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ANALYTIC ACCURACY ANALYSIS FOR UNSTRUCTURED MESH FINITE VOLUME METHODS WITH APPLICATION TO AERODYNAMIC SIMULATIONS

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The long-term objective of the research program of which this project was a part is to provide prescriptive guidance for generating meshes for full aircraft configurations that will reduce solution error for a given number of degrees of freedom compared with meshes generated using today's best practices. To achieve this goal, we must be able to identify features in unstructured meshes that have an adverse effect on solution quality for commonly used numerical methods for computational aerodynamics and we must develop techniques to modify meshes to reduce those effects. During the term of this sponsored project, we completed the first step: identifying mesh features that negatively impact the accuracy of common discretization schemes, including identifying which discretization approaches are particularly sensitive to variations in mesh properties.

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Analytic Accuracy Analysis for Unstructured Mesh Finite Volume Methods, with Application to Aerodynamic Simulations
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Carl Ollivier-Gooch
The University of British Columbia*

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The long-term objective of the research program of which this project was a part is to provide prescriptive guidance for generating meshes for full aircraft configurations that will reduce solution error for a given number of degrees of freedom compared with meshes generated using today's best practices. To achieve this goal, we must be able to identify features in unstructured meshes that have an adverse effect on solution quality for commonly used numerical methods for computational aerodynamics and we must develop techniques to modify meshes to reduce those effects. During the term of this sponsored project, we proposed to take the first step: identifying mesh features that negatively impact the accuracy of common discretization schemes, including identifying which discretization approaches are particularly sensitive to variations in mesh properties.

This report summarizes the work completed during the term of this award. Full details can be found in the publications cited; any that are not readily available online can be obtained by contacting the PI.

1 Truncation Error Analysis

To quantify the interactions between mesh and solution scheme, we relied on analytic accuracy analysis of the truncation error, which is defined as the difference between the continuous partial differential operator and its discrete equivalent. Analysis of truncation error for structured meshes is based on Taylor series analysis. This analysis approach, which is applicable to finite difference, finite volume, and finite element methods alike, is based on the underlying assumption that the solution is smooth and therefore well represented locally by a Taylor series expansion. This assumption is a property of the solution, not the mesh, and so the approach should extend to unstructured meshes. This section gives a brief outline of how this can be done for finite volume methods. For simplicity and compactness, discussion here will focus on linear model problems in two dimensions, which can be written as

$$\frac{\partial U}{\partial t} + \mathcal{L}(U) = 0,$$

where $\mathcal{L}(U)$ is some linear spatial operator that an be written in flux divergence form: $\mathcal{L}(U) = \nabla \cdot \vec{F}$. This PDE can be discretized in space using the finite volume method and written as

$$\frac{d\overline{U}_i}{dt} = -\frac{1}{A_i}\oint_i \vec{F} \cdot \hat{n}\, dl \tag{1}$$

where $\overline{U}_i$ is the control volume average of the solution in control volume i, and the right-hand side of the equation is the discrete flux integral around the two-dimensional control volume. The computation of the flux integral is the key step in determining spatial accuracy for finite volume methods; regardless of the

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order of accuracy of the scheme, the flux integration process produces a linear combination of control volume averages:

$$\frac{d\overline{U}_i}{dt} = -\sum_j a_{ij}\overline{U}_j \tag{2}$$

The coefficients a_{ij} are the entries of the global flux Jacobian matrix and will depend on both the problem and the discretization scheme. However — for a linear problem — the a_{ij} are strictly geometric terms and therefore depend only the mesh topology and geometry in the neighborhood of control volume i. In a structured mesh context, this sum would be readily recognizable as a collection of discrete spatial derivatives. For unstructured meshes, the sum is again a collection of discrete spatial derivatives, but much less easily recognizable, especially for general stencils or for higher-order schemes.

