



Computational Science and Engineering (Int. Master's Program)

Technische Universität München

Master's Thesis

Towards A Spatial Adaptive Combination Technique

Mahyar Valizadeh





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Author:	Mahyar Valizadeh
1 st examiner:	Univ.-Prof. Dr. Hans-Joachim Bungartz
2 nd examiner:	Univ.-Prof. Dr. Thomas Huckle
Advisor:	Christoph Kowitz, M.Sc. (hons)
Assistant advisor:	Alfredo Parra Hinojosa, M.Sc.
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Disclaimer

I hereby declare that this thesis is entirely the result of my own work except where otherwise indicated. I have only used the resources given in the list of references.

Ich versichere, dass ich diese Master's Thesis selbständig verfasst und nur die angegebenen Quellen und Hilfsmittel verwendet habe.

September 14, 2016

Mahyar Valizadeh

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Abstract

1. This new algorithmic concept is based on the independent solution of many problems with reduced size and their linear combination. [4]
2. The basic idea of combination technique is same as for multilevel splitting of finite element spaces is to replace the usual nodal bases of the finite element spaces by hierarchical bases.[2]
3. nearly of the same optimal computational complexity as the conventional multigrid methods but which is free of many of its restrictions. [2]
4. We think that one of the main advantages of our method is its robustness and the fact that its speed of convergence does not depend on the regularity properties of the considered boundary value problem or on a regular refinement.[2]
5. The natural coarse grain parallelism of the combination method makes it perfectly suited for MIMD parallel computers and distributed processing on workstation networks.[4]
6. Consequently, one of the main advantages of the combination technique stems from the properties of sparse grids [1] In comparison to the standard full grid approach the number of grid points can be reduced significantly. Another advantage has to be seen in the simplicity of the combination concept its inherent parallel structure and its framework property allowing the integration of existing solvers for partial differential equations.[10]
7. In elliptic problems the smoothness of the solution may be disturbed where the data is non-smooth. The form of the domain or the need for local refinement may make the use of uniform meshes difficult. The local smoothness of the solution is a basic characteristic of many elliptic problems, so that extrapolation can be used locally, even when the global solution is non-smooth.[11]
8. The simulation of complex real life experiments usually needs a great deal of computing time and returns vast amounts of data. Thus, in order to obtain sufficiently accurate simulation results, it is necessary to find algorithms which economize on both computing time and storage space.[12]
9. One way of using sparse grids efficiently involves hierarchical, tree-like data structures and special algorithms for both the discretization and the solution. Since conventional solvers usually do not provide means for dealing with hierarchical data structures, they cannot be employed for solving problems on sparse grids. Thus, new algorithms and new codes have to be developed in order to compute solutions on sparse grids efficiently

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Outline of the Thesis

Part I: Introduction and Theory

CHAPTER 1: INTRODUCTION

This chapter presents a general overview of the thesis, what has been the reason and motivation behind this research, and its main objectives which are basically what we are trying to achieve.

CHAPTER 2: RELATED WORKS

As any scientific work requires, this chapter presents all the related works and gives comprehensive literature review of published works. It can be seen how the research evolves to this point that now we try to push it further forward. All the material will be presented in the order of how progress has been done.

CHAPTER 3: METHODS

By methods in this chapter we mean the basic underlying principles and theories required to achieve the goal. All presented materials will be shown how they are related to the work at hand. Three primary methods presented are idea of sparse grid method and its relation to hierarchical basis, combination technique used to give another representation for sparse grid methods and finally data structure of trees specifically quadtrees in two-dimensional case. Finally some general important points will be discussed on what are the important factors at play in this kind of problem.

Part II: Implementation, Results and Conclusion

CHAPTER 4: MY IMPLEMENTATION

This chapter presents the general idea of how combination technique is implemented in this case and more importantly how we are going to achieve the spatial adaptivity. Lastly, in this chapter different schemes are described.

CHAPTER 5: RESULTS

Firstly in this chapter we verify the result of the main block used in the implementation and later we present the results of implementation presented under circumstances of different given schemes and effects of the two factors of adaptivity level and accuracy will be studied.

CHAPTER 6: CONCLUSION

In similar to all scientific researches last chapter is dedicated to summary of what have been accomplished, what usage it can have and how to proceed from here for future related research and developments.

Part I.

Introduction and Theory

1. Introduction

This chapter presents a very general and broad overview of the current thesis. Firstly, we present how the author thinks the method at hand, i.e. combination technique, had came to life. As it happens in every particular area of science several researchers have basically done similar and closely related works but they have articulated their methods differently and in result multiple names have been introduced. The author, here, have chosen the name combination technique based on the fact that multiple results on grid have been combined and projected to one final grid. Secondly, the reason and motivation behind this research will be presented in details based on several arguments marking benefits of the method in use.

Clearly motivation is important only when we are transparent about the objectives and goals of the project. So, we state these goals in detail.

1.1. Motivation

In numerical or computational science and more specifically numerical mathematics efficient discretization procedures are of crucial importance for different types of problems we encounter in various applications. All of these applications have multiple tasks in common. Definition of sets of points, also known as grid generation, computation and evaluation of function values on these point, interpolation of function to estimate a value at an arbitrary point, or integrating or differentiating functions for solving differential equations using different schemes are all examples of these tasks.

