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Title: Final Report of the Project "From the finite element method to the virtual element method"

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Abstract
The Finite Element Method (FEM) is a powerful numerical tool that is being used in a large number of engineering applications. The FEM is constructed on triangular/tetrahedral and quadrilateral/hexahedral meshes. Extending the FEM to general polygonal/polyhedral meshes in straightforward way turns out to be extremely difficult and leads to very complex and computationally expensive schemes. The reason for this failure is that the construction of the basis functions on elements with a very general shape is a non-trivial and complex task. In this project we developed a new family of numerical methods, dubbed the Virtual Element Method (VEM) for the numerical approximation of partial differential equations (PDE) of elliptic type suitable to polygonal and polyhedral unstructured meshes. We successfully formulated, implemented and tested these methods and studied both theoretically and numerically their stability, robustness and accuracy for diffusion problems, convection-reaction-diffusion problems, the Stokes equations and the biharmonic equations.

Background and Research Objectives
In over sixty years since its introduction, a clear theoretical foundation of the FEM has been developed for many Partial Differential Equations (PDEs) and the existence of a clear theory with rigorous error bounds has become one of the attractions of this methodology. Finite Elements are a powerful numerical tool that is being used in a large number of engineering applications. The classical FEM is constructed on triangular/tetrahedral and quadrilateral/hexahedral meshes. Extending the FEM to general polygonal/polyhedral meshes in straightforward way turns out to be extremely difficult and leads to very complex and computationally expensive schemes. The reason for this failure is that the construction of the basis functions on elements with a very general shape is a non-trivial and complex task. Nonetheless, there are many advantages in using polygonal/polyhedral meshes over purely triangular/tetrahedral or quadrilateral/hexahedral ones:

(a) polygonal/polyhedral meshes significantly simplify the partitioning of domains with complex geometry;

(b) they can reduce the complexity of adaptive mesh refinement and coarsening algorithms as no special treatment of hanging nodes is required to maintain the conformity of the mesh;

(c) they may be dictated by the data coming from multi-physics applications. Therefore, extending the finite element techniques to polygonal/polyhedral meshes while keeping their solid theoretical foundation is of great interest to the community of physicists and engineers.

However, doing that in a computationally efficient way without sacrificing the accuracy of the numerical approximation is a formidable task for the reasons that we will explain below. Instead, the virtual element approach is a very effective strategy to accomplish this task. To explain the challenge in extending finite elements to general polygonal/polyhedral meshes let us summarize the basic steps involved in the construction of a finite element method:

(1) rewrite the PDE in a weak form: multiply by a test function, integrate over the domain, integrate by parts moving one derivative from the unknown onto the test function;

(2) partition the domain into elements and identify the degrees of freedom, e.g., the solution values at the vertices of the elements;

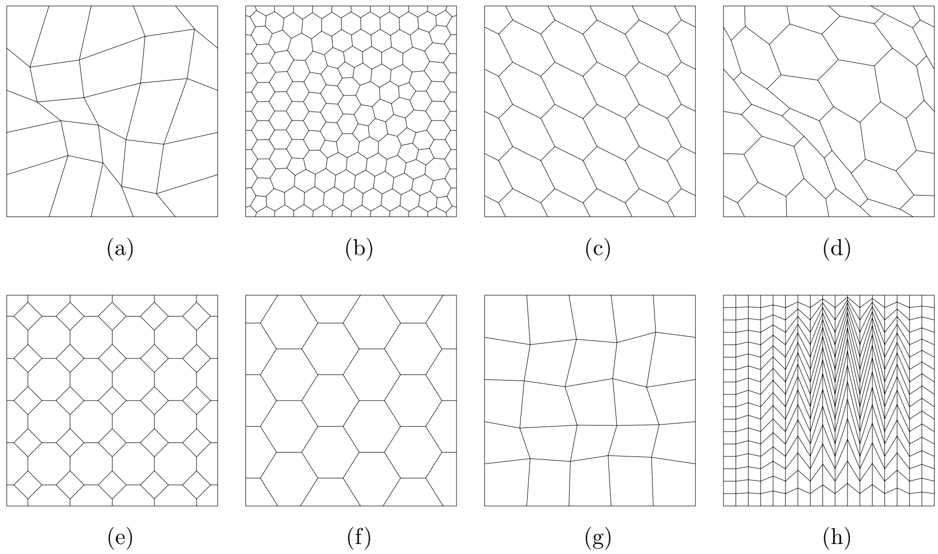

Figure 1: *Example of 2D meshes with very general shape cells:* (a) *smoothly remapped quadrilateral cells;* (b) *voronoi cells;* (c) *oblique hexagonal cells;* (d) *smoothly remapped hexagonal cells;* (e) *quadrilateral and octagonal cells;* (f) *regular hexagonal cells;* (g) *randomized quadrilateral cells;* (h) *highly skewed quadrilateral cells. The VEM works on all these kinds of meshes.*