To determine the spatial accuracy of the scheme, we must evaluate how accurately the sum in Equation 2 approximates the control volume average of the linear operator $\mathcal{L}(U)$ over control volume i:

$$\mathrm{TE}_i = \frac{1}{A_i}\iint_i \mathcal{L}(U)\, dA - \sum_j a_{ij}\overline{U}_j. \tag{3}$$

As written, the truncation error is a combination of differential and discrete terms. These can both be written in terms of derivatives of the solution at the reference location $\vec{x}_i$ for control volume i.[1]

To begin this process, we write the control volume average $\overline{\phi}_i$ of a smooth function ϕ as

$$\begin{aligned}\overline{\phi}_j \equiv \frac{1}{A_j}\int_j \phi(\vec{x}-\vec{x}_i)\,dA \quad &= \quad \phi|_i + \left.\frac{\partial\phi}{\partial x}\right|_i \widehat{x}_{ij} + \left.\frac{\partial\phi}{\partial y}\right|_i \widehat{y}_{ij} \\ &\quad + \left.\frac{\partial^2\phi}{\partial x^2}\right|_i \frac{\widehat{x^2}_{ij}}{2} + \left.\frac{\partial^2\phi}{\partial x\,\partial y}\right|_i \widehat{xy}_{ij} + \left.\frac{\partial^2\phi}{\partial y^2}\right|_i \frac{\widehat{y^2}_{ij}}{2} + \cdots \end{aligned} \tag{4}$$

where the geometric terms in this equation are of the general form

$$\begin{aligned}\widehat{x^n y^m}_{ij} \quad &\equiv \quad \frac{1}{A_j}\int_j \left((x-x_j)+(x_j-x_i)\right)^n \cdot \left((y-y_j)+(y_j-y_i)\right)^m \, dA \\ &= \quad \sum_{l=0}^{m}\sum_{k=0}^{n} \frac{m!}{l!\,(m-l)!}\frac{n!}{(n-k)!}\left(x_j-x_i\right)^k \cdot \left(y_j-y_i\right)^l \cdot \overline{x^{n-k}y^{m-l}}_j\end{aligned}$$

This general form can be used directly to replace the control volume averages $\overline{U}_j$ in Equation 3 with a linear combination of derivatives of the solution at $\vec{x}_i$. For the control volume average of the linear operator, we simplify the general case to give a control volume average in i:

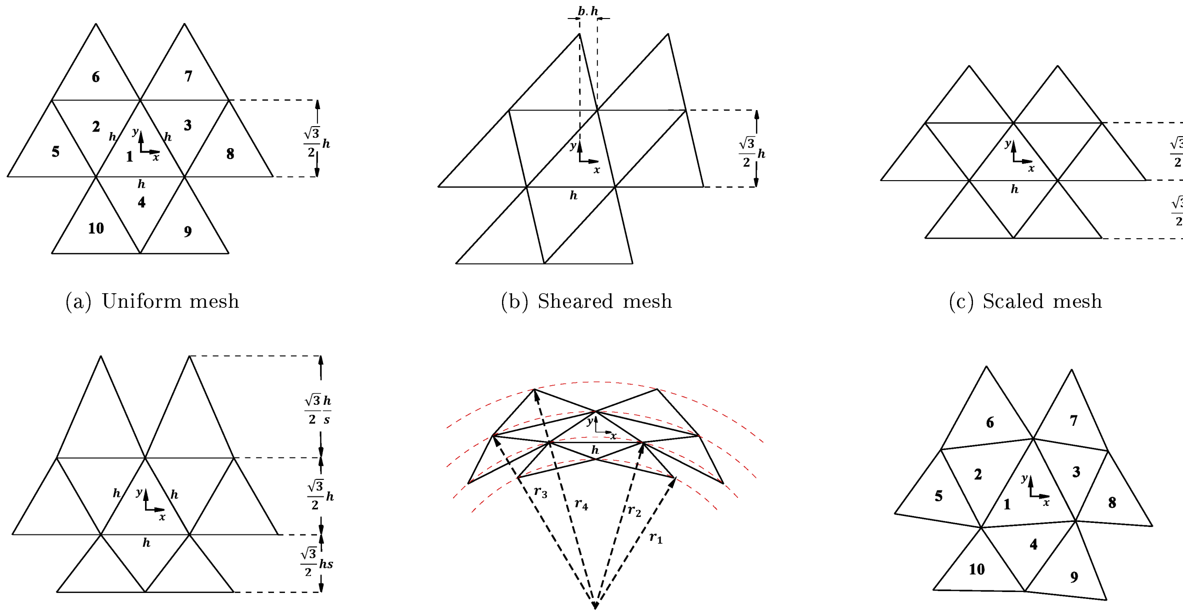
$$\begin{aligned}\overline{\phi}_i \equiv \frac{1}{A_i}\int_i \phi(\vec{x}-\vec{x}_i)\,dA \quad &= \quad \phi|_i + \left.\frac{\partial\phi}{\partial x}\right|_i \overline{x}_i + \left.\frac{\partial\phi}{\partial y}\right|_i \overline{y}_i \\ &\quad + \left.\frac{\partial^2\phi}{\partial x^2}\right|_i \frac{\overline{x^2}_i}{2} + \left.\frac{\partial^2\phi}{\partial x\,\partial y}\right|_i \overline{xy}_i + \left.\frac{\partial^2\phi}{\partial y^2}\right|_i \frac{\overline{y^2}_i}{2} + \cdots \end{aligned} \tag{5}$$