In particular we are interested in interpolation problem in our research certainly because it is the baseline problem to prove the method can even be used for other more advanced problems. Through extensive search and review of previous related works, it seems the origin of idea for base of our method comes from classical Richardson extrapolation[11]. On the other hand, Russian mathematician Smolyak using the basic of Richardson extrapolation presented a method which he used for numerical integration. One can imagine this gave birth to a foundation of sparse grids [1]. The underlying idea of Richardson was to use of different discretizations with different resolution such that fine mesh approximations are fine-tuned recursively by approximations on coarser levels. This idea is really close to multigrid methods and uses the same hierarchical structure. Such strategies, where multiple distinct grids participate to define a combined result, are generally called extrapolation methods such as Classical Richardson extrapolation.

Classical Richardson extrapolation can be extended and generalized in many ways. if this generalization is being done using mesh widths in the different dimensions coordinate directions as the major playing parameters it will leads to the so-called multivariate extrapolation[11]. Note that combination extrapolation can be interpreted as a special case

of multivariate extrapolation.[4, 7]. Even further, it has been shown that one case of combination extrapolation is exactly the combination technique proposed in [6]. The primary idea of combination technique is identical for multilevel splitting of finite element spaces and it is to replace hierarchical bases of the finite element spaces instead of the usual nodal ones.[2]. As explained earlier various names, such as (discrete) blending method [21], Boolean method [11], sparse grid method [56].[15], technique of hyperbolic crosses [2][16], or splitting extrapolation' [20] are practically interchangeable. As the name is just a representation for the idea, we stick to the combination technique introduced by Zenger et. al in [6]

The advantages of this method discussed extensively in literature are as follows:

1. **Reduction of number of grid points:** Main advantages of the combination technique borrows this characteristic from the properties of sparse grids in that comparing to the full grid approach, the number of grid points (unknowns) can be drastically reduced.
2. **Inherently parallelizable:** Since the grids to be combined are usually independent of each other, it makes it easy to imagine how it can be parallelized using MIMD[5], Network[4] or GPGPUs[30]. The coarse grain parallelism of the combination method makes it perfectly suited for MIMD parallel computers and distributed system on workstation networks. parallelization of combination technique supports both modularity and portability by separation of sequential modules. The gain is expected to be even more dramatic for higher dimensions. However, the collection of the results is not trivial as we need a strategy like trees to combine the solutions.
3. **Simplicity of the concept:** its framework allows the usage and integration of existing solvers and methods[10].
4. **Good accuracy:** the combination technique usually doesn't require as much storage space and computing time as the usual full grid but achieves nearly the same accuracy[12].
5. **Robustness:** Later it will be shown how this method can be exploited to various problems under certain conditions. Specially compared to sparse grids since it doesn't involves hierarchical, tree-like data structures and special algorithms for both the discretization and the solution it can be used in conjunction with conventional solvers.
6. **Speed of convergence:** its speed of convergence does not depend on the regularity properties of the considered boundary value problem or the refinement resolution[2].
7. **Optimal computational complexity:** The computational complexity of combination technique is almost the same as the conventional multigrid methods but without their restrictions[2].

Given these many advantages we are going to proceed and to set goals for this project. Note that only major draw back which can not be ignored here is the error and convergence analysis. Later we see for various applications, there are certain conditions needed to be ensured of convergence.

1.2. Goals

As you will observe, comprehensive literature review has been on subject and while there are plenty works on different areas such as error analysis and convergence, solution in complicated domains, numerical Integration, regression and data fitting problem, eigenvalue problems, parallelization schemes, data mining and machine learning, fluid mechanics, heat transfer and some stochastic or random partial differential equations, and finally adaptive sparse grid methods been presented throughout years, it hasn't been any attention to possibility of introducing a spatial adaptive combination technique. Perhaps, the reason is it requires more complex data structure, projection and interpolation methods to achieve it. However in this research we will tackle this idea with a greedy but simple algorithm. Details of the algorithm is explained later in the implementation chapter.

2. Related Works

Comprehensive literature study will be presented here. The author tries to categorize the researches in separate sections. By doing so, faster access to the different applications for a seeking scientist can be achieved. While each work is referenced, we try to give major important remarks and conclusions of that research so that it can be a good preparation and start for deeper search.

2.1. Works on Complicated Domains

The combination technique is not restricted to the unit square. Successfully treatment of problems on distorted quadrilaterals, triangles, polygonal boundaries domain have been investigated by Griebel. The solution of problems with a nonlinear operator and partial differential equations like the Stokes and Navier-Stokes equations have been presented. [5, 8]

It has been shown that to some extent the combination technique works even in the case of non-smooth solutions like complicated domains explained earlier but replacement of h_i^2 and h_j^2 by h_i^α , h_j^β with appropriate α and β in the given problem is required. Because of the properties of the combination technique the major error terms still cancel each other this way. However, for the problems with severe singularities, the appropriate combination of adaptively refined grids is recommended[5]. This results that our research can also be applied to this type of problems.

2.2. Works on Error Analysis and Convergence

Although, the implementation of the combination technique seems trivial, General convergence of the method cannot be proved with usual standard arguments from finite element theory. Therefore, there has been a lot of works which we present in chronological order to give insight on what has been done. Recent studies [36] uses more general convergence scheme with definition of error bounds but still there are plenty of assumptions there. Convergence and error analysis of the combination technique for the finite element solution of Poisson's equation and 2nd-order elliptic differential equations which is general form of Poisson equation has been investigated in early works and it has been the base for error analysis of the combination technique.[9, 13]

Bungartz et al have investigated a model problem of Laplace equation on the unit square with a Dirichlet boundary function based on finite difference and Fourier techniques on a pointwise manner [10]. They proposed it there exist an error splitting if the Dirichlet boundary function satisfies a certain smoothness requirement i.e. Fourier coefficients in case of Laplace equation. Multiple numerical solutions for both smooth and nonsmooth boundary functions have been studied the convergence of the pointwise error.[10]

