



International Journal of Applied Mathematics and Numerical Research

Finite Element Methods for High-Dimensional Partial Differential Equations

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Article Info

Volume: 01

Issue: 03

May-June 2025

Received: 02-06-2025

Accepted: 27-06-2025

Page No: 15-17

Abstract

Partial Differential Equations (PDEs) are fundamental in modeling phenomena across physics, engineering, finance, and biology. The Finite Element Method (FEM) is a powerful and flexible numerical technique for approximating solutions to PDEs, especially in complex geometries. However, as the dimensionality of the problem increases, FEM faces significant computational challenges due to the curse of dimensionality. This article provides a comprehensive overview of finite element methods for high-dimensional PDEs, discussing their mathematical foundations, discretization strategies, computational challenges, and recent advances—including hybrid approaches with machine learning. We highlight applications, current research directions, and the future outlook for FEM in tackling high-dimensional problems.

Keywords: Finite Element Method (FEM), High-Dimensional PDEs, Sparse Grids, Computational Modeling, Physics-Informed Neural Networks (PINNs)

1. Introduction

Partial differential equations describe the evolution of systems with multiple variables and are ubiquitous in science and engineering. Classical examples include the heat equation, wave equation, Maxwell's equations, and the Black-Scholes equation in finance. Many real-world problems, such as those in quantum mechanics, uncertainty quantification, and high-dimensional data analysis, naturally lead to PDEs in high-dimensional spaces.

The Finite Element Method (FEM) is a widely used approach for numerically solving PDEs. Its flexibility in handling complex domains and boundary conditions has made it the method of choice for many engineering applications¹²⁶. However, when the number of dimensions increases, FEM faces severe computational hurdles, primarily due to the exponential growth in degrees of freedom—a phenomenon known as the curse of dimensionality²⁸.

This article explores the theoretical underpinnings of FEM, its extension to high-dimensional PDEs, the computational bottlenecks encountered, and recent innovations aimed at overcoming these challenges.

2. Mathematical Foundations of the Finite Element Method

2.1. Variational Formulation

FEM is grounded in the variational (or weak) formulation of PDEs. For a prototypical elliptic PDE:

$$-\nabla \cdot (A(x) \nabla u(x)) = f(x), x \in \Omega \subset \mathbb{R}^n, -\nabla \cdot (A(x) \nabla u(x)) = f(x), x \in \Omega \subset \mathbb{R}^n,$$

with boundary conditions (e.g., Dirichlet: $u|_{\partial\Omega} = 0$), the weak form seeks u in a suitable function space V (often a Sobolev space) such that:

$$a(u, v) = l(v) \forall v \in V, a(u, v) = l(v) \forall v \in V,$$

2.2. Discretization

The domain Ω is partitioned into simple geometric elements (simplices in higher dimensions), and the infinite-dimensional space V is approximated by a finite-dimensional subspace V_h spanned by basis functions (e.g., piecewise polynomials)²⁶. The solution is then sought as: $u_h(x) = \sum_{i=1}^N U_i \phi_i(x)$, where $\{\phi_i\}$ are basis functions and U_i are the unknown coefficients.

The resulting system of equations is typically sparse and can be solved using direct or iterative solvers⁶.

3. FEM in Higher Dimensions: Theory and Practice

3.1. Simplicial Elements and Mesh Generation

In two and three dimensions, mesh generation and basis function construction are well-understood and supported by commercial and open-source software². In higher dimensions ($n > 3$), the domain is partitioned into n -simplices (generalizations of triangles and tetrahedra). A linear function on an n -simplex is uniquely determined by its values at the $n+1$ vertices, making piecewise linear basis functions a natural choice².

However, mesh generation in high dimensions is nontrivial, and the number of simplices grows rapidly with dimension, exacerbating storage and computational costs.

3.2. Curse of Dimensionality

The primary challenge in high-dimensional FEM is the exponential growth in degrees of freedom. For a mesh with m subdivisions per dimension in an n -dimensional domain, the total number of elements is m^n . This makes even moderately high-dimensional problems intractable for classical FEM²⁸.

3.3. Variants and Generalizations

Several extensions of FEM have been developed to address specific challenges:

- **Generalized Finite Element Method (GFEM):** Uses local spaces with non-polynomial functions to improve approximation in domains with complex boundaries or microstructures⁶.
- **Mixed FEM:** Introduces additional variables to handle problems with constraints or multiple physical fields⁶.
- **hp-FEM:** Combines mesh refinement (h-refinement) with increasing polynomial degree (p-refinement) for improved accuracy.
- **CutFEM and XFEM:** Designed to handle complex geometries and interfaces with minimal mesh generation effort⁶.

4. Computational Strategies for High-Dimensional FEM

4.1. Sparse Grids

Sparse grid techniques reduce the number of basis functions by exploiting the structure of the solution space, especially when the solution exhibits anisotropy or low effective dimensionality. Sparse grids achieve polynomial rather than exponential scaling with dimension for certain classes of problems.

4.2. Model Reduction and Low-Rank Approximations

Model reduction methods, such as Proper Orthogonal Decomposition (POD) and tensor decompositions,

approximate the solution in a lower-dimensional subspace, significantly reducing computational cost.

4.3. Adaptive Methods

Adaptive mesh refinement (AMR) and adaptive basis enrichment focus computational resources on regions where the solution exhibits high variability, improving efficiency and accuracy.