Equation 5 can be applied to each of the terms in $\mathcal{L}(U)$ to evaluate the integral term in the truncation error.

1.1 Interior Schemes

We have applied this approach to study the interaction between mesh quality and solution discretization schemes for several model problems. Our initial work focused on diffusion operators, because of the wide range of schemes in common use for such problems [6, 5]. We used the mesh fragments shown in Figure 1 to test the sensitivity of different discretization schemes to deviations from a perfect, uniform, equilateral triangular mesh, using cell-centered control volumes. Our results showed that least-squares reconstruction produces more accurate solution gradients — and therefore more accurate diffusive fluxes — compared with

[1] Typically, the vertex for a vertex-centered scheme or the cell centroid for a cell-centered scheme.



(a) Uniform mesh (b) Sheared mesh (c) Scaled mesh

(d) Stretched mesh (e) Curved mesh (f) Randomly perturbed mesh

Figure 1: Uniform and distorted meshes for analytic tests.

Green-Gauss gradient calculations on meshes with any nonuniformity. Also, we found that, when using second-order linear reconstruction, flux integrals were second order accurate only on uniform meshes. For sheared and scaled meshes, the flux integrals were first-order accurate, and for our stretched, curved, and randomly perturbed test meshes, the flux integrals were zero order accurate. These results are consistent with other work in the literature (for instance, [2, 3]) and also with our subsequent numerical experiments on full-scale unstructured meshes. We also found that averaging the cell gradients based on cell volume when computing a single face gradient for the flux is consistently significantly less accurate than using either arithmetic averaging or weighting each cell's gradient with the other cell's size.[2] Including Nishikawa's jump term [10], designed to account for the difference in the two reconstructed solution values at the face, in the flux also improves accuracy, regardless of mesh type. Unsurprisingly, we found that the optimal value for the free coefficient in the jump term formulation is different for unstructured meshes than the value Nishikawa recommends for sturctured meshes. This work was later extended to vertex centered control volumes, with similar results [17].