A technique to analyze the convergence rate of the combination technique applied to general second order elliptic differential equations in two dimensions and its proof for Poisson's equation convergences in arbitrary dimensions is later inspected by Pflaum [18]. The difference to his early work is the removal of requirement that the normal derivative of some coefficients should be zero at the boundary. The significant consequence is the proof the convergence of the combination solution on a complicated domain or more precisely curvilinear bounded domain. The scheme is to divide the curvilinear bounded domain in several blocks and to transform each block onto the unit square. [18]

Further improvement has been done which is the base for the Introduction of optimized combination technique. Since we hardly know about the reasons of this effectiveness or divergence criteria of the combination technique. A technique which inherently uses the error terms has been introduced which is the so-called optimized combination technique. This is based on the fact that the combination technique gives an exact result in the case of a projection into a sparse grid space if their partial projections commute. They have analysed the performance of the combination technique in a projection framework and used the C/S decomposition. Based on that analysis modified optimal combination coefficients are derived and substantially expand the applicability and performance of the combination technique.[28]

Most recently in the error analysis of combination technique has been shown that it requires derivation of a specific multivariate error expansions on Cartesian grids and for linear difference schemes through an error correction technique. By this an error formulae will be derived to use for analysis of the convergence. Note that its dependence on dimension and smoothness in case of linear elliptic and parabolic problems has been on the focus. Finally, introduction of a new framework to analyze error bounds for general difference schemes in arbitrary dimensions is given. [36]

2.3. Works on Parallel Environment

Coarse grain parallelism which basically is kind of decomposition of tasks for the combination method makes it perfectly suited for MIMD parallel computers and distributed processing on workstation networks. There has been early studies parallel for the solution of elliptic partial differential equations on MIMD structured computers and parallel sparse grid preconditioning or solution of partial differential equations on Workstation networks [4, 5].

Concept of parallelization can be applied to different parts of solutions, for instance, the parallelization of the basic iterative method, the parallelization of the preconditioning step and so on. However, most types of preconditioners are not parallelizable that efficiently. They require modifications of the numerical algorithms resulting in slower convergence rates. and well parallelizable preconditioner using combination technique has been introduced by Griebel. They have compared their method with preconditioners inefficiently parallelizable and with preconditioner like classical multigrid which are well parallelizable but do not possess the natural parallel characteristic of the combination method. In contrast to these techniques, the parallelism in the combination technique is more explicit. Similar to the domain decomposition approach, the combination method possesses a sim-

ple parallelization potential, because all the subproblems are independent[4].

Further parallel experiments on MIMD-machines and networks, however, have shown that it is insufficient to achieve substantially better efficiency rates for combination method. Therefore idea of complex or advanced load balancing strategy is necessary to exploit the benefits of massive parallel systems equipped with quick communication hardware.[4]

Till that point of time, no comparison has been done with usual sparse grid methods, simply because the parallelization of a sparse grid code usually is non-trivial and requires a substantial effort on coding. Early works on this regard to compare it with combination technique is investigated in[20]. A parallel version of a finite difference discretization of partial differential on arbitrary, adaptively refined sparse grids is proposed. The efficient parallelisation is based on a dynamic load-balancing approach with space-filling curves. with applications can be in higher-dimensional problems such as financial engineering, in quantum physics, in statistical physics and in general relativity. Presented issue there is usually hierarchies of refined grids in neighbour nodes may reside on different processors so it needs to be managed. One solution can be creation and updating of appropriate ghost nodes on a communication operation. The space-filling curve is simply a unique mapping of nodes to processors so it immediately shows which processor needs to be communicated with [20]. Relevantly, A load model for linear initial value runs with GENE is introduced for effective load balancing for the combination technique in [37].

Another interesting concept is the idea of using GPGPUs also known as multicore programming. In multi dimensional option pricing problems of computational finance the sparse grid combination technique can be a practical tool to solve arising PDEs. Using Hierarchization leads to linear systems smaller in size compared to standard finite element or finite difference discretization methods. Excessive demands memory for direct methods which challenges the iterative methods suggests the usage of massive parallelism of general purpose Graphics Processing Units (GPGPU)s. It also requires proper data structures and efficient implementation of iterative solvers. Performance analysis and the scalability of combination technique based solvers on the NVIDIA's CUDA platform compared to CPUs for certain applications shows promising results. because of locality and linearity properties.[30]

Advanced idea of hierarchization as preprocessing step to facilitate the communication needed for the combination technique has been presented in [33]. The derived Parallel hierarchization algorithm outperforms the baseline drastically and achieves good performance. The algorithm needs iterative hierarchization and dehierarchization. (For further details please check [33])

Lastly, in discussion of fault tolerance methods we know extreme scale computing usually leads to the increase in probability of soft and hard faults. Parallel fault tolerant algorithms with modification of sparse grid combination method is in focus to solve partial differential equations in the presence of faults. It modifies combination formula to accommodate the loss of few component grids. A prototype implementation within a MapReduce framework using the dynamic process features and asynchronous message passing of MPI is presented.[35].