(3) identify the shape functions and their gradients on each element;

(4) compute the elemental mass matrix and stiffness matrix by computing or approximating the integrals of the pairwise products of the shape functions and their gradients;

(5) assemble all the elemental matrices, solve the resulting linear system and post-process the numerical solution (if needed).

A straightforward extension of steps 1-5 to polygonal meshes has led to the development of the Polygonal Finite Element Methods (PFEMs) and how to perform an effective, accurate and robust polyhedral extensions is still an open issue. Moreover, PFEM are a generalization of the linear Galerkin FEM and thus provides a low-order approximation. How to build higher-order accurate approximations, e.g., quadratic, is also an open issue. The critical point in the PFEM approach is represented by step 3: the construction of the elemental shape functions. On triangular/tetrahedral and quadrilateral/hexahedral elements the basis functions are determined as the unique solution of a polynomial interpolation problem for the degrees of freedom; hence, they are polynomials and are expressed by relatively simple formulas. For example, the shape functions of the linear Galerkin FEM on a triangle and a tetrahedron are the linear Lagrangian interpolants whose value is one at a given vertex and zero at the other vertices. The situation is completely different on general polygonal and polyhedral elements because:

- the solutions of such interpolation problems are no longer polynomials;
- they are not uniquely determined, i.e., many different constructions for such interpolants are possible such as the Wachspress interpolants, the Sybson interpolants, the natural neighbor interpolants, the harmonic interpolants (just to mention a few);

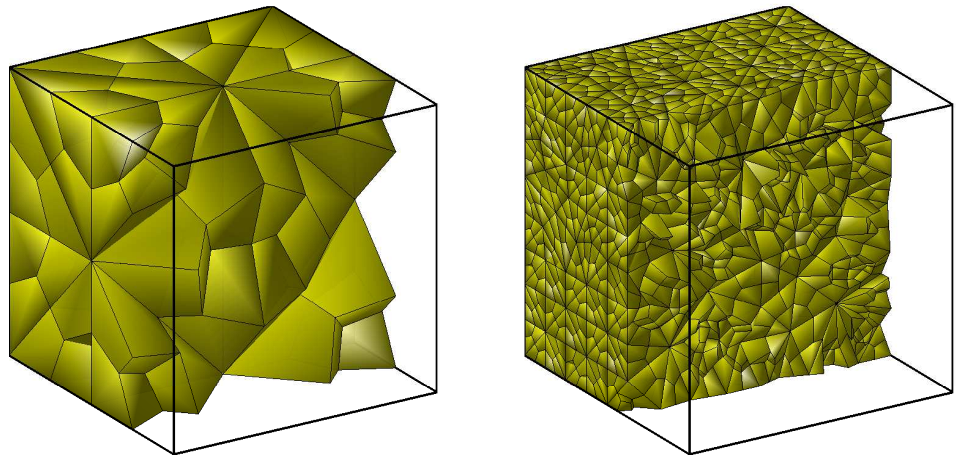

Figure 2: *Example of 3D unstructured meshes of polyhedral cells*

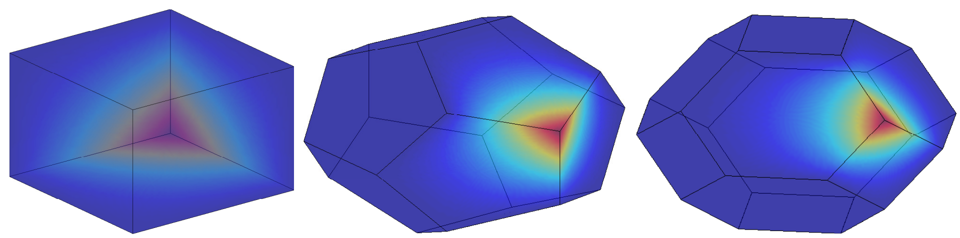

Figure 3: *Example of 3D shape functions used in the Polyhedral Finite Element Method*

- no explicit formula is available for such interpolants and their gradients.