4.4. Parallel and High-Performance Computing

Modern FEM solvers leverage parallel computing architectures and distributed memory systems to tackle large-scale high-dimensional problems. Libraries such as FEniCS and DUNE provide scalable implementations⁵.

5. FEM vs. Emerging Machine Learning Approaches

Recent years have seen the emergence of machine learning methods, particularly deep learning, for solving high-dimensional PDEs⁴⁷⁸. Physics-Informed Neural Networks (PINNs) and deep Galerkin methods use neural networks to approximate solutions, often bypassing the need for mesh generation.

However, studies show that, in terms of solution time and accuracy, classical FEM remains highly competitive, especially for problems where mesh-based discretization is feasible and well-understood⁵. Hybrid approaches that combine FEM with deep learning are an active area of research, aiming to harness the strengths of both paradigms⁷.

6. Applications of High-Dimensional FEM

6.1. Quantum Mechanics and Chemistry

The Schrödinger equation for multi-particle systems is a high-dimensional PDE. FEM, combined with model reduction and symmetry exploitation, is used to approximate electronic structure and molecular dynamics.

6.2. Uncertainty Quantification

In engineering and finance, PDEs with random inputs lead to high-dimensional stochastic PDEs. FEM, combined with stochastic collocation or polynomial chaos expansions, enables the computation of statistical properties of solutions.

6.3. Financial Mathematics

Option pricing models, such as the multi-asset Black-Scholes equation, are high-dimensional PDEs. Sparse grid FEM and low-rank methods are used to compute option prices and risk measures efficiently.

6.4. Data Science and Machine Learning

High-dimensional PDEs arise in manifold learning, diffusion maps, and kernel methods. FEM provides a principled approach to discretizing differential operators on data manifolds.

7. Recent Advances and Research Directions

7.1. Deep Learning and Neural FEM

Hybrid methods that integrate FEM with deep learning architectures are gaining traction. For example, neural networks can be used to approximate basis functions or solution coefficients, enabling efficient solution of parametric or nonlinear high-dimensional PDEs⁴⁷.

7.2. Physics-Informed Neural Networks (PINNs)

PINNs embed the PDE and boundary conditions into the loss function of a neural network. While promising for some high-dimensional problems, current research suggests that FEM often outperforms PINNs in terms of accuracy and solution time for many practical cases⁵.

7.3. Automatic Mesh Generation and Adaptivity

Advances in mesh generation algorithms, including those based on machine learning, are making it easier to construct high-quality meshes in high dimensions, further extending the reach of FEM.

7.4. Tensor-Based and Low-Rank FEM

Tensor decomposition methods, such as the tensor train and hierarchical Tucker formats, are being explored to represent high-dimensional solution spaces compactly, reducing storage and computational requirements.

8. Case Study: Solving a High-Dimensional Elliptic PDE

Consider the following model problem:

$$-\Delta u(x_1, \dots, x_n) = f(x_1, \dots, x_n), x \in [1, n], -\Delta u(x_1, \dots, x_n) = f(x_1, \dots, x_n), x \in [1, n],$$

with homogeneous Dirichlet boundary conditions.

A classical FEM approach would discretize the domain into n -simplices and approximate the solution using piecewise linear basis functions. For $n=6$ and a modest mesh resolution, the number of degrees of freedom can easily exceed millions, requiring substantial computational resources.

Sparse grid FEM or low-rank tensor methods can reduce this burden, making the problem tractable on modern hardware. Alternatively, a neural network-based approach might represent the solution as a function approximator trained to minimize the PDE residual and boundary errors.

9. Challenges and Limitations

9.1. Scalability

Despite advances, the curse of dimensionality remains a major obstacle for classical FEM in very high dimensions ($n > 5$). Algorithmic innovations and hardware advances continue to push these limits, but fundamental barriers persist.

9.2. Mesh Generation

Constructing high-quality meshes in high dimensions is challenging, both in terms of computational cost and geometric complexity.

9.3. Error Estimation and Adaptivity

Reliable a posteriori error estimation and adaptive refinement strategies are less developed in high dimensions, complicating the design of efficient and accurate solvers.

9.4. Integration with Data-Driven Methods

Seamlessly combining FEM with data-driven or machine learning approaches requires new theoretical frameworks and software tools.

10. Future Outlook

The future of FEM for high-dimensional PDEs will likely involve a synergy of classical numerical analysis, high-

performance computing, and machine learning. Promising directions include:

- **Hybrid FEM-ML Solvers:** Combining the interpretability and robustness of FEM with the flexibility of neural networks.
- **Automated Mesh Generation:** Using AI to generate and adapt meshes in high-dimensional spaces.
- **Tensor Methods:** Further development of efficient tensor-based representations for high-dimensional functions.
- **Open-Source Ecosystems:** Continued growth of scalable, user-friendly FEM libraries for research and industry.

11. Conclusion

Finite Element Methods remain a cornerstone of numerical PDE analysis, offering unparalleled flexibility and rigor for a wide range of problems. In high dimensions, FEM faces significant computational challenges, but ongoing research in sparse grids, model reduction, tensor methods, and machine learning is expanding its capabilities. As scientific and engineering problems grow in complexity and dimensionality, FEM—augmented by new computational paradigms—will continue to play a central role in simulation, analysis, and discovery.

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