MATHEMATICAL AND NUMERICAL ANALYSIS OF SOME PARAMETER-DEPENDENT MODELS

— A SUMMARY OF MY RECENT WORK

SHENG ZHANG

1. A general formulation of the problems

Much of my recent work is on mathematical models that fit in a general form. In this section, I describe this form and list the problems related to my work as examples. In many dimensionally-reduced models for the deformation of a thin elastic body—including the Timoshenko beam, the Reissner–Mindlin plate, and the Koiter and Naghdi shell models—the solution can be characterized variationally as the minimizer over an appropriate Hilbert space of a strain energy expression formed as a combination of separate terms (representing energy due to bending, membrane, or transverse shear deformation) which scale differently with respect to the thickness of the body. Many other parameter-dependent variational problems, such as problems of anisotropic heat conduction, nearly incompressible elasticity, domain embedding methods for Dirichlet/Neumann boundary value problems based on penalty/regularization, regularization of some ill-posed PDE boundary value problems on singular domains, and numerous other singular and regular perturbation also involve minimization of an energy with differently scaled terms. All these problems can be put in the general form (1.1): given $f \in H^*$, the dual space of a Hilbert space H, and $\epsilon > 0$, find $u^\epsilon \in H$, such that

$$\epsilon^2 (Au^\epsilon, Av)_U + (Bu^\epsilon, Bv)_V = \langle f, v\rangle \quad \forall\, v \in H. \tag{1.1}$$

Here A and B are continuous linear operators from H to Hilbert spaces U and V, respectively, and $B(H)$, the range of B, is dense in V. For all the aforementioned examples, it can be proved that there exist constants C_1 and C_2 such that

$$C_1 \|u\|_H \le \|Au\|_U + \|Bu\|_V \le C_2 \|u\|_H \quad \forall\, u \in H,$$

so that (1.1) has a unique solution $u^\epsilon \in H$ for all $f \in H^*$ and $\epsilon > 0$. The dependence of u^ϵ on ϵ when $\epsilon \to 0$ is quite complicated, and the behavior of u^ϵ could be drastically different depending on the space H, the space V, the operator B, and the functional f. The various behaviors of u^ϵ can be classified into five cases mainly depending on whether $f|_{\ker B} = 0$

Department of Mathematics, Wayne State University, Detroit, MI 48202, `sheng@math.wayne.edu`.

and whether $B(H) = V$. Some of the key features are as follows. If $f|_{\ker B} \neq 0$, then u^ϵ blows up in H at the rate $\mathcal{O}(\epsilon^{-2})$, and $\epsilon^2 u^\epsilon$ converges to a finite limit in H. If $f|_{\ker B} = 0$, then u^ϵ itself converges in H if $B(H) = V$. In this case, if $B(H) \neq V$ then u^ϵ converges in a weak norm if $f \in B^*(V^*)$, or u^ϵ converges in an even weaker norm if $f \notin B^*(V^*)$. The condition $B(H) = V$ distinguishes regular perturbation problems from singular perturbation problems. The five cases, and examples in each case, are listed below. The elusiveness of the behaviors of u^ϵ increases in this order. Most of these examples are related to my work, and some of them were put to their positions in the list by my work.

1. $B(H) = V$ and $f|_{\ker B} \neq 0$: Bending dominated Timoshenko beams, bending dominated Koiter and Naghdi arches, penalty based domain embedding for Dirichlet problems in which the complement of the original domain in the fictitious domain is Lipschitz, and nearly incompressible elasticity.
2. $B(H) = V$ and $f|_{\ker B} = 0$: Shear dominated Timoshenko beams, membrane dominated Koiter arches, membrane-shear dominated Naghdi arches, regularization based domain embedding methods for Neumann problems defined on Lipschitz domains.
3. $B(H) \neq V$ and $f|_{\ker B} \neq 0$: Bending dominated Reissner–Mindlin plates, bending dominated Koiter and Naghdi shells, hot-state anisotropic heat conduction, penalty based domain embedding for Dirichlet problems in which the complement of the original domain in the fictitious domain is not Lipschitz.
4. $B(H) \neq V$, $f|_{\ker B} = 0$, and $f \in B^*(V^*)$: Shear dominated Reissner–Mindlin plates, membrane dominated Koiter shells, membrane-shear dominated Naghdi shells, cool-state anisotropic heat conduction, regularization based domain embedding for Neumann problems defined on non-Lipschitz domains, and general domain regularization.
5. $B(H) \neq V$, $f|_{\ker B} = 0$, and $f \notin B^*(V^*)$: Reissner–Mindlin plates subject to stress boundary conditions with a dominating twisting moment that does not induce pure bending, intermediate Koiter and Naghdi shells, regularization of ill-posed boundary value problems on singular domains, and numerous singular perturbation problems. The problem could be as simple as $-\epsilon^2 D^2 u^\epsilon + u^\epsilon = f$ with $u^\epsilon \in H^1_0(0,1)$ and $f \notin L^2(0,1)$, or as hard as the Scordelis-Lo roof whose solution behaves like a “monster”.