2.4. Works on Fluid Mechanics, Heat Transfer and other PDEs

Arguably, one of the most important application areas for combination technique can be in solution for partial differential equations with high dimension, high computation complexity or high memory demands regarding high order number of grid points. As first demonstration of the advantages of combination approach investigation on modal problem has been done in two dimensional cases [6]. Modal problems are as follows:

1. Smooth Solution
2. Singular Solution
3. Boundary layer (solution of combination technique is equal to full grid, in general holds for solution only depends on one direction or boundary layer)
4. Distorted quadrilateral and triangular elements
5. Nonlinear heat transfer

In case of nonlinear heat transfer, the combination technique produces good solutions. The error quotient is major factor to check here. It has been shown that the efficiency, the degrees of freedom, the run time and the achieved accuracy for the combination technique is far better than the full grid approach. Also note that additional Newton iterations seems to be a remedy the approach even further [6].

First studies of the sparse grid combination technique as an efficient method for the solution of fluid dynamics problems has been done in [12]. It shows the numerical experiments for the application of the combination method to CFD problems e.g. two-dimensional laminar flow problems with moderate Reynolds numbers. The research is based on the fact that implementation of the combination technique can be based on any black-box solver. Usually, fluid dynamics problems have to be solved on rather complex domains, thus, a reasonable approach is to decompose the domain into blocks to handle the problem. Obviously, the combination technique works on such block structured domains as well as complicated domains like a graded grids. Since the sparse grid methods are highly economical on storage requirements, given that they produce a fairly accurate solution, the usage is highly recommended [12].

In [17], promising numerical results are presented for the combination technique applied to a constant coefficient advection equation for four test cases of. Their work differs from [17] in that it also presents error estimates [19].

1. Horizontal advection
2. Diagonal advection
3. Time dependent advection
4. The Molenkamp-Crowley test case

Similar to heat transfer problem explained above, in [21] a significant progress in the numerical simulation of systems of partial differential equations in the advection diffusion reaction equations of large-scale transport problems in the modeling of pollution of the

atmosphere, surface water and ground water has been achieved. Since these models are three dimensional and modeling transport and chemical exchange over long time periods requires very efficient algorithms computational capacity is a restricting factor. For example in simulation of global air pollution huge numbers of grid points is needed, each of which many calculations must be carried out in. The application of sparse grid combination techniques might be a solution. However, in their research they only considered pure advection and left the diffusion and reaction processes to future research[21].

More recently, a convection diffusion problems on the conventional unit square has been investigated and observed using a sparse grid Galerkin finite element method in[29].

Lastly, application to probabilistic equations like the stochastic collocation method based is on the horizon. For instance, an anisotropic sparse grid solution is an important tool to solve partial differential equations with random input data[38].

2.5. Works on Numerical Integration

Based on original idea of Smolyak there has been some similar work in numerical integrations. For example [15] they review and compare existing algorithms for the numerical integration with the the ones of multivariate functions over multi-dimensional cubes using several variants of the sparse grid method.[15, 1]

Multivariate integrals arise in many application fields, such as statistical mechanics, computational finance and discretization of partial differential and integral equations or the numerical computation of path integrals. The so-called curse of dimension are also in play in these conventional numerical algorithms for computation of integrals there. So the rectifying remedy of sparse grid combination method is used in [15].

2.6. Works on Regression Problem

In the context of regression or basically fitting the function to given values there has been some works, in [22], they compared the iterative algorithm for multidimensional sparse grid regression with penalty and showed the improving performance compared to iterative methods based on the combination technique.

The combination technique approach shows instabilities in some situations and is not guaranteed to converge specially with higher discretization levels. As stated before the optimized combination technique can repairs these instabilities. based on the fact that combination coefficients also depend on the function to be reconstructed, thus a nonlinear solution. It has been shown that the computational complexity of the optimized method still scales in linear manner to the number of data.[24]

In [31] there has been investigation in theory and experiment of the reason why combination technique solution for regularized least squares fitting is not as effective as it is in the case of elliptic partial differential equations. Their argument is that this is due to the irregular and random data distribution, and dependency of number of data to the grid resolution. They note that overfitting can arises when the mesh size goes to zero. So they conclude an optimal combination coefficients can prevent the amplification of the sampling noise present.

2.7. Works on Data Mining and Machine Learning

Data is currently produced with a huge rate. The issues in data processing sciences are mainly the ncreasing amount of data recorded and also the increasing complexity of these data. Application of analysis of image, multimedia, or spatial data are some examples of it.. An important task in data modelling is to develop prediction models or functional relationships between their selected features. The so-called curse of dimensionality arises when one want to identify such predictive models. In [23], Hegland discusses, how to choose the function spaces with an iterative approach to increase complexity of functions. His approach is to use adaptive complexity management closely related to the Analysis of Variance, also known as ANOVA decomposition. As the sparse grid approximations is good framework in this regards it has been combined with regression trees and multivariate splines to analyze the complexity of solution

Similar to the idea above the generative dimensionality reduction methods in machine learning has been investigated in [39]. They propose a framework to build a mapping from a lower dimensional space problem to higher dimensional data space and vice versa to achieve a dimension adaptive sparse grid reduction method. The reason to do so in data analysis is because some directions are play more important role than the others than others and it is reasonable to refine the underlying discretization space only in these directions based on the value of reconstruction error in that dimension.

2.8. Works on Eigenvalue Problems

In computational physics the concept of eigenvalue problem arise for example for the Born-Oppenheimer approximation of the stationary Schrödinger equation for atoms. A discrete eigenvalue problem is based on finite element discretization of the problem. The authors of [27] propose to use optimized combination technique to be used for the solution of this problem but directly applying to eigenvalue problems is not possible. Their remedy is to use partial solutions as ansatz functions and reconstruct the projection of the optimized combination technique as a Galerkin-approach[27].