As no explicit formula is available, using such interpolants as basis functions is awkward: PFEMs are necessarily based on numerical quadratures and at each quadrature node the evaluation of a basis function requires the numerical resolution of an implicit and non-linear problem. As a result, depending on the accuracy of the quadrature rule and the number of quadrature nodes we may obtain either poor accuracy of the approximation (too few nodes) or a very expensive scheme (too many nodes). These issues become even more pronounced in 3D, making straightforward generalization of PFEMs prohibitively complex and computationally expensive. Instead, in the virtual element formulation, only the part of the finite element space that refers to polynomials is constructed, while the behavior of the method on the rest of the space is approximated following a stability criterion. This fact has a dramatic impact on the computational complexity that is greatly simplified as the implementation of VEM does not require the explicit construction of the shape functions.

The VEM is characterized by an order of accuracy higher than one in the energy norm and an order of regularity higher than zero (numerical solutions with continuous derivatives). The high order of accuracy is achieved by ensuring the exactness of the methods when the solution is a polynomial of degree higher than one. This property is normally achieved in the finite element

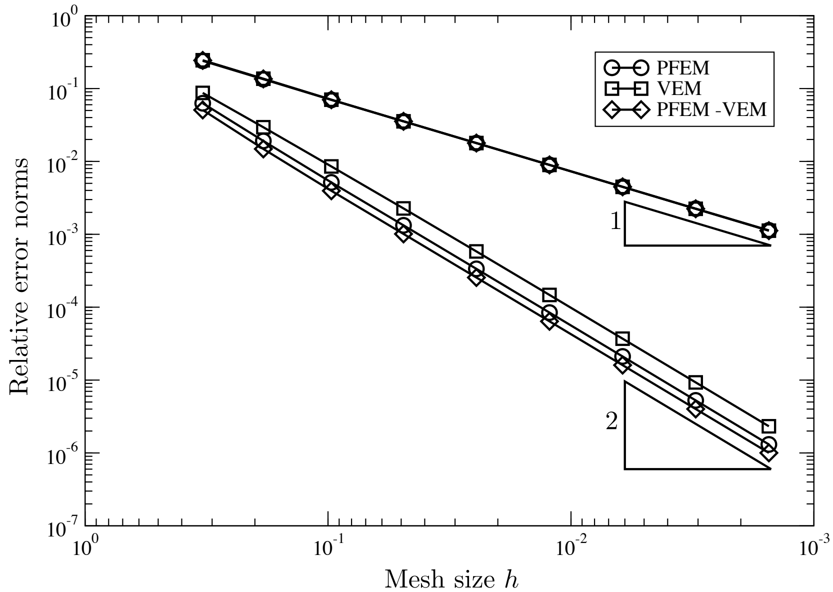

Figure 4: *Comparison of the convergence curves versus the mesh size parameter h for the VEM, the PFEM, and the combination VEM-PFEM when solving a benchmark problem for the Poisson equation. The relative errors are evaluated by using the L^2 norm (steepest slopes) and H^1 norms (top slopes).*

method only on meshes of triangles and quadrilaterals in 2D and tetrahedra and hexahedra in 3D. The high order of regularity is normally achieved by a suitable choice of the degrees of freedom and, consequently, of the definition of the projection operators.

Scientific Approach and Results

We discuss the three major points where we were particularly successful, the dissemination activity and the follow up of this project.

(1) **Comparison with Polygonal/Polyhedral FEMs and hourglass stabilization**

Generalized barycentric coordinates such as Wachspress and mean value coordinates have been the unique available finite element formulation for polygonal and polyhedral meshes for about three decades. The VEM is an alternative, consistent and stable finite element method that works on polygonal and polyhedral elements. In the VEM, we use a projection operator to decompose the stiffness matrix into two terms: the consistency matrix and the stability matrix. This latter matrix must be positive semi-definite and is only required to scale like the consistency matrix. The VEM decomposition still provides a robust and efficient generalized barycentric coordinate Galerkin method if we adopt the consistent VEM matrix and we compute the stabilization term by using the generalized barycentric coordinates. This facilitates post-processing of field variables and visualization in the VEM, and on the other hand, provides a means to exactly satisfy the patch test with efficient numerical integration in polygonal and polyhedral finite elements. In [12] we compare the accuracy and performance of the method with respect to the traditional polygonal/polyhedral FEMs and for Poisson problems in the two- and three-dimensional space we establish that linearly complete generalized barycentric interpolants deliver optimal rates of convergence in the L^2 norm

