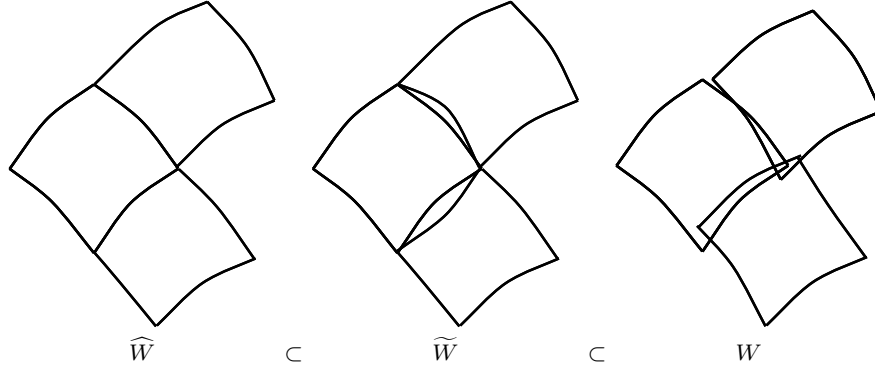
An implementation was also made available online. SA AMG was used in industry and included, for example, in ANSYS [64]. At national laboratories, the SA AMG method was further developed by a team including Marian Brezina [9] and became a widely used workhorse solver.

## 9 FETI-DP and BDDC

FETI-DP [18] treats degrees of freedom at corners as primal variables, while enforcing continuity of the remaining interface components by Lagrange multipliers. Continuing with Tezaur, we proved its convergence with the standard condition number bound [57]. While visiting Sandia to give a lecture on coupled fluid-solid scattering [50], I was introduced to Clark Dohrmann, who created a similar, simpler method [13] without Lagrange multipliers, and we proved its condition number bound and coined the name BDDC [43].

The first indication that these two approaches were fundamentally equivalent came from numerical experiments rather than theory. I built BDDC and FETI-DP prototypes in MATLAB from exactly the same components, and compared the eigenvalues of the preconditioned operators. The spectra matched exactly except for 0 and 1. This was far too specific to be accidental. With Dohrmann and Tezaur [44], we gave a proof, but it was quite technical.





**Fig. 3** Schematic drawing of continuity conditions between substructures, in the case of corner coarse degrees of freedom only: all degrees of freedom continuous (the fully assembled space  $\widehat{W}$ ), only the coarse degrees of freedom need to be continuous (the partially assembled space  $\widetilde{W}$ ), and no continuity conditions (the unassembled space  $W$ ). BDDC constructs the preconditioner on  $\widetilde{W}$  by solving the variational problem on  $\widetilde{W}$ , equivalent to solving the local subdomain problems and a the coarse problem, followed by an averaging (or projection) back to  $\widehat{W}$ . From [53].

Subsequent work focused on simplifying this picture. Li and Widlund [30] gave a clearer interpretation based on block Cholesky factorizations, making the correspondence between the primal and dual formulations more transparent. Brenner and Sung [8] further reduced the argument, eliminating much of the matrix-level machinery.

Inspired by those works, with my student Bedřich Sousedík, we have stripped down the proof and formulation of FETI-DP/BDDC even more [53], based on only the 3 spaces  $\widehat{W} \subset \widetilde{W} \subset W$  in Fig. 3, which is probably the easiest way to understand FETI-DP and BDDC. From this viewpoint, BDDC can be interpreted as preconditioning the fully assembled problem by solving in the partially assembled space  $\widetilde{W}$ . The choice of coarse constraints – corners, later edge and face averages, and eventually adaptive methods with Sousedík and Jakub Šístek [52, 54, 55] – determines the size of  $\widetilde{W}$  and hence the quality of the preconditioner. The adaptive methods again follow the design principles set out in Fig. 2.

## 10 Running Out of Dimensions: To Probability and Wildfires

The focus of computational modeling shifted over time: from two to three dimensions, multiscale models, multiphysics, then the dominant difficulty became uncertainty. I started working with statisticians, and when the opportunity arose, I moved into data assimilation, wildfire modeling, weather simulation, and satellite data.

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