Similarly, in the context of hot fusion plasmas there is a five-dimensional gyro-kinetic equations. As five dimensional problem in plasma needs a lot grid points and it is exponentially grown because of factor five one will encounter the curse of dimensionality. However as shown before the combination technique can be applied to this eigen-value problem for the gyro-kinetic code GENE[34].

2.9. Works on Adaptive Methods

This section is in major importance since it is closely related to the work of author of this project, in that they are also adaptive methods. First major study in this regard has been done by Griebel [16]. Adaptive Sparse Grid Multilevel Methods for Elliptic PDEs Based on Finite Differences: They have investigated how to use standard operations between two functions, i.e. addition or subtraction, scalar multiplication, and Division. This is done by

transformation of values to nodal basis and accumulation in nodal basis and then returning to hierarchical basis representation. By this setup we can estimate the error indicators and perform adaptive multilevel treatment of PDEs. First hand usage of hash table benefits in the case of adaptive multilevel treatment are also another important part of the research[16].

Another important research has been in the context of machine learning and regression [26]. Note that we included this work here rather than in regression section simply because of importance of their work in correspondence with the research at hand. It has been proposed how to use hierarchy of generalized sparse grids and choose the partial functions with adaptive iterative procedure. By doing so, one can pick out features insignificant to the prediction and thus the adaptivity.

3. Methods

1. The basic idea of combination technique is same as for multilevel splitting of finite element spaces is to replace the usual nodal bases of the finite element spaces by hierarchical bases.[2]

1. This new algorithmic concept is based on the independent solution of many problems with reduced size and their linear combination. [4]

3.1. sparse grid method and hierarchical basis

5. At first sight one gets rather dense and complicated discretization matrices when using hierarchical bases but The trick is not to assemble the discretization matrix but to use a factorization of it into the usual nodal basis stiffness matrix and some other very simple and sparse matrices.[2]

3. Using this type of hierarchical basis the calculation with functions defined on different grids and spaces is simplified. For example, the addition of two functions defined on different grids is reduced to the addition of the single coefficients. This is due to the fact that now the basis functions that are associated with the grid points which belong to both grids are just the same. [6]

4. The transformation of the coefficients of a function on grid represented in standard nodal basis to its representation in hierarchical basis can be implemented by a constant number of operations per grid point. The transformation to the hierarchical basis representation is done by the algorithm in [6]. This gives further insight to our hierarchical basis.

5. Following the argumentation in [3] we use as our finite element space the direct sum of the subspaces where the contribution to the error is equal or larger than some prescribed tolerance and results in an approximation space that corresponds to a sparse grid instead of a full grid. Now we will give a different motivation of the sparse grid approach. To this end we seek a certain linear combination of full grid spaces so that the sparse grid space is created. This gives the idea to represent any sparse grid function as a linear combination of its interpolants on the regular full grids. This approach has the advantage that only regular data structures must be used. There is no need for more complicated data structures than a few arrays to store a sparse grid function.[6]

6. Efficient discretization techniques are of crucial importance for most types of problems in numerical mathematics, starting from tasks like how to define sets of points to approximate, interpolate, or integrate certain classes of functions as good as possible, up

to the numerical solution of differential equations. Introduced by Zenger in 1990 and based on hierarchical tensor product approximation spaces, sparse grids have turned out to be a very efficient approach in order to improve the ratio of invested storage and computing time to the achieved accuracy for many problems in the areas mentioned above.[14]

3.2. Combination Technique

1. Altogether combination technique involves $O(h_n^{-1} \log(h_n^{-1}))$ unknowns in contrast to $O(h_n^{-2})$ unknowns for the conventional full grid approach. Additionally, combination solution is nearly as accurate as the standard solution. It can be proven that error is only slightly worse than for the associated full grid.[5, 6]

2. to some extent the combination technique even works in the case of non-smooth solutions. Now, h_i^2 and h_j^2 have to be replaced by h_i^α , h_j^β with appropriate α and β , but because of the properties of the combination technique the leading error terms still cancel. However, for the problems with severe singularities, the appropriate combination of adaptively refined grids is recommended.[5]

3. We have seen that in many situations the combination technique leads to the cancellation of certain error terms in the asymptotic error expansion[6]

4. Using bilinear interpolation for each single component function, we can extend the domain of definition to the union of all participating grids. This is possible, because bilinear interpolation can be shown to be compatible with the error splitting.[11]

3.3. Tree and in special Quadrees

20. (1. The sparse grid method is a special discretization technique, which allows to cope with the curse of dimensionality of grid based approaches to some extent. It is based on a hierarchical basis, a representation of a discrete function space which is equivalent to the conventional nodal basis, and a sparse tensor product construction. The method was originally developed for the solution of partial differential equations [Zen91, Gri91, Bun92, Bal94, Ach03]. It can be used in all finite element approaches, finite differences and finite volume approaches. Besides working directly in the hierarchical basis a sparse grid representation of a function can also be computed using the combination technique [GSZ92], where a certain sequence of partial functions is linearly combined.[25]

2. For the representation of a function f defined over a d -dimensional domain the sparse grid approach employs $O(h_1 \log(1/h_1))$ grid points in the discretization process, where h_n denotes the mesh size. It can be shown that the order of approximation to describe a function f , under certain smoothness conditions, is $O(h_2 \log(h_1/d))$. This is in contrast to conventional grid methods, which need $O(h^d)$ for an accuracy of $O(h^2)$. Since the curse of

dimensionality of full grid method arises for sparse grids at this much smaller extent they can be used for higher dimensional problems.[25]

3. Sparse grid: Motivated by the relation (13) of the importance of the hierarchical components Zenger [Zen91] and Griebel [Gri91] introduce the so-called sparse grids, where hierarchical basis functions with a small support, and therefore a small part in the function representation, are not included in the discrete space of level n anymore.[25]