In the above examples, the beam, arch, plate, and shell models are approximations to the three-dimensional elasticity theory. A fundamental question with these models is about their accuracy compared with the theory of elasticity. I have made some contributions to clarifying the situation around this question, and I am continuously working in this direction.

Numerical analysis of these models is an active and fast progressing field, which is full of challenges and open problems, especially for shells. This is a field to which I have devoted some efforts in recent years, and is the main direction of my current work.

Domain embedding method yields approximations to boundary value problems on complex domains. There is some problems about the accuracy of these approximations, and about the efficiency of numerical schemes based them. I have devoted some work to this method.

I derived sharp estimates on the behavior of u^ϵ, the solution of (1.1), on an abstract level. These estimates actually play a central role in much of my work and my thinking. Applying these estimates to specific problems yielded a number of new results. It continues to serve as a guide for me to understand some more difficult problems, like shells. I describe these in the following sections, in which all the comments on my work are quoted from paper referee reports, NSF proposal reviewer reports, NSF panel reports, or the MathSciNet. I also use some statements and conclusions in the literature in the background descriptions of my work, without explicitly citing their authors.

2. Estimates on u^ϵ on an abstract level [1]

In analyzing the asymptotic behaviors of solutions of parameter-dependent equations of the form (1.1), the most widely used method is based on weak convergence. The method was developed by the Lions school and has been extensively used in plate and shell analysis, and in the theory of domain embedding methods. The method is very powerful and very general (it solves problems that do not fit in the form of (1.1)), but not easy to apply, and requires several steps to reach a conclusion. In [1] I established two sharp (equivalent) estimates on the solution of (1.1) in terms of interpolation spaces, dealing with the asymptotic behavior of u^ϵ that falls into case 4 or 5, respectively. However, these estimates easily yield sharp and stronger estimates for behaviors of u^ϵ in the other three cases.

In this way, I established sharp estimates on the behaviors of Timoshenko beam, Naghdi arch, and domain embedding solutions of boundary value problems defined on Lipschitz domains. These behaviors fall in cases 1 and 2. These estimates furnish the basis for my investigation of these models. Sharp estimates on the Reissner–Mindlin plate model are also obtained in this way, the behaviors of which could fall into case 3, 4, or 5. The results play an important role in my investigation in the Reissner–Mindlin plate model. Application of the estimates to shells leads to estimates that accurately capture the asymptotic behaviors of shell solutions in all cases. Particularly, they clearly reveal that even in the intermediate case the shell model solution converges to a limit at a rate that is related to the classification index of an intermediate shell, in a weak norm. This was a situation not clear before. This led me to conceive a method to deal with the intermediate shells.

3. On Timoshenko beam and Naghdi arch models [2]

Timoshenko beam model and its generalization to arches are widely used in engineering computations and have been extensively analyzed in the literature. However, there are important issues regarding these models that have been left open: The forms of these models have not been completely determined; The relative merits of these models comparing to the more classical fourth order beam or arch bending model have not been clarified. The variety of forms of each of these models are not always asymptotically consistent with each other. Without the correct choice of the form of a model, any numerical scheme, not matter how accurate it is to the model, would not be able to produce the desired results.

