

A Thesis

entitled

Verification and Validation Method for  
an Acoustic Mode Prediction Code for Turbomachinery Noise

by

Jeffrey Severino

Submitted to the Graduate Faculty as partial fulfillment of the requirements for the  
Masters of Science Degree in Mechanical Engineering

---

Dr. Ray Hixon, Committee Chair

---

Dr. Chinhua Sheng, Committee Member

---

Dr. Soric Cioc, Committee Member

---

Dr. Patricia R. Komuniecki, Dean  
College of Graduate Studies

The University of Toledo

- 2022

Copyright 2022, Jeffrey Severino

This document is copyrighted material. Under copyright law, no parts of this document may be reproduced without the expressed permission of the author.

An Abstract of  
Verification and Validation Method for  
an Acoustic Mode Prediction Code for Turbomachinery Noise

by  
Jeffrey Severino

Submitted to the Graduate Faculty as partial fulfillment of the requirements for the  
Masters of Science Degree in Mechanical Engineering

The University of Toledo  
- 2022

Over the last 20 years, there has been an increase in computational fluid dynamic codes that have made numerical analysis more and more readily available, allowing turbomachine designers to create more novel designs. However, as airport noise limitations become more restrictive over time, reducing aircraft takeoff and landing noise remains a prominent issue in the aviation community. One popular method to reduce aircraft noise is using acoustic liners placed on the walls of the engine inlet and exhaust ducts. These liners are designed to reduce the amplitude of acoustic modes emanating from the bypass fan as they propagate through the engine. The SWIRL code is a frequency-domain linearized Euler equation solver that is designed to predict the effect of acoustic liners on acoustic modes propagating in realistic sheared and swirling mean flows, guiding the design of more efficient liner configurations. The purpose of this study is to validate SWIRL using the Method Of Manufactured Solutions (MMS). This study also investigated the effect of the integration and spatial differencing methods on the convergence for a given Manufactured Solution. In addition, the effect of boundary condition implementation was tested. The improved MMS convergence rates shown for these tests suggest that the revised SWIRL code provides more accurate solutions with less computational effort than the original formulation.

# Acknowledgments

This work is supported by the NASA Advanced Air Transport Technologies (AATT) Project. I would like to thank Edmane Envia of the NASA Glenn Research Center, who is the technical monitor of this work. A very special thanks goes to Dr. Ray Hixon who supervised and guided me through out my course work and Master's Thesis. His rigor and tenacity in his profession has been the model example for an aspiring aeroacoustician. I would like to also thank all of my committee members, Dr. Chunhua Sheng and Dr. Sorin Cioc. Their contributions have been instrumental. Thanks to Dr. Clifford Brown for his programatic insights.

I would also like to thank my focus group peers, Zaid Sabri, Matthew Gibbons , and Gabriel Gutierrez for their patience and support over the years. I wish them the best in all of their endeavours.

# Contents

Abstract	iii
Acknowledgments	iv
Contents	v
List of Tables	vi
List of Figures	vii
List of Symbols	viii
List of Abbreviations	x
Preface	xi
<b>1 Introduction</b>	<b>1</b>
<b>2 Literature Review</b>	<b>2</b>
<b>3 Theoretical Framework and Methods</b>	<b>3</b>
3.1 Introduction . . . . .	3
3.2 Governing Equations for Compressible, Inviscid Flow . . . . .	3
3.3 Nonuniformities from swirling mean flow . . . . .	5
3.4 Linearizing the Governing Equations . . . . .	6
3.5 Non-Dimensionalization . . . . .	8

<b>4</b>	<b>Verification and Validation Techniques for Numerical Approxima-</b>	<b>12</b>
	<b>tions</b>	
4.1	Introduction . . . . .	12
4.1.1	Examining Convergence Using Multiple Grids . . . . .	14
4.1.2	Calculation of Observed Order-of-Accuracy . . . . .	15
4.2	Methods . . . . .	18
4.2.1	Procedure . . . . .	19
4.2.2	Tanh Summaion Formulation . . . . .	20
4.3	General form of a Hyperbolic Tangent . . . . .	20
4.4	Setting Boundary Condition Values Using a Fairing Function . . . . .	26
4.4.1	Using $\beta$ as a scaling parameter . . . . .	26
4.4.2	Minimum Boundary Fairing Function . . . . .	28
4.4.3	Max boundary polynomial . . . . .	30
4.4.4	Corrected function . . . . .	30
4.4.5	Symbolic Sanity Checks . . . . .	31
4.4.6	Min boundary derivative polynomial . . . . .	32
4.4.7	Polynomial function, max boundary derivative . . . . .	33
4.4.8	Putting it together . . . . .	35
<b>5</b>	<b>Results and Discusssion</b>	<b>36</b>
5.1	Verification of Numerical Schemes using the Method of Manufactured	
	Solution . . . . .	36
5.1.1	Introduction . . . . .	36
	<b>References</b>	<b>38</b>