4. Sparse grid combination technique : The so-called combination technique [GSZ92], which is based on multi-variate extrapolation [BGR94], is another method to achieve a function representation on a sparse grid. The function is discretized on a certain sequence of grids using a nodal discretization. A linear combination of these partial functions then gives the sparse grid representation. This approach can have numerical advantages over working directly in the hierarchical basis, where e.g. the stiffness matrix is not sparse and the on-the-fly computation of the matrix-vector-product, which complexity scales better, is challenging in the implementation [Ach03, Bal94, Bun98].[25]

5. Note that in the original [GSZ92] and other papers as well, a slightly different definition was used, again due to Dirichlet boundary conditions, [25]

6. The resulting function f_{nc} lives in the sparse grid space V_{ns} , the combined interpolant is identically with the hierarchical sparse grid interpolant.[25]

7. Note that the solution obtained with the combination technique f_{nc} for the numerical treatment of partial differential equations is in general not the sparse grid solution f_{ns} . However, the approximation property is of the same order as long a series expansion of the error[25]

8. Sparse grids in python: We give the listing of some python code for a sparse grid without functions on the boundary, i.e. according to formula (16).[25]
)

27. (1. The approach is obtained from a multi-scale basis by a tensor product construction and subsequent truncation of the resulting multi-resolution series expansion[32]

2. Combination technique is another method to achieve a function representation on a sparse grid. The function is discretized on a certain sequence of grids using a nodal discretization.[32]

3. sparse grid representation of a function can also be computed using the combination technique [25], here a certain sequence of partial functions represented in the conventional nodal basis is linearly combined.[32]

4. The number of basis functions which describe a function in nodal or hierarchical basis is $(2^n + 1)^d$.[32]

5. Note that a practical realization of sparse grids involves suitable data structures and special algorithms, e.g. for efficient matrix-vector multiplications in Galerkin methods for the numerical solution of partial differential equations. Also note that sparse grid functions do not possess some properties which full grid functions have, e.g. a sparse grid function need not be monotone [32, 34]. [32]

6. The sparse grid structure introduced so far defines an a priori selection of grid points that is optimal if certain smoothness conditions are met, i.e. if the function has bounded second mixed derivatives, and no further knowledge of the function is known or used. [32]

7. If the aim is to approximate functions which do not fulfill this smoothness condition, or to represent functions that show significantly differing characteristics, e.g. very steep regions beyond flat ones, spatially adaptive refinement may be used as well. Depending on the characteristics of the problem and function at hand adaptive refinement strategies decide which points, and corresponding basis functions, should be incrementally added to the sparse grid representation to increase the accuracy. [32]

8. In the sparse grid setting, usually an error indicator coming directly from the hierarchical basis is employed [14, 23, 34, 35]: depending on the size of the hierarchical surplus it is decided whether a basis function should be marked for further improvement or not. This is based on two observations: First, the hierarchical surplus gives the absolute change in the discrete representation at point x_{lj} due to the addition of the corresponding basis function ϕ_{lj} , it measures its contribution in a given sparse grid representation (15) in the maximum-norm. And second, a hierarchical surplus represents discrete second derivatives according to (12) and hence can be interpreted as a measure of the smoothness of the considered function at point [32]

9. Further details on spatially adaptive sparse grids, their realization and the state of the art can be found in [14, 34, 35]. [32]

10. two different hierarchy presented. [32]

11. one can build such a representation for a given function in an adaptive fashion, i.e. one chooses which component functions up to which ANOVA order are used for a reasonable approximation of some f . If the ANOVA order can be limited to q with $q \leq d$, the complexity estimates do not depend on the dimension d but on the ANOVA order q , allowing the treatment of even higher dimensional problems. An ANOVA-based dimension adaptive refinement algorithm in the hierarchical sparse grid basis is presented and evaluated in [14]. [32]

12. This approach can have numerical advantages over working directly in the hierarchical basis, where e.g. the stiffness matrix is not sparse and efficient computations of the matrix-vector-product are challenging in the implementation [1, 3, 6, 14, 34, 44]. [32]

13. The resulting function f_{nc} lives in the sparse grid space V_{ns} , where the combined interpolant is identical with the hierarchical sparse grid interpolant f_{ns} (proof in page 73).

but solution obtained with the combination technique fnc for the numerical treatment of partial differential equations, i.e. when the solutions on the partial grids are combined according to the combination formula (28), is in general not the sparse grid solution fns . However, the approximation property is of the same order as long as a certain series expansion of the error exists [25]. Its existence was shown for model-problems in [9].[32]

14. one can view the combination technique as an approximation of a projection into the underlying sparse grid space. The combination technique is then an exact projection into the sparse grid space if and only if the partial projections commute, i.e. the commutator $P_{V1} P_{V2} W_D P_{V1} P_{V2} P_{V2} P_{V1}$ is zero for all pairs of involved grids [27].[32]

15. so-called dimension adaptive procedure one considers an index set I which only needs to fulfill the following admissibility condition and one especially assumes here that $q_{j|d}$, so that the computational complexity depends on the so-called superposition (or effective) dimension q . The size of each grid l is now of order $O(q...)$ (page 76 and 77), Further details on dimension adaptive algorithms and suitable refinement strategies for the sparse combination technique can be found in [17, 19, 21]. [32]

16. Optimized combination coefficients are in particular relevant for dimension adaptive approaches [17, 19]. build functional and minimize it. [32]

17. Optimized combination technique requires the solution of a system with an overhead and results in an increase in computational complexity. In specific situations the computational complexity can be smaller though [16].[32]

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Finally some general important points and remarks will be discussed. These remarks will show the important factors at play in these kind of problems and maybe give insight for future work.