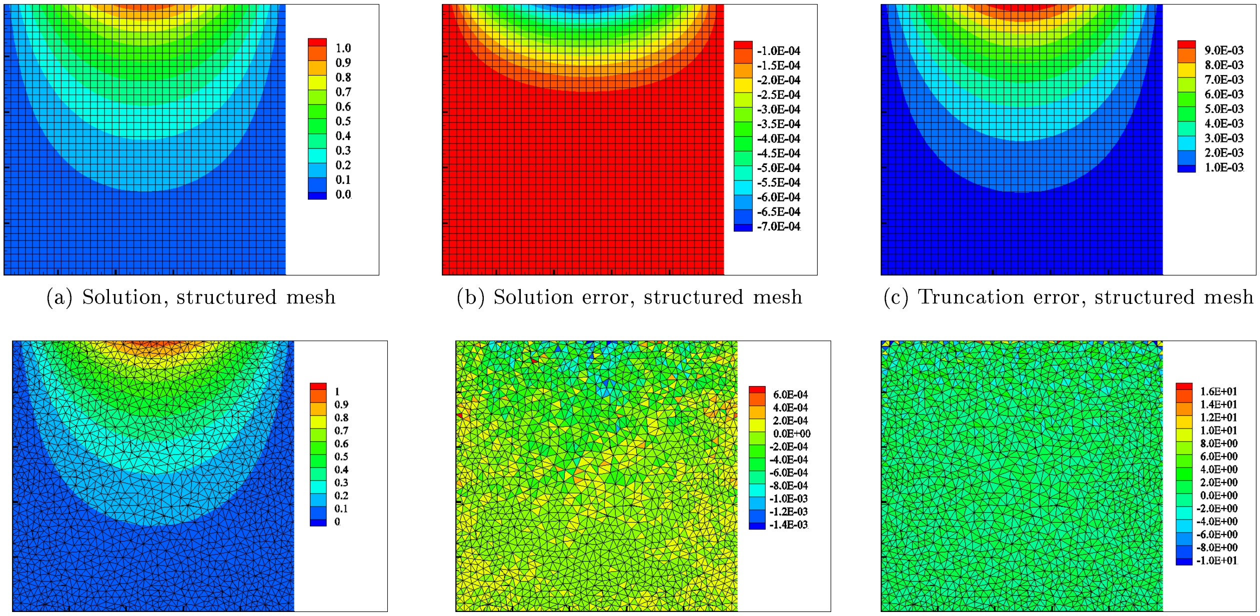
We extended this analysis to advection problems, both the linear advection equation and Burgers' equation [5, 7]. Because Burgers' equation is nonlinear, the truncation error includes not only terms like $u_{x_i x_j}$ but also its cousins $u_{x_i} u_{x_j}$ and $u u_{x_i x_j}$, where the indices i and j indicate coordinate direction. For these problems, our primary interest was in comparing the accuracy of upwind and centered flux formulations. Our results showed that, for realistic unstructured meshes, there is no statistically significant difference in truncation error between these schemes.

For non-linear problems more complex that Burgers' equation, the task of identifying all the terms in the truncation error expansion and sorting out their effects in numerical experiments becomes infeasible. Rather than wasting effort by continuing to try to solve an intractable problem, we turned our attention instead to using our truncation error estimates to improve solution error, as I will describe in Section 2.

1.2 Boundary Condition Enforcement

Our experience showed us that the largest truncation error typically occurs at or near the domain boundary because of asymmetry in stencils there, so we turned our attention to error analysis near boundaries and on

[2]The latter is equivalent to linear interpolation of the gradient in the direction perpendicular to the face.



(a) Solution, structured mesh

(b) Solution error, structured mesh

(c) Truncation error, structured mesh

(d) Solution, unstructured mesh

(e) Solution error, unstructured mesh

(f) Truncation error, unstructured mesh

Figure 2: Error comparison for structured versus unstructured meshes for a simple Poisson test case.

mixed element meshes [12, 11]. We found that the truncation error near the boundary is strongly dependent on the boundary condition implementation. Our tests used a manufactured solution, projected onto the mesh by control volume averaging, and Dirichlet boundary conditions. The weakest boundary condition implementation we used simply performed least-squares reconstruction as normal in boundary cells and computed a flux based on the gradient. This scheme uses no direct information about the boundary condition, and performs poorly even for this simple flux integral test. Adding constraints to enforce the boundary condition at flux quadrature points along the boundary gives a strong boundary condition and reduces truncation error by about a factor of two. Better still is to return to the weak implementation but add to the boundary flux a Nishikawa-style jump term that accounts for the difference between the reconstructed solution and the physical boundary condition; using the same jump term coefficient as in the interior of the domain reduces error by about a factor of four compared with the strong BC, while a separate jump coefficient for only the boundary faces can be tuned to reduce error by a further factor of about 1.5. These trends also apply at the interface between quadrilateral and triangular mesh regions.

