

Preface

Simply stated, the purpose for preparing this book was to document the experience within the fields of grid generation and enhancement accrued over the past years by members of the U. S. Department of Energy's Advanced Simulation and Computing (ASC) Setup Project at the Los Alamos National Laboratory.¹

This work was motivated by the desire to achieve better results when modeling fluid dynamics and heat transfer problems, high-speed fluid flows, along with other applications. Generally, these problems were discretized by multi-dimensional structured and/or unstructured meshes, usually possessing highly-curved external and internal boundary definitions. Furthermore, the vast majority of these two- and three-dimensional meshes were required by the final simulation application to contain predominantly quadrilateral or hexahedral elements. It has been our challenge to meet these, seemingly increasingly complex, requirements. While unstructured mesh generation and enhancement methods present the most difficult challenges, structured meshes continue to have challenges of their own.

Note that we use the terms mesh and grid interchangeably to mean the set of cells, faces, and/or nodes that represent the discretization of physical space contained and defined by geometrical surfaces, *etc.* to be used by an approximate numerical algorithm for the purpose of simulating a physical process. The reader will also note that we have drawn a distinction between grid generation and grid enhancement. Historically, the term *grid generation* has been used to designate both operations. It is our view that grid generation refers to the process of creating an initial grid based directly

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on domain geometry information. Grid enhancement refers to the operations involved in modifying the initial mesh to improve its computability or ability to meet the requirements of the ultimate simulation application.

It is our goal in writing this monograph that anyone wishing to understand the basics of grid smoothing and enhancement using elliptic methods may find this book useful. Our intent is not to present an exhaustive survey of the field by looking at all elliptic methods; we limit this presentation to those approaches that we are most familiar with or have used successfully. To this end, the book:

- Presents basic background information on grids and terminology as well as on approximation methods for differential equations.
- Includes a discussion of solving the resulting non-linear algebraic equation systems.
- Because the emphasis is upon elliptic enhancement methods which rely on spatial metrics, several chapters (and an appendix) are presented that focus on differential geometry of surfaces.
- These topics are followed by a discussion of existing elliptic enhancement methods, placing them in context of the general Laplace-Beltrami elliptic system (LBES) for grid enhancement.
- The last two chapters detail how the LBES is implemented for structured and unstructured grids and provide motivation for our use of this approach by comparing results with other selected elliptic methods.

This book, therefore, presents information on the computational geometry and mesh enhancement aspects of the Numerical Simulation Process.

Specifically, the introductory chapter on basic concepts places grid generation and enhancement within the numerical simulation process, describes an elliptic enhancement methodology, and presents a primer on meshes and associated terminology. It also briefly summarizes several grid generation methods and introduces the concept of grid quality.

In order to define an initial mesh and to properly enhance it, a detailed description must exist of the geometric objects that define the computational domain. This includes the external boundaries of the mesh as well as the internal geometries defining specific material interfaces. Chapter 2 presents information about curves and surfaces and operations that may be performed upon them. The focus is on parametric curves and surface descriptions, but some information is also provided on constructive solid

geometry. An overview of geometric data structures is also given.

The chapter on numerical approximation methods for differential equations (Chapter 3) is rather extensive, covering finite difference methods and methods of weighted residuals, also called weak solution methods. Weighted residual methods include finite volume and finite element methods as special cases. These approximation methods are central to the mesh topology definition and are used to solve the LBES as well as within the final physics application. Consequently, we have given a thorough introduction to these methods so that the reader can obtain sufficient information to support our stated goals in preparing this book.

As a result of applying the numerical approximations to the LBES, systems of, generally, non-linear algebraic equations for the unknown coordinates of each mesh node are formed. These must then be solved in a reliable and accurate manner. The next chapter (Chapter 4) presents a discussion of the methods we have found effective for obtaining such solutions.

The next two chapters, Chapters 5 and 6, revisit surface geometry by focusing upon the two fundamental differential geometric forms required to understand the metric tensor used in the LBES. A discussion of isothermal coordinates and their generalization, harmonic coordinates, is also presented. An appendix (Appendix A) provides a summary of the mathematical concepts used in discussions on differential geometry and special coordinates.

Before we present the LBES for structured and unstructured meshes, a discussion of selected existing elliptic mesh enhancement methods is given in Chapter 7. They are shown to be derivable from our general perspective. This places the LBES in historical perspective.

Chapter 8 presents the implementation and results for applying the LBES to structured meshes, while Chapter 9 does so for unstructured mesh enhancement. For structured meshes, the LBES results are compared with several existing elliptic results. For unstructured meshes, the finite element method is used to solve the LBES. Results are presented for two- and three-dimensional meshes.

Topics omitted as falling beyond the goals of the monograph include

- parallel processing
- parallel mesh decomposition algorithms
- data structures for unstructured meshes
- application-specific criteria defining “mesh quality”
- solution-adaptive mesh enhancement methods

- embedding solution features into the mesh

The authors are indebted to many who made the development of this material possible. First, we wish to thank the ASC Program at Los Alamos National Laboratory for supporting this work and motivating the development of more effective approaches at mesh enhancement. We wish to acknowledge the Setup Team and its customer base for their roles in the development of this material, which ranged from providing customer requirements to contributing technical and application details, algorithms, assorted codes, and often detailed insight into various problems that were encountered. We specifically thank Alan Stagg, William Hachfeld, and Ahmed Khamayseh for their many contributions, including the *Altair* grid generation capability, the Modified Interpolated Control Function grid enhancement method, impedance matching, element Jacobian development, and countless other approaches and algorithms that they contributed to the Setup Project. We also thank Doran Greening and Randy Bos who motivated the development of several approaches considered here; contributing ideas, algorithms, and theoretical development to this effort, and who spent many hours in the advancement of these approaches. We finally wish to thank Will Dearholt who read early drafts of the manuscript and provided valuable feedback on its improvement.

Ultimately, it is our desire that this monograph will be a useful addition to the mesh generation and enhancement literature and its methods used to enhance meshes of broad application.

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