HIGHER-ORDER DGFEM TRANSPORT CALCULATIONS ON POLYTOPE MESHES FOR MASSIVELY-PARALLEL ARCHITECTURES

A Dissertation

by

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1. INTRODUCTION

1.1 Motivation and Purpose of the Dissertation

Accurate solutions of the neutral particle transport equation are important for multiple fields, including medical imaging, radiotherapy, nuclear power, and other industrial applications.

1. Polytope mesh cells are now being employed in other physics communities - most notably computational fluid dynamics (CFD) [1];

2. They are believed to reduce the number of unknowns to solve with equivalent accuracy;

3. They can reduce cell/face counts which can reduce algorithm wallclock times depending on the solution method;

4. They can allow for transition elements between different portions of the domain (e.g., tetrahedral elements bordering hexahedral elements at the border of the boundary layer);

5. They can easily be split along cut planes - allowing the mesh to be partitioned into regular or irregular divisions as well as be generated by simplical meshing techniques across processor sets in parallel;

6. Hanging nodes from non-conforming meshes, like those that naturally arise from locally refined/adapted meshes, are no longer necessary.

1.2 Current State of the Problem

1.2.1 Background on the Multigroup DGFEM S_N Transport Equation

Multigroup goes here...

Angular discretization goes here...

DGFEM Sn goes here...

1.2.2 Diffusion Synthetic Acceleration

1.2.3 Polytope Grids Formed from Voronoi Mesh Generation

Since this dissertation work is on the solution of the transport equation on polytope meshes, we next describe how these grids can be generated. Traditionally, FEM calculations have been performed on simplical (triangles and tetrahedra) and tensor based meshes (quadrilaterals and hexahedra). In fact, it is still a standard practice to refer to any type of mesh as a *triangulation* in some communities [2]. Many different mesh generation software has been developed to build these simple grids [3, 4, 5, 6]. However, multiple fields including *computational fluid dynamics* (CFD) and *solid mechanics* are now finding benefits to utilizing polygonal and polyhedral meshes for their calculations.

However, polytope mesh generation is still in its infancy.

1.2.4 Adaptive Mesh Refinement for the DGFEM S_N Transport Equation

1.3 Organization of the Dissertation

In this introductory chapter, we have presented a summary of work performed. We also gave our motivation for choosing this work as well as a brief discussion of previous work that has directly influenced this dissertation. We conclude this intoduction by briefly describing the remaining chapters of this dissertation.

In Chapter **??**, we present the DGFEM formulation for the multigroup, S_N transport equation. We then describe the transport equation's discretization in energy, angle, and space. We have left the FEM spatial interpolation function as arbitrary at this point to be defined in detail in Chapter **??**. For the spatial variable, we provide the theoretical convergence properties of the DGFEM form. We also detail the elementary assembly procedures to form the full set of spatial equations. We conclude by providing the methodology to be used to solve the full phase-space of the transport problem.

In Chapter **??**, we present all the finite element basis functions that we will use in this work. In two dimensions, we present four different linearly-complete polygonal coordinate systems that we will use to generate our finite element basis functions. We then present the methodology that converts each of these linear coordinate systems into quadratically-complete coordinates for use as higher-order basis functions. We also present the single linearly-complete polyhedral coordinate system that we will use for the 3D transport problems.

In Chapter **??**, we present the methodologies to be used for DSA preconditioning of the DGFEM transport equation for optically thick problems. We give a discontinuous form of the diffusion equation which can be used on 2D and 3D polytope grids. The theoretical limits of the DSA scheme are analyzed and we conclude with a real-world problem of accelerating the thermal neutron upscattering of a large multigroup, heterogeneous transport problem. In doing so, we demonstrate that our methodology will work on massively-parallel computer architectures.

We then finalize this dissertation work by drawing conclusions and discussing open topics of research stemming from this dissertation in Chapter 2. We note that our detailed literature reviews, numerical results, and conclusions pertaining to each topic are presented in their corresponding chapter.

Additional material that is not included in the main body of the dissertation for the sake of brevity is appended for completeness. The appendices are organized in a simple manner:

- Appendix **??**: addendum to Section **??**, corresponding to additional material relating to the multigroup S_N equations.
- Appendix **??**: addendum to Section **??**, corresponding to additional material relating to the various polytope coordinate systems to be utilized as finite element basis functions.
- Appendix **??**: addendum to Section **??**, corresponding to additional material relating to DSA preconditioning on polytope grids.

2. CONCLUSIONS

2.1 Conclusions

In this dissertation, we have performed work to advance the state-of-the-art in solving the DGFEM S_N transport equation on polytope meshes using massively-parallel computer architectures. We have done this by investigating two different topical areas. First, we investigated four different linearly-complete polygonal coordinate systems to be used as FEM basis functions. Then,

1.
2.
3.
4.

2.2 Open Items

While the work in this dissertation answered several open questions related to the calculation of the DGFEM S_N transport equation on massively-parallel architectures, several items remain for ongoing research. We now list the open items that we have identified:

1. *Quadratic serendipity basis functions on 3D polyhedra:*

   The direct extension of the work involving the 2D quadratic serendipity basis functions would be to form quadratically-complete, analogous serendipity coordinates for arbitrary 3D polyhedra. To maintain quadratic completeness in 3D, the coordinates would be beholden to the ten quadratic 3D constraints which would require exact interpolation of the $\{1, x, y, z, xy, xz, yz, x^2, y^2, z^2\}$ span of functions. Along a polyhedral face, the methodology presented in Chapter **??** has a direct 3D analogue. However, careful consideration is required to remove all of the diameter nodes within the polyhedron and is an open area of research in the applied mathematics community.

2. *Higher-order 2D serendipity polygonal basis functions:*

   The quadratic serendipity basis functions were formed by taking pairwise products of the linear barycentric basis functions, followed by removal of the interior nodes. For a given polynomial order p, the monomials that the basis functions need to exactly interpolate are $x^\sigma y^\tau$, where $\sigma + \tau = p$. We can see that all of the higher-order functional spaces can be generated by taking pairwise products of terms from lower-order functions. Mukherjee and Webb have just recently developed a means to generate these higher-order polygonal finite elements through a hierarchical approach [**?**].

3. *Alternate integration schemes on polygons:*

   For this work, our quadrature integration scheme on arbitrary polygons consisted of a simple triangulation scheme where each sub-triangle had points mapped onto it from the reference triangle. We did not focus on efficiency for this work, but instead simply used a high-order reference quadrature set. However, by performing our integration this way, the basis function values and gradients must be computed for each polygon in the mesh. This becomes computationally expensive for meshes with many cells containing polygons with large vertex counts. An alternative approach could consist of the use of Schwarz-Christoffel Conforming Maps (SCCM) [**?**, **?**]. Generation of the polygonal basis functions and gradients could be computed on reference (regular) polygons and then conformally mapped to any arbitrary polygon for integration [**?**].

4. *Mixed-mode parallelism with DSA preconditioning:*

   In this work, the only parallelism used was

5. *Further preconditioning the MJA method:*

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