3.4. Some General Discussions and Points

1. The resulting algorithm can be used as a solver and within a preconditioner. it can also be applied as a preconditioner for the full grid problem to speed up a basic iterative solver. [4]

3.4.1. Argument of error and convergence

1. We show that the condition number of such a stiffness matrix for multilevel splitting of finite element spaces behaves like $O((\log \kappa)^2)$ where κ is the condition number of the stiffness matrix with respect to a nodal basis. [2]
2. error satisfies $O(h_n^2 \log(h_n^{-1}))$ (pointwise and with respect to the L_2 - and L_∞ -norm).[6]

3. For the Poisson equation on the unit square it is proved that the combined solution converges with order $O(h)$ in the energy norm and with order $O(h^2 \log h)$ in the L^2 -norm. (journals 5 and 9 are very similar aka poisson vs. second-order elliptic differential equations-9 general of 5) [9]

3.4.2. Argument of Preconditioner plus solver

1. The resulting algorithm can be used as a solver and within a preconditioner. it can also be applied as a preconditioner for the full grid problem to speed up a basic iterative solver. [4]

2. In addition to being a solver in its own right, the combination method can be used as a parallel preconditioner for the full grid problem. Then, a basic iterative method is accelerated substantially and shows nearly optimal, i.e. multigrid-like convergence behavior, if the accuracy of the solution is required only up to the truncation error.[4]

Argument of relation between hierarchical basis and nodal basis

1. As the representation of a finite element function with respect to a hierarchical basis can be converted very easily and quickly to its representation with respect to a nodal basis, our results mean that the method of conjugate gradients needs only logarithm of the dimension of the finite element space steps and computer operations to reduce the energy norm of the error by a given factor if one uses hierarchical bases or related preconditioning procedures. [2]

2. Two dimensional sparse grids contain only $O(h^{-1} \log(h^{-1}))$ grid points in contrast to the usually used full $O(h^{-2})$ grids, whereas for a sufficiently smooth function the accuracy of the representation is only slightly deteriorated. from $O(h^2)$ to $O(h^2 \log(h^{-1}))$. [6]

3. Using this type of hierarchical basis the calculation with functions defined on different grids and spaces is simplified. For example, the addition of two functions defined on different grids is reduced to the addition of the single coefficients. This is due to the fact that now the basis functions that are associated with the grid points which belong to both grids are just the same. [6]

4. The transformation of the coefficients of a function on grid represented in standard nodal basis to its representation in hierarchical basis can be implemented by a constant number of operations per grid point. The transformation to the hierarchical basis representation is done by the algorithm in [6].

5. The advantage of using the hierarchical basis representation during the combination process is that no interpolation to additional grid points has to be performed explicitly: For each 'missing' grid point, the interpolated value would be zero in hierarchical basis representation, and thus can be omitted during the combination of solutions[12]

6. One of the main advantages of hierarchical bases compared with standard nodal point bases is probably the fact that the basis gets a multilevel structure. Thus, we can now distinguish between high-level basis functions with a large support that usually (in the smooth case, at least) already contain a significant part of the information, and functions living on lower levels whose contribution to an interpolant or a finite element approximation is rather small. The decrease of the hierarchical coefficients from level to level can be used, of course, to control adaptive grid refinement, but, if it is combined with a tensor product approach for the higher dimensional case, it can be used for an a priori reduction of the number of grid points involved in the calculation, too.[14]

7. The hierarchical coefficient or hierarchical surplus itself can be used to indicate the smoothness of u at the corresponding grid point and, consequently, the necessity to refine the grid here.[14]

8. The elements of the sparse grid space can be represented in a hierarchical basis [27] and many algorithms for hierarchical basis methods including wavelets can be used for the solution [5,20]. Compared to the commonly used nodal basis, a hierarchical basis of, e.g. multilinear functions has its disadvantages, as the corresponding matrices have reduced sparsity and a less regular structure. This is due to the fact that the supports of the lower level basis functions are large and intersect nontrivially with many higher level basis functions. These difficulties increase with dimension. An efficient way to avoid the problem of reduced sparsity is given by the combination technique. [28]

Part II.

**Implementation, Results and
Conclusion**

4. Current Implementation

1. for non smooth solutions and more complex problems theory is still missing. Here like for the standard grid adaptive refinement seems to be necessary to get around solution method. First attempts in this direction are promising[6]

2. Consequently, one of the main advantages of the combination technique stems from the properties of sparse grids [1] In comparison to the standard full grid approach the number of grid points can be reduced significantly. Another advantage has to be seen in the simplicity of the combination concept its inherent parallel structure and its framework property allowing the integration of existing solvers for partial differential equations.[10]

3. we have implicitly assumed that this is the coarse mesh with spacing h that is naturally embedded in the fine mesh, so that the fine mesh solution may be transferred to the coarse mesh with injection.