1.3 Eigenanalysis of Error

Error analysis for unstructured mesh finite volume methods reveals two key differences between error on structured versus unstructured meshes. First, for a structured mesh solution with error of order p, the truncation error is also order p, whereas a unstructured mesh solution of the same order will have truncation error of order $p-d$, where d is the highest number of derivatives in the governing partial differential equation. Second, the structured mesh truncation error is smooth, whereas the unstructured mesh truncation error is extremely noisy. Both of these features are illustrated in Figure 2. The reason that unstructured mesh truncation error is asymptotically larger than the discretization error is relatively well-known: mesh irregularities prevent any cancellation of error from occurring. When this project began, to our knowledge, there was no rigorous explanation of why the discretization error is asymptotically smaller than the truncation error. We were able to accomplish this by applying eigenanalysis [14, 8, 9] to the generalized error transport equation in discrete form [13]:

$$\frac{\partial R}{\partial U}\varepsilon = \tau$$

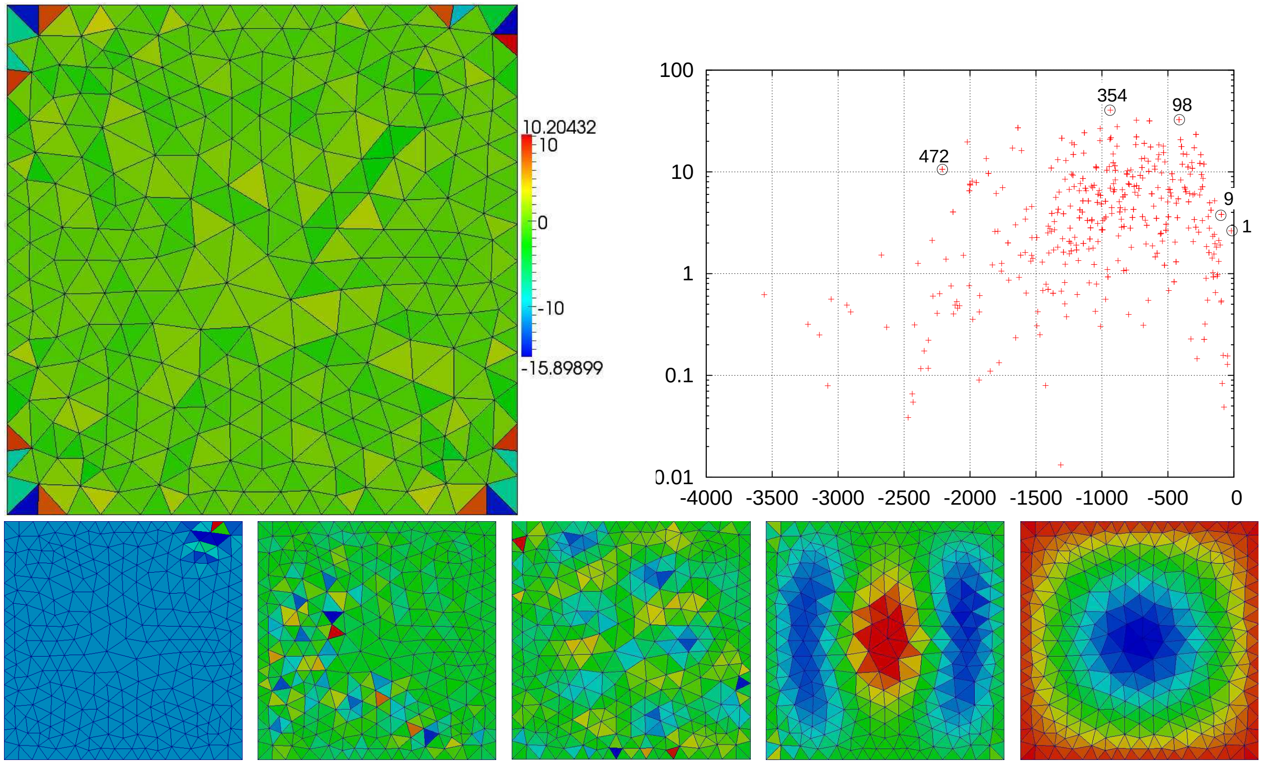


Figure 3: Truncation error for a Poisson problem in a square. Top left: truncation error. Top right: magnitude of coefficients in the eigendecomposition. Bottom row: eigenvectors associated with the eigenvalues labeled above.

where τ is the truncation error, ε is the discretization error, and $\frac{\partial R}{\partial U}$ is the global flux Jacobian. An example eigendecomposition for the truncation error for a second-order discretization for a Poisson problem is shown in Figure 3.