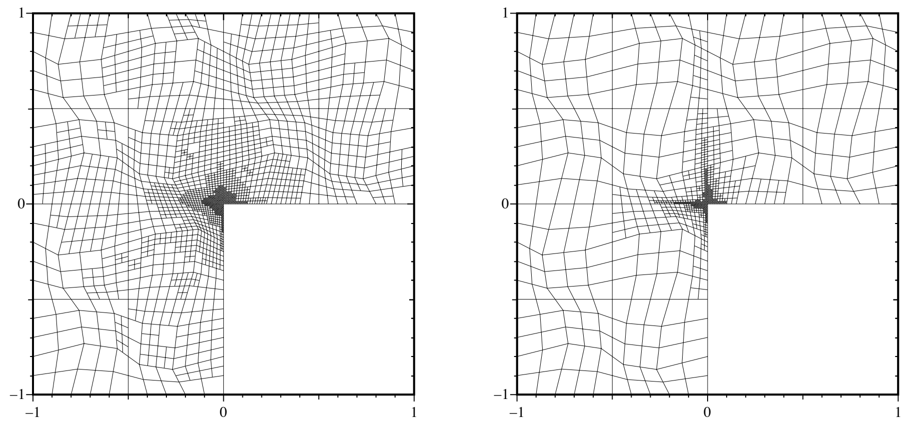

Figure 5: *Example of a local mesh refinement driven by the residual-based a posteriori estimator, see [3]*

and the H^1 seminorm.

In [9] we investigate the connections between the VEM and the hourglass control techniques that was developed by Belytschko and collaborators in the early '80s to stabilize underintegrated C^0 Lagrange finite element methods. In particular, we prove theoretically that the variational approach adopted in the VEM affords a generalized and robust means to stabilize underintegrated finite elements and the virtual element formulation is the natural theoretical setting to explain the hourglass stabilization techniques. In this work we mainly focus on the heat conduction equation and we develop the virtual element method and assess its performance for the isoparametric 4-node quadrilateral and the 8-node hexahedral element. In addition, we show quantitative comparisons of the consistency and stabilization matrices in the VEM with those in the hourglass control method of Belytschko and coworkers. Numerical examples in two and three dimensions for different stabilization parameters reveal that the virtual element method satisfies the patch test and delivers optimal rates of convergence in the L^2 norm and the H^1 seminorm for Poisson problems on quadrilateral, hexahedral, and arbitrary polygonal meshes.

(2) **Conforming VEM: grid adaptivity using residual based a posteriori estimators and methods with arbitrary regularity**

A posteriori error estimation and adaptivity are very useful in the context of the virtual element and mimetic discretization methods due to the flexibility of the meshes to which these families of numerical schemes can be applied. Nevertheless, developing error estimators for virtual and mimetic methods is not a straightforward task due to the lack of knowledge of the basis functions. In the new virtual element setting, we developed a residual based a posteriori error estimator that immediately applies also to its mimetic counterpart [3]. For such estimator we proved the reliability and we showed the numerical performance when it is combined with an adaptive strategy for the mesh refinement.

In a second work, we developed and analyzed a new family of virtual element methods on unstructured polygonal meshes for the diffusion problem in primal form, that use arbitrarily regular discrete spaces. The degrees of freedom are (a) solution and derivative values of various degree