Using the sharp estimates obtained from those in [1], I can clearly see the inconsistency in the different forms of the Naghdi type arch model, of which Timoshenko beam is a special case. Which form of the model is the right one is a question that can only be answered by comparing it with the three-dimensional elasticity theory. In [2], I presented a theory that completely resolved all the uncertainties regarding the beam and arch models. The background of the paper is best described in one of the paper referee's reports: "The paper develops a dimensionally reduced model of an elastic arch with rectangular cross section and arbitrary central curve. The model is of Naghdi type, encorporating bending, membrane, and transverse shear effects. Such models are well-known, but appear in various variations, justified by a variety of ad hoc arguments. In particular the infamous shear correction coefficient has been introduced in various ways through various arguments, but there has been no agreement on what its correct value is, or whether it matters. This is particularly complicated by the fact that the arch allows different asymptotic regimes (bending dominated and membrane/shear dominated), and asymptotic arguments made for one regime may not be legitimate for the other." The referee wrote that "The present paper uses rigorous analysis to bring clarity to this situation. It shows that in the shear-dominated case, where the use of such Naghdi models is justified, the shear correction factor should not be used (or should be set equal to one), otherwise the method does not converge to the solution of the 3D elasticity model, while in the bending dominated case it doesn't matter asymptotically what value is used. This is a valuable and original contribution." "The analysis, while complicated, is clear and carefully presented, using a nice mix of variational and asymptotic techniques." Another referee commented on the method I used: "This paper presents some very interesting results regarding the distance between arch solutions and the corresponding 3D solutions, in particular in the energy norm." "These error estimates are obtained by a clever construction of statically/kinematically admissible fields allowing to use the Prager–Synge theorem, while some necessary corrector terms near the arch ends are handled using (a rigorous form of) the Saint-Venant's principle."

The behaviors of Timoshenko beam, Naghdi, and Koiter arch models fall into either the case 1 or 2. The theory [2] proved the validity of these models in both the two cases, with the shear correction factor being set to 1. It is a peculiar feature for these models to have a closed-ranged B operator, thus fall into the simplest two cases. Thanks to this feature, the theory is complete. We shall see that such a status can not be achieved for the Reissner–Mindlin plate. The situation is much worse for shells.

4. On Kirchhoff–Love and Reissner–Mindlin plate models [3, 4, 5]

It has long been a question whether the Reissner–Mindlin plate bending model is more accurate than the Kirchhoff–Love model, and what is the best value of a shear correction factor in the Reissner–Mindlin. In [3], together with D.N. Arnold and A.L. Madureira, we, for the first time, proved that when a plate is totally clamped the Reissner–Mindlin has a wider range of applicability than the Kirchhoff–Love: When a dominant shear is involved in the plate deformation, the Reissner–Mindlin is accurate while the Kirchhoff–Love fails. Since the clamping boundary condition was assumed, this paper does not address a problem that is very important to the Reissner–Mindlin plate model. It is about its ability of resolving the twisting moment applied on the plate boundary. Twisting moment is one of the three Poisson resultants, which is suppressed by the Kirchhoff contraction in reducing the three conditions to the two Kirchhoff resultants. Reissner–Mindlin plate model was originally conceived as a result of efforts to directly incorporate the twisting moment in the model. The problem is whether the Reissner–Mindlin indeed has the ability to resolve the twisting moment. Another problem with this paper is about the shear correction factor. To accommodate the well-known value of 5/6 for this factor, the resultant loading functional in the Reissner–Mindlin model in [3] is forced to have a messy expression hardly explainable in terms of mechanical terminologies.

Motivated by these considerations, I wrote the paper [4], which addresses the form and accuracy problems of the Reissner–Mindlin plate model when a plate is subjected to stress boundary conditions. A striking difference between the stress boundary condition and clamping boundary condition is that solution of the former could fall into three cases: bending dominated (case 3), shear dominated (case 4), or intermediate (case 5), while solution of the latter only falls into case 3 or 4. Using the sharp estimates that follow from those in [1], I proved that in the bending dominated case, Reissner–Mindlin and Kirchhoff–Love have the same order of accuracies; In the shear dominated case, Kirchhoff–Love is totally useless and Reissner–Mindlin is accurate if one sets the shear correction factor to 1 (with the resultant loading functional being the standard); In the intermediate case, which tests the ability of a model in resolving the twisting moment, Kirchhoff–Love is useless but Reissner–Mindlin is not consistent with the 3D elasticity either, asymptotically. The latter is a negative statement on the Reissner–Mindlin's fulfilling its original goal — resolving the twisting moment. The paper was regarded as "very valuable" by the journal referee. In the Math Reviews (MathSciNet), the reviewer said that the paper "involves a surprising result of Zhang regarding the shear correction factor. He shows that the widely accepted value of 5/6 should be actually replaced by 1, otherwise Reissner-Mindlin fails to converge in the transverse shear dominated regime." And "This is an interesting paper that must be read by anyone interested in modeling plates and shells."