If we expand substitute eigenvector decompositions of $\tau = \sum_i a_i x_i$ and $\varepsilon = \sum_i b_i x_i$, where the x_i are right eigenvectors of $\frac{\partial R}{\partial U}$, we get

$$\begin{aligned}
\frac{\partial R}{\partial U} \sum_i b_i x_i &= \sum_i a_i x_i \\
\sum_i b_i \frac{\partial R}{\partial U} x_i &= \sum_i a_i x_i \\
\sum_i b_i \lambda_i x_i &= \sum_i a_i x_i \\
b_i \lambda_i &= a_i
\end{aligned}$$

In other words, the coefficients in the eigendecomposition of the discretization error are smaller than their counterparts for the truncation error by a factor of the eigenvalue. This result holds, of course, for both structured and unstructured meshes. Unstructured mesh discretizations see an improvement in accuracy between the truncation error and discretization error because the dominant truncation error modes are rough modes, associated with eigenvalues that scale like $1/h^d$. For structured meshes, on the other hand, the dominant terms in the truncation error are smooth modes, with eigenvalues that are $\mathcal{O}(1)$. We have also been able to use eigenanalysis to explain why, in some cases, a scheme with lower truncation error produces solutions with higher discretization error [8]. As a spin-off from this eigenanalysis work, we are now beginning to study mesh impacts on solver stability by examining the behavior of the eigenvalues and attempting to systematically modify the mesh to improve stability.

2 Error Reduction for Unstructured Mesh Methods via the Error Transport Equation

Ultimately, the goal of CFD is to compute quantities of engineering interest accurately and efficiently. In computational aerodynamics, those quantities are typically integrals of boundary tractions, like lift, drag, yawing moment, etc. The current state-of-the-art for improving the accuracy of these schemes on a single mesh is adjoint methods, which are specific to the output quantity desired. There are well-known techniques for combining the truncation error for the primal problem with the solution to the adjoint problem to improve the accuracy of output quantities. This approach has been shown by many researchers to be quite successful for both steady and unsteady problems. For unsteady problems, the drawback to adjoint methods is that the adjoint problem must be integrated backwards in time, and so the primal solution must be available at all times to be able to solve the unsteady adjoint problem.

The twin disadvantages of the adjoint method, then, are its specificity to a single output quantity and the data storage challenge for the unsteady adjoint problem. To address both of these issues, we have begun work on solving the error transport equation, which computes the discretization error in the original physical problem. This approach allows us to improve the solution everywhere (freeing us to compute any output quantity more accurately) and is integrated forwards in time (making the memory requirement much smaller). We begin with a PDE written in flux divergence form:

$$\partial_t U + \nabla \cdot f(U) = S \tag{6}$$

We would like to estimate the discretization error $\varepsilon(x,t) = U(x,t) - \tilde{U}(x,t)$ where U is the exact solution of the PDE and $\tilde{U}$ is some approximate solution. Substituting into the PDE and re-arranging, we get the error transport equation:

$$\partial_t \varepsilon + \nabla \cdot (f(\varepsilon + \tilde{U}) - f(\tilde{U})) = -(\partial_t \tilde{U} + \nabla \cdot f(\tilde{U}) - S) \tag{7}$$

Note that the source term in this equation for the discretization error is the truncation error present for the approximate solution $\tilde{U}$. If f is nonlinear, the difference on the left-hand side can not be simplified, although it can be linearized. In solving the error transport equation discretely, there are three choices one must make: the order of accuracy p for the primal flow problem (Eq. 6); the order of accuracy q for the error transport equation (Eq. 7); and the order of accuracy r for the residual evaluation (right-hand side of Eq. 7).

For structured meshes, there is a relatively large amount of work on the error transport equation; for a particularly good treatment, see Banks et al [1]. The principal result is that, for problems with smooth solutions and therefore well-behaved truncation error, the order of accuracy of the corrected solution $\tilde{U} + \varepsilon$ (equivalently, the order of accuracy of the error estimate ε) is $\min(p+q, r)$. Because the computational cost for the ETE is comparable to the cost of the primal problem, this implies that, for the cost of two second-order flow solutions plus a single fourth-order residual evaluation, we can get a fourth-order solution. In practice, for linear problems defect correction methods are equivalent to the ETE solution with $p = q$.