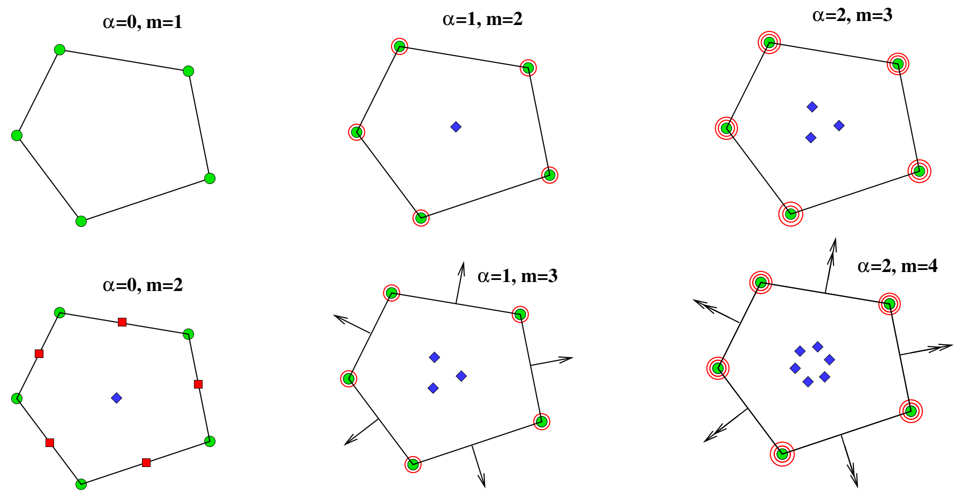

Figure 6: *Degrees of freedom on a pentagonal cell for the VEM with regularity* $\alpha = 0,1,2$ *(left, middle, and right panel) and accuracy provided by polynomials of degree* $m = 1,2,3$*, see [4]*

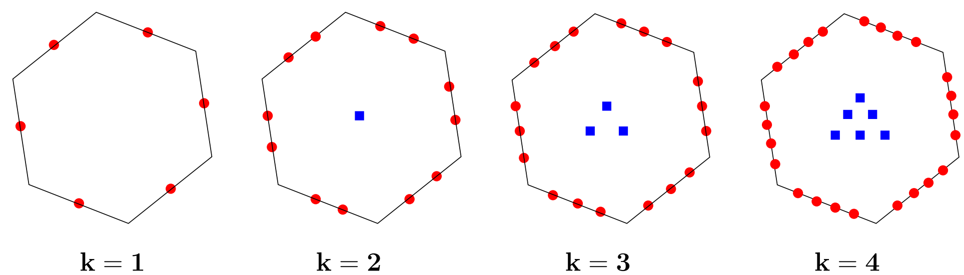

Figure 7: *Nonconforming degrees of freedom for an hexagonal cell for the polynomial degree* $k = 1,2,3,4$.

at suitable nodes and (b) solution moments inside polygons. The convergence of the method was proven theoretically, an optimal error estimate was derived and the proper behavior of the method was confirmed through numerical experiments.

(3) **The nonconforming virtual element formulation**

The first virtual element formulation can be considered as an extension of the classical conforming FEM, which is usually stated on simplicial and quadrilateral/hexahedral elements, to polygonal and polyhedral elements. During the first year of this project we realized that a nonconforming formulation is also possible. The nonconforming formulation offers a major advantage with respect to the conforming one: it does not require a hierarchical construction of the virtual element space when the number of dimensions is increased. Therefore, the total number of degrees of freedom is smaller in 3D than that required by the conforming VEM. Moreover, as in the case of Stokes equations, the method is the same for any number of space dimensions. In [2] we first developed the nonconforming VEM for the approximation of second order elliptic problems (Poisson equation). The method is designed in two and three dimensions (but the formulation is indeed the same for

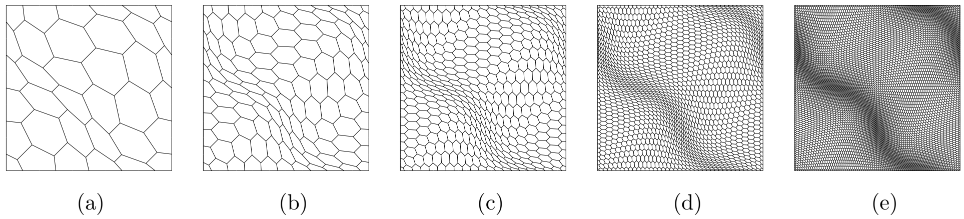

Figure 8: *An example of a sequence of remapped hexagonal meshes used for convergence tests.*