The inconsistency between the Reissner–Mindlin and the 3D elasticity in the intermediate case shows that the theory of Reissner–Mindlin plate model can not be as complete as that of Timoshenko beam and Naghdi arch models. This discovery has a very negative impact on my confidence in the theory of Naghdi and Koiter shell models. If it is an exceptional case for the Reissner–Mindlin solution to fall in to the intermediate case, it is a general rule for shell solutions to fall into this case. For general shells, the Naghdi and Koiter models have been justified in the bending and membrane/shear dominated cases in the literature, and (lower) convergence rates have been established. We can also prove that the best value for the shear correction factor in the Naghdi model is 1, which is solely determined by the shell behavior in the membrane-shear dominated regime. (This requires a systematic modification of my thesis [9].) However, it seems that there is no decisive conclusion about the validity of Naghdi or Koiter shell model in the intermediate case. The negative result on the Reissner–Mindlin suggests that these models are unlikely valid approximations to the 3D elasticity if their solutions fall into the intermediate regime.

Based on all the above, one may conclude that the theory of mathematical modelling is complete for beams and arches, it is almost complete (or slightly open) for plates, and it is still wide open for shells. I shall come back to this problem from time to time in my future work.

In case a plate is polygonal and simply supported on its boundary, the Kirchhoff-Love model is equivalent to a biharmonic boundary value problem. The latter can be decoupled to two Poisson equations and solved by Poisson solvers. With Zhimin Zhang, we proved a negative result claiming the invalidity of this method when the plate is not convex [5].

5. Domain embedding methods [6, 7, 8]

This is a strategy of numerical computations that takes advantages of fast numerical solvers developed only for special domains, FFT for Poisson equation on rectangles, for example. A major step in domain embedding is (approximately) replacing the original boundary value problem by one defined on a larger, fictitious, say, rectangular, domain. A class of domain embedding methods, namely penalty for Dirichlet problems and regularization for Neumann or Robin problems, can be put in the form of (1.1). Depending on the type of boundary conditions and regularity of the original domain, the behaviors of the domain embedding solution could run through all the five cases listed at the beginning of this summary. We can establish sharp estimates for all the possible behaviors. In [8], I reported my results of estimates on the solution of domain embedding methods under the assumption that the original domain boundary is Lipschitz. This mild assumption confines the behavior of the domain embedding solutions in the simplest case 1 (for Dirichlet problems) or 2 (for Neumann and Robin problems). The estimates are all sharp, and better than what one finds in the key references in this field. Since the parameter (ϵ) severely affects the condition number of the matrix resulting from discretization of the domain embedding formulations, the sharp estimates are valuable in that they provide crucial information for one to optimize the overall cost of a numerical method based on domain embedding. Domain embedding for mixed boundary value problems, however, imposes new challenges. The formulation involves two parameters, one is small and the other large. It does not fit in the form of (1.1). I generalized the results of [1] to handle such a situation, and obtained sharp estimates on the rate of convergence for mixed boundary value problems as well. The result was announced in [6], which was presented by Professor Roland Glowinski who is the leader in this field.

The domain embedding formulations only furnish a basis for numerical methods. In [7], I derived error estimates for finite element discretization of these domain embedding equations. The fictitious rectangular domain is partitioned by uniform meshes. The straightforward discretization achieves the full accuracy for Neumann and Robin problems. For Dirichlet problems, however, there is a locking phenomena that needs to be addressed. It turns out that a local mesh adjustment around the original domain boundary completely unlock the numerical scheme and achieves full accuracy when the original domain is convex. If the domain is not convex, the accuracy is a little lower. The latter result crucially depends on the sharp estimates established in [6, 8].

Domain embedding methods can be put under the general theme of regularization of rough domains, on which I plan to write a report.

6. Numerical analysis of shells and some work in progress

Numerical analysis of beams, arches, plates, and shells is a major part of computational mathematics and scientific computing. For beams, arches, and plates there are many efficient methods sitting on solid mathematical foundations, and new methods continuously appear. For shells, despite decades of efforts and much progress, the theory of numerical analysis is, however, still far from satisfactory. “In contrast to plates, the theory of shells is still in-mature. There is no provably reliable numerical method yet for shells, particularly one that would work in the three possible regimes, bending-dominated, membrane-dominated or intermediate.” Partially, this is because (quote from NSF reviewer reports on my proposal) “the behavior of shells, particularly intermediate shells, have been elusive even to the most prominent numerical analysts in the field.” “Mathematically, the simulation of thin shells is a very challenging problem, and progress towards efficient methods would have large impact in the mathematical and engineering sciences.”

My current work attempts to make some contribution to the shell numerical analysis. The work is supported by the NSF because its panel review sees that I am “in a good position to understand the delicacies involved in modeling shells and in developing related numerical methods.” And I “have the best ideas that the reviewers have seen for attacking the intermediate regime”.

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