4. In elliptic problems the smoothness of the solution may be disturbed where the data is non-smooth. The form of the domain or the need for local refinement may make the use of uniform meshes difficult. The local smoothness of the solution is a basic characteristic of many elliptic problems, so that extrapolation can be used locally, even when the global solution is non-smooth. With this background, several interesting new extrapolation-based approaches have been developed within the past few years, including the sparse grid combination technique and multivariate extrapolation. In this paper we will focus on explicit extrapolation methods that are based on the (linear) combination of solutions on different grids. Implicit extrapolation methods, in contrast, obtain higher order by applying the extrapolation idea on quantities like the truncation error or the numerical approximation of the functional. Such methods are discussed in Rude[11, 7]

5. Using bilinear interpolation for each single component function, we can extend the the domain of definition to the union of all participating grids. This is possible, because bilinear interpolation can be shown to be compatible with the error splitting.[11]

6. Obviously, an algorithm is needed which combines the advantages of both methods: low storage requirements, a low number of operations involved, but still simple data structures. In the following, we present an algorithm that fulfills these requirements[12]

7. Firstly, the block structure of a grid reduces main memory requirements. In an inner iteration step, the problem is solved one block at a time. An outer iteration establishes the overall solution. Secondly, the block structure of a grid is a natural basis for the parallelization of the solver. Each processor solves the problem on one of the blocks, and communication is necessary merely along block interfaces, in order to achieve a smooth solution on the whole domain.[12]

8. The hierarchical coefficient or hierarchical surplus itself can be used to indicate the smoothness of u at the corresponding grid point and, consequently, the necessity to refine the grid here.[14]

4.1. General Ideas

4.2. Different Schemes

5. Results

In this chapter we present the result of our implementation and discuss in details about the important matters which can be observed. we try to tackle the different schemes and naturally compare it to a full grid method.

The problem at hand might seem very trivial at first as we are investigating the interpolation problems in two dimension. However, the flexibility of the implementation shows how it can easily be extended to the higher dimension. Not only, the solution at hand is the base for higher dimension it can also be a base for solution on different applications such as regression and data fitting problem in Data mining, a partial differential equation solver for elliptic, parabolic problem, projection method and preconditioner for multigrid-like methods, and more importantly in computational mechanics, chemistry or physics. However, first we need to realize that this hierarchy of complexity of problem starts with interpolation problem which is the task discussed here. The author acknowledges the drawbacks of method mainly in regard to convergence but tries to discuss the reasons he believe this current implementation can resolve a part of those problems.

As we discussed earlier in the implementation chapter, the idea here is to project the result of the combination technique to the full grid. This has already been done by the fact that the underlying idea of the current implementation is to first project the function values of different level vector grids all to be combined with into a corresponding full grid and then combine them pointwise. This way we have some advantages and some disadvantage compared to other combination schemes presented in the literature.

Firstly, the obvious disadvantage would be the fact that by projection of all grids to a full grid we have a lot of extra memory consumption and this is exactly against the idea of rectifying curse of dimensionality. However, there is a solution to this problem though more clear after showing that the adaptive refinement strategy works. Assuming it works for now, it gives the rise to idea to use a coarse full grid and use adaptive refinement in the areas needed. This way, Same order of general error will be achieved but less storage than same full grid which needs higher resolution in the first place. In the worst case scenario, we get to the full grid resolution resulting the storage required be exactly the number of grids added plus subtracted multiplied by the storage required for the full grid.

In contrast, the advantage we achieve in this method is that since we perform tasks needed for each of the grids in the hierarchy of combination method separately, the extra effort is just from a projection. Therefore, using a very efficient projection method there are not that many operation added to the solution which basically means less computational effort compared to solution on normal full grid method.

Another advantage of this, as discussed earlier, can be possibility to start with a coarse grain solution and adaptively refine to areas needed. Probably later investigation of using lower resolution schemes for lower subtree problems can show better result for storage space and memory usage.

5.1. Verification of components

In any case, as for any scientific approach we first need to verify that our implementation works as expected. This has been done by comparison of the solution to normal full grid problem. we present here different test cases to be sure that in all different cases we get proper results.

1. $f(x) = x^2 + y^2$
2. $f(x) = x^2 \cdot y^2$
3. $f(x) = \sqrt[2]{x} \cdot \sqrt[2]{y}$
4. $f(x) = 16 \cdot x(1 - x)y(1 - y)$

In each case we try to compare the error of combination technique given the default scheme of $\vec{l} = (4, 4)$.

In every case we will draw the figures of the difference to observe better how the error is spread in the domain. For special test case 1 since the bilinear interpolation is used we can see the combination technique gives the perfect solution. The reason obviously is the nature of problem. Since bilinear interpolation is performed in one direction first and later in other direction it can be observe that interpolation of a function which is not of terms $x^{even} \cdot y^{even}$ gives no error.

Test Case Number	Function	General Error
1	$f(x) = x^2 + y^2$	error1
2	$f(x) = x^2 \cdot y^2$	error2
3	$f(x) = \sqrt[2]{x} \cdot \sqrt[2]{y}$	error3
4	$f(x) = 16 \cdot x(1 - x)y(1 - y)$	error4

5.2. results of local refinement (spatial adaptivity)

Based on the

5.2.1. error indicator based on solution of combination technique

5.2.2. error indicator based on predefined error function

5.3. Error and Accuracy

implementing a linked quad tree data structure together with 1. Firstly, the block structure of a grid reduces main memory requirements. In an inner iteration step, the problem is solved one block at a time. An outer iteration establishes the overall solution. Secondly, the block structure of a grid is a natural basis for the parallelization of the solver. Each processor solves the problem on one of the blocks, and communication is necessary merely along block interfaces, in order to achieve a smooth solution on the whole domain.[12]

6. Conclusion

6.1. Conclusion

final conclusion is written here

6.2. Suggestions for future works

Appendix

A. Detailed Descriptions

Here come the details that are not supposed to be in the regular text.

A.1. List of Figures

List of Figures

A.2. List of Tables

List of Tables

A.3. Source Code

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