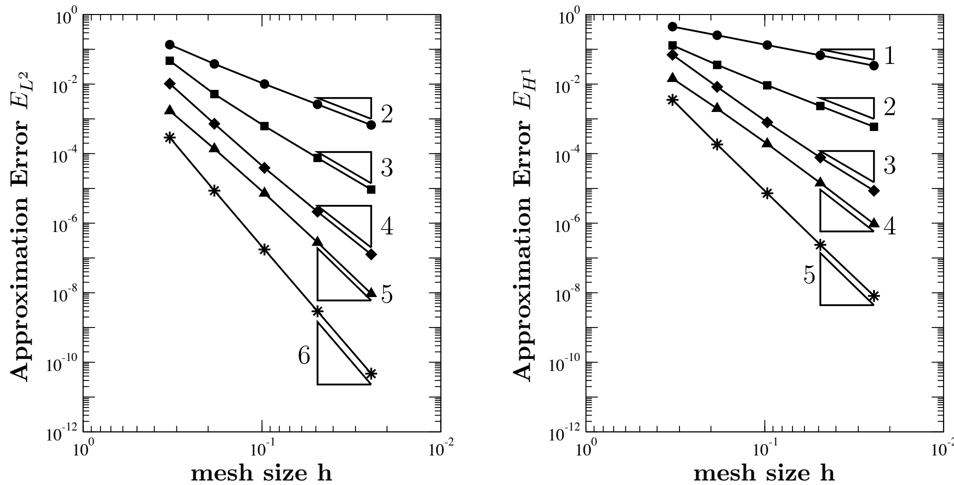

Figure 9: *Convergence curves for the nonconforming VEM applied to a benchmark problem for the Poisson equation. The relative errors are measured by using the L^2 norm (left panel) and the H^1 norm right panel*

any number of spatial dimensions), and in [] we highlight the main differences with the conforming VEM and the classical nonconforming finite element methods. For this method, we provide the complete error analysis and establish the equivalence with the family of mimetic finite difference methods previously developed by the PI with other authors. Furthermore, we verified the theory and validated the performance of the proposed method by a set of numerical experiments.

The nonconforming formulation is currently one of the three major VEM formulations, the other two being the conforming formulation and the mixed formulation. During this project we developed a unified framework for the conforming and nonconforming VEM and extended the nonconforming formulation to general second order elliptic problems in two and three dimensions. In our approach, cf. [10], we split the differential operator of the continuum setting into its symmetric and non-symmetric parts and established conditions for stability and accuracy on their discrete counterparts. Under these conditions, we may provide optimal H^1- and L^2-error estimates, which are confirmed by numerical experiments on a set of polygonal meshes. The accuracy of the numerical approximation provided by the two methods was also shown to be comparable. An example of these results, extracted from [10], is shown in Figure 9; the calculations are carried on the sequence of meshes depicted in Figure 8. In the second and third year of the project, we continued the development of the nonconforming virtual element formulations and designed new VEM for the *Stokes equations* and the *biharmonic problem*.

In the Stokes equations, the pressure is approximated using discontinuous piecewise polynomials, while each component of the velocity is approximated using the nonconforming virtual element space. On each mesh element the local virtual space contains the space of polynomials of up to a given degree, plus suitable non-polynomial functions. The virtual element functions are implicitly defined as the solution of local Poisson problems with polynomial Neumann boundary conditions. As typical in VEM approaches, the explicit evaluation of the non-polynomial functions is not required. This approach makes it possible to construct nonconforming (virtual) spaces for any polynomial degree regardless of the parity, for two-and three-dimensional problems, and for meshes with very general polygonal and polyhedral elements. In [7] we show that the nonconforming VEM is inf-sup stable and establish optimal a priori error estimates for the velocity and pressure approximations in the energy norm. Numerical examples confirm the convergence analysis and the effectiveness of the method in providing high-order accurate approximations.

Finally, we developed the nonconforming virtual element method for the numerical resolution of the biharmonic problem [1]. This work began during the final stages of project and was finished and published after the end of the project. This method uses both internal and boundary degrees of freedom locally defined on each mesh element to represent the functions of a special finite element space. The convergence of the method is theoretically proved by deriving optimal convergence rates, and a set of numerical experiments confirms the theoretical expectations.

(4) **Dissemination of results**

- In 2014 the PI has been invited to be the Guest Editor of the special issue on *Recent techniques for PDE discretization on polyhedral meshes* for the international journal *Mathematical Models & Methods in Applied Sciences*, cf. [5], co-Editors Prof. N. Bellomo and Prof. F. Brezzi;

- during the FY14-FY15-FY16 the PI co-organized the following minisymposia at international conferences:

  2016.
  Co-organizer with A. Cangiani and S. Weisser of the minisymposium ”PDE Discretisation Methods on Polygonal and Polyhedral Meshes” within the MAFELAP 2016 Conference (The Mathematics of Finite Elements and Applications), to be held at Brunel University, Uxbridge (London), June 14-17, 2016.