The situation is more difficult for unstructured meshes, because the structured mesh behavior just discussed requires that the solution be smooth and that the truncation error be smooth and of the same order as the discretization error [4]. As we have seen, this is not the case for unstructured meshes, so the same results can not be expected to apply. Our experiments began with model problems on randomly non-uniform meshes in 1D. We evaluated solution and gradient data for the residual by using high-order reconstruction ($r > p$). To improve accuracy asymptotically, we must found that we had to use $q = r > p$, which resulted in order q accuracy. In other words, we had to solve the error equation to higher accuracy than the primal equation [16]. This result also holds for model problems in multiple dimensions.

For linear problems, solving the error transport equation to high order is identical to solving the primal problem to high order, and so is not worthwhile. For non-linear problems, we have shown that the steady ETE gains an advantage, in two ways. First, applying a Newton linearization of the Eq. 7 allows us, for steady problems, to solve the ETE for the cost of a single linear solve of the high-order linearized system while retaining the same asymptotic accuracy as the fully non-linear solution, provided that $2p \geq q = r$. Second, the low-order primal solution is typically more robust and faster to converge than the high-order primal solution; the combination of a low-order primal solve followed by the linearized ETE retains this robustness advantage. Overall, we see a speedup of a factor of two or more for using a low-order primal solution and the linearized ETE to compute the high-order solution compared with solving the high-order primal problem directly. These results are based on solutions to the Euler and laminar Navier-Stokes equations [15]

We are currently working to extend these results to unsteady flows. We expect that we will be able to achieve structured-like results for the time advance, because step size will at worst vary smoothly. We also expect to retain a robustness advantage compared with high-order solutions. The comparison in effort and results with unsteady adjoint methods remains to be seen.

3 Personnel Involved

Several graduate students have participated in this research. Alireza Jalali (MASc 2012) did the initial work on error analysis for interior schemes on cell-centered meshes (Sec. 1.1) as well as the impact of eigenstructure on error (Sec. 1.3).[3] On the latter topic, he was assisted by Mahkame Sharbatdar (PhD anticipated 2016). Varun Puneria (MASc 2015) performed the studies on error near boundaries (Sec. 1.2). Mr. Gary Yan, Mr. Puneria, and Mr. Jalali collaborated on the analysis of vertex-centered methods.

Gary Yan (PhD anticipated 2017) began his research work looking at Taylor series analysis for non-linear problems. Since that proved to be a blind alley, he has shifted his focus to the error transport equation.

Mr. Puneria and Mr. Yan have been funded from this project throughout their studies at UBC. Ms. Sharbatdar has been primarily funded from other sources, and Mr. Jalali has been entirely funded from other sources.

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1.

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Annual Report

Primary Contact E-mail
Contact email if there is a problem with the report.

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Primary Contact Phone Number
Contact phone number if there is a problem with the report

765-494-5130

Organization / Institution name

Purdue University

Grant/Contract Title
The full title of the funded effort.

Development and Applications of Acoustic Metamaterials with Locally Resonant Microstructures

Grant/Contract Number
AFOSR assigned control number. It must begin with "FA9550" or "F49620" or "FA2386".

FA9550-10-1-0061

Principal Investigator Name
The full name of the principal investigator on the grant or contract.

C. T. Sun

Program Manager
The AFOSR Program Manager currently assigned to the award

Byung-Lip Les Lee

Reporting Period Start Date

04/15/2011

Reporting Period End Date

04/14/2012

Abstract

An elastic metamaterial which exhibits simultaneously negative effective mass density and bulk modulus was first presented with a single unit structure made of solid materials. The doubly negative properties were achieved through a chiral microstructure that is capable of producing simultaneous translational and rotational resonances. The dynamic characteristic of the chiral metamaterial was illustrated using a representative mass-spring lattice model. The negative effective mass density and effective bulk modulus were numerically determined and confirmed by the analysis of wave propagation. The left-handed wave propagation property of this metamaterial was demonstrated by the left-handed refraction of acoustic waves.
A microstructure design of anisotropic resonant inclusions was investigated for the elastic metamaterial plate with the aid of the numerically-based effective medium model. Experimental validation was then conducted in the anisotropic metamaterial plate through both harmonic and transient wave testing, from which the anisotropic effective dynamic mass density, group and

