A discourse on variational and geometric aspects of stability of discretizations

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Abstract

These lectures are devoted to variational and geometrical aspects of stable discretizations for Partial Differential Equations problems.

Variational principles have been in the arsenal of finite element methods since their inception in the early fifties. They are a powerful tool for stability and error analysis, and indeed, variational principles have remained unsurpassed in their ability to generate sharp error estimates. One of the main reasons for the tremendous success of variational methods lies in the fundamental connection that exists between variational principles, on one hand and optimization problems and the structure of PDE's on the other hand.

Differential complexes serve to provide another tool that can be used to encode PDE structure. Differential forms model global quantities rather than fields, and in many ways their formalism is closer to the first principles used to describe physical phenomena. Two decades ago Bossavit pointed out that differential forms can and should be used to analyze and develop discretizations that mimic the topological structure of the underlying PDE. This viewpoint proved to be the key to successful application of finite element methods in electromagnetics.

Since then there has been an increased interest in the use of such *geometrical* methods for the discretization of PDE's. The main goal of these lectures is to show how variational and geometric approaches can complement each other in the quest for accurate and stable discretizations.

We begin with a review of basic facts about variational methods and take time to consider three special cases of variational settings. Then we provide examples of finite element methods in each setting and discuss their stability. In particular, we show how variational principles associated with a given PDE are propagated to the discrete problems, thus forming the basis of the *variational approach* to stability of discretizations.

The lectures contain a necessarily brief introduction into the elements of differential forms calculus. After these preliminaries we embark on a mission to apply this formalism to describe topological structure of PDE problems. We choose the Kelvin

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principle as a model problem and derive factorization diagrams for the associated first-order optimality system. Using these diagrams we define *compatible* discretizations of the PDE equation and show how the structure encoded in the factorization diagram is being propagated through a wide range of different discretizations, thus forming the basis of the *geometrical approach* to stability of discretizations.

The last part of these lectures highlights the fundamental connection between geometrical structure of PDEs and variational characterizations of their stable discretizations. Our examples are based on the grid decomposition property and the commuting diagram property for the Kelvin principle.

We conclude with examples of alternative discretization methods that are capable of circumventing the rigid constraints imposed by geometrical structures upon finite dimensional representations of PDEs and explain why such methods are useful.

1 Introduction

Partial Differential Equations (PDE) are a fundamental modeling tool in science and engineering. Their applications range from design and modeling of semiconductor devices to global climate simulations. As a result, approximate numerical solution of PDE's is a task of tremendous practical importance.

A numerical solution of a PDE problem, which we will write symbolically as

$$\mathcal{L}U = F \tag{1}$$

involves two principal ingredients:

> a *discretization* step, wherein the continuous problem is replaced by a finite dimensional algebraic equation

$$\mathcal{L}^h U^h = F^h \tag{2}$$

and

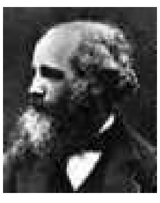
> a *solution* step, wherein the algebraic problem (2) is solved either by a direct or an iterative solution method.

In (2) we follow the accepted custom of using h to denote a small positive parameter whose reciprocal h^{-1} is related to the dimension of the space where U^h is sought.

In these lecture notes our main focus will be on the first, discretization step and the three dominant paradigms that exist in the construction of (2):

- finite element methods where *projection* or *quasi-projection* principles are restricted to finite dimensional subspaces;
- finite difference methods where *differential operators* are approximated by algebraic operators;
- finite volume methods where *integral fluxes* are approximated by quadrature.

While both ingredients are vital to the success of computer simulations, it is the discretization step that ultimately holds the key to all fundamental properties, both desirable and undesirable, of any numerical method for PDE's. Our main goal will be to explain why some discretization choices work well, while some other perform poorly or lead to downright disasters. Such an undertaking cannot be accomplished without a keen appreciation of the mathematical structure of the PDE. This structure governs well-posedness of the PDE and reflects intrinsic properties of the physical phenomena that are being modeled, e.g., conservation laws, solution symmetries, positivity, and maximum principles. Importance of well-posedness has been noted long before the dawn of the computer age by Maxwell who in 1873 wrote[3]



There are certain classes of phenomena, as I have said, in which a small error in the data only introduces a small error in the result. Such are, among others, the larger phenomena of the Solar System, and those in which the more elementary laws in Dynamics contribute the greater part of the result. The course of events in these cases is stable.

[3] J. C. Maxwell. *Does the progress of Physical Science tend to give any advantage to the opinion of Necessity (or Determinism) over that of the Contingency of Events and the Freedom of the Will?* in [64, pp.434-463].