  2015.
  (*i*) Co-organizer with N. Sukumar, A. Gillette, J. Bishop of the minisymposium ”Polygonal and Polyhedral Discretizations in Computational Mechanics”, at the 13th US National Congress of Computational Mechanics, to be held in San Diego, California, 26-30 July, 2015;

  (*ii*) Co-organizer with K. Lipnikov of the minisymposterium ”Advanced discretizations for complex applications”, at the SIAM Conference on Computational Science, to be held in Salt Lake City, Utah, 14-18 March 2015;

2014.
Co-organizer with L. Beirao da Veiga, A. Buffa, A. Ern, M. Gerritsma, J. Evans, of the minisymposium “Structure-preserving and polyhedral discretizations”, at the XI World Congress of Computational Mechanics, held in Barcelona, Spain, 20-25 July 2014;

- during the project the Pi and the co-Pi was invited in several international workshops, congresses and domestic and foreign research institutions to deliver talks an poster presentations on the research activity of the project.

(5) **Follow up**
The virtual element methodology developed in this project has paved the way to some interesting further applications and developments, that we briefly review here. Most of this work was carried out after the end of the project, and, thus, was not funded directly by the project.

- The connection between the VEM and other schemes for solving PDEs on unstructured polygonal/polyhedral mesh has been investigated in [11]. The major result of this work is that the VEM, the Hybrid High-Order (HHO) method by Di Pietro and Ern and the Hybridizable Discontinuous Galerkin (HDG) method by Cockburn and collaborators are in fact just different instances of a more general family of numerical methods call *Gradient Discretisations* by Droniou and coauthors;
- the VEM method developed in [6] for the advection-diffusion-reaction equation in diffusive regime has been extended to the advection-dominated regime by introducing the Streamline Upwind/Petrov-Galerkin stabilization. Theoretical and experimental investigations have shown the optimality of the method so that optimal convergence rates and robustness also in presence of strong advective layers in the solution have been shown.
- The new LDRD project *Novel Algorithms for Ab-Initio DFT Calculations of Large-Scale Material Systems*, #20180428*ER*, have been funded for the FY18-FY19-F20 to develop the VEM technology for solving the Schrodinger and Kohn-Sham equations for the numerical modeling of applications from Computational Quantum Chemistry;
- at the end of the project the Pi and the co-Pi were invited to write a chapter in the book *Generalized barycentric coordinates in computer graphics and computational mechanics*, edited by Prof. K. Hormann and Prof. N. Sukumar, and published by CRC Press in October 2017, see [8]. This chapter offers a short overview of the VEM and the results obtained during the project.

Anticipated Impact on Mission
This research has provided unique capabilities in the DOE complex by developing world-class algorithms with a strong theoretical foundation for the numerical treatment of partial differential equations. These algorithms can be ported to high-end HPC technologies and have natural connections with potential large proposals in the Co-Design and Extreme-Scale Solvers categories. Even if our project was mainly focused to the design and analysis of new numerical methods and their implementation and testing were carried out mostly on academic problems, these new

capabilities position us uniquely towards future opportunities in the areas mentioned above. We expect indeed that virtual element algorithms may impact the numerical modeling in a wide range of multi-physics applications, including climate and environmental modeling (e.g., climate, ocean and sea-ice modeling, ASCEM Project), plasma physics (e.g., Fokker-Planck equation in inertial confinement fusion simulations) and other CFD-based applications. This will lead to new funding in fundamental research on numerical methods by working with Office of Science ASCR managers.

Conclusion

In this project we developed a new type of finite elements, dubbed Virtual Element Method (VEM), that is particularly suitable to the numerical treatment of variational problems in weak form on very general meshes. The new family of numerical methods have been studied from the theoretical and numerical viewpoint, and stability, robustness and accuracy have been assessed for general elliptic problems like convection-reaction-diffusion equation in the diffusive domain, the Stokes equations and the biharmonic equations. The work carried out in the project led us to the development of the nonconforming VEM, which is currently one of the three major formulations. As a follow up of this project, we mention the study of the connections between the VEM and other numerical techniques suitable to polygonal/polyhedral meshes, the development of the SUPG-VEM for advection-diffusion problem for the advection-dominated regime, and new LDRD-ER project funded to development the VEM for Schrodinger and Kohn-Sham equations.

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