phase velocities were determined as functions of frequency. The strongly anisotropic mass density along two principal orientations was observed experimentally and the prediction from the experimental measurements agreed well with that from the numerical simulation. Finally, based on the numerically obtained effective dynamic properties, a continuum theory was developed to simulate different guided wave modes in the elastic metamaterial plate. Particularly, high-order guided wave coupling and repulsion as well as the preferential energy flow in the anisotropic elastic metamaterial plate were discussed. Two continuum methods were investigated for modeling the dynamic behavior of an acoustic metamaterial in the form of a composite material with internal resonators. First, an effective homogeneous classical continuum model was proposed. The effective elastic constants for this continuum are obtained by taking the static equivalence between the continuum and the composite, while the effective mass density adopts the form of a second order tensor. The second model is also a continuum model that is described by two displacement variables. In addition to the usual displacement vector, a displacement vector for the motion of the resonator mass is included, thus making this multi-displacement model quite different from the classical model for elastic solids. It was shown that the dispersion relations predicted by the proposed two approaches were practically the same. The accuracy of the dispersion curves was verified by finite element analyses. Simplicity is the main advantage of the first approach. However, it has to adopt an unusual frequency-dependent effective mass density which may become negative in certain frequency range. On the other hand, the multi-displacement model can be constructed based on the actual material properties of the composite and, in general, is more versatile for further extensions to complex microstructures.

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Archival Publications (published) during reporting period:

• H. H. Huang and C. T. Sun, "Locally Resonant Acoustic Metamaterials with 2D Anisotropic Effective Mass Density," Philosophical Magazine, Vol. 91, No.6, 2011, pp. 981-996.
• H. H. Huang and C. T. Sun, "A study of Band-gap Phenomena of Two Locally Resonant Acoustic Metamaterials," J. Nanoengineering and Nanosystems, 2011.
• X. N. Liu, G. K. Hu, C.T. Sun, and G. L. Huang, "Wave Propagation Characterization and Design of Two-Dimensional Elastic Chiral Metacomposite," J. of Sound and Vibration, 330, pp. 2536-2553, 2011
• X.N. Liu, G. K. Hu, G. L. Huang, and C.T. Sun, "An Elastic Metamaterial with Simultaneously Negative Mass Density and Bulk Modulus," Applied Physics Letters, 98, 251907, 2011.
• H.H. Huang and C.T. Sun, "Behavior of an Acoustic Metamaterial with Extreme Young's Modulus," J. Mechanics and Physics Solids, doi:10.1016/j.jmps.2011.07.002, 2011.
• R. Zhu, G. L. Huang, H.H. Huang, and C. T. Sun, "Experimental and Numerical Study of Guided Wave Propagation in a Thin Metamaterial Plate," Physics Letters A, 375, , 2011, pp. 2863-2867
• H.H. Huang and C.T. Sun, "Continuum Modeling of a Composite Material with Internal Resonators," Mechanics of Materials, 46, 2012, pp.1-10.
• Hsin-Haou Huang and C. T. Sun, "Anomalous Wave Propagation in a One-dimensional Acoustic Metamaterial Having Simultaneously Negative Mass Density and Young's Modulus," to appear in the Journal of the Acoustical Society of America, 2012

Changes in research objectives (if any):

Change in AFOSR Program Manager, if any:

Extensions granted or milestones slipped, if any:

AFOSR LRIR Number

LRIR Title

Reporting Period

Laboratory Task Manager

Program Officer

Research Objectives

Technical Summary

Funding Summary by Cost Category (by FY, $K)

	Starting FY	FY+1	FY+2
Salary			
Equipment/Facilities			
Supplies			
Total			

Report Document

Report Document - Text Analysis

Report Document - Text Analysis

Appendix Documents

2. Thank You

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Http Referrer:	http://www.wpafb.af.mil/library/factsheets/factsheet.asp?id=9389
Page Path:	1 : (SKU: 1) 2 : Thank You (SKU: 2)
SessionID:	1449761602_56699b4201e748.00661104

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