# List of Tables

# List of Figures



# List of Symbols

$A$ .....	mean flow speed of sound
$A_T$ .....	speed of sound at the duct radius
$\tilde{A}$ .....	dimensionless speed of sound, $\frac{A}{A_T}$
$D/Dt$ .....	material derivative, $\partial/\partial t + V \cdot \nabla$
$D_N$ .....	derivative matrix using $N$ points
$\mathbf{e}_x, \mathbf{e}_\theta$ .....	unit vectors for the axial and tangential directions
$k_x$ .....	perturbation axial wavenumber
$k$ .....	reduced frequency, $\omega r_{max}/A_T$
$m$ .....	number of nodal diameters, i.e. azimuthal mode number
$M_x$ .....	axial Mach number
$M_\theta$ .....	tangential Mach number
$P$ .....	mean pressure
$p'$ .....	perturbation pressure
$r$ .....	radial coordinate
$r_{min}$ .....	hub radius, i.e. minimum radius
$r_{max}$ .....	hub radius, i.e. maximum radius
$\bar{r}$ .....	dimensionless radial coordinate, $r/r_{max}$
$\bar{r}_{Shankar}$ .....	dimensionless radial coordinate in ?? , $r/b = r/(r_{max} - r_{min})$
$S$ .....	mean entropy
$s'$ .....	perturbation entropy
$t$ .....	time
$\vec{V}$ .....	mean flow velocity vector
$v$ .....	mean flow velocity
$v'$ .....	perturbation flow velocity
$v_x$ .....	axial component of mean flow velocity
$v_\theta$ .....	tangential component of mean flow velocity
$v'_r$ .....	axial component of perturbation velocity
$v'_x$ .....	axial component of perturbation velocity
$v'_\theta$ .....	tangential component of perturbation flow velocity
$v_\phi$ .....	phase velocity, $k/\bar{\gamma}$
$v_g$ .....	group velocity, $dk/d\bar{\gamma}$
$x$ .....	axial coordinate

### *Greek Symbols*

$\bar{\gamma}$ .....	dimensionless axial wavenumber, $k_x r_{max}$
$\Gamma$ .....	free vortex strength
$\bar{\Gamma}$ .....	$\Gamma/(r_T A_T)$
$\delta$ .....	Kronecker delta
$\eta_H$ .....	hub acoustic liner admittance (at $r_{min}$ )
$\eta_T$ .....	tip acoustic liner admittance (at $r_{max}$ )
$\Theta$ .....	circumferential/azimuthal coordinate
$\kappa$ .....	ratio of specific heats
$\kappa_{m\mu}$ .....	modal separation constant
$\lambda$ .....	eigenvalue, $-i\bar{\gamma}$
$\mu$ .....	radial mode index
$\bar{\rho}$ .....	mean density
$\rho'$ .....	perturbation density
$\sigma$ .....	hub-to-tip radius ratio, $r_{min}/r_{max}$
$\Omega$ .....	angular frequency for solid body swirl
$\bar{\Omega}$ .....	$\Omega r_T/A_T$
$\omega$ .....	perturbation angular frequency

# List of Abbreviations

CAA .....	Computational Aeroacoustics
CFD .....	Computational Fluid Dynamics
MMS .....	Method of Manufactured Solutions
TSM .....	Tanh Summation Method
NS .....	Navier-Stokes
RK .....	Runge-Kutta

# Preface

# Chapter 1

## Introduction

# Chapter 2

## Literature Review

# Chapter 3

## Theoretical Framework and Methods

### 3.1 Introduction

This chapter will outline the steady and unsteady aerodynamic models used for this study. The MMS procedure as it is used in this study will be described. The summation method used to generate symbolic expression will be briefly described. This chapter will also present the use of fairing functions to impose the equivalent boundary conditions used in the numerical approximation. The procedure for calculating the approximated rate of convergence for a system of equations is also presented.

### 3.2 Governing Equations for Compressible, Inviscid Flow

The governing equations for an isentropic, inviscid, compressible gas with density,  $\rho$ , velocity,  $\vec{V}$ , and pressure,  $p$  describe the conservation of mass, momentum, and energy for a given domain in Equations (3.1, 3.2, 3.2) respectively.

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \vec{V} \quad (3.1)$$

$$\frac{D\vec{V}}{Dt} = -\frac{\nabla p}{\rho} + \vec{g} \quad (3.2)$$

$$\frac{Ds}{Dt} = 0 \quad (3.3)$$

where  $D/Dt$  is the material derivative operator,,

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \nabla \cdot \vec{V} \quad (3.4)$$

For this model, the domain is assumed to be uniformly cylindrical. Therefore the flow is assumed to be asymmetric, then the radial velocity component is zero. With this considered, the velocity vector , $\vec{V}$  in cylindrical coordinates become,

$$\vec{V}(r, \theta, x) = v_x(r)\hat{e}_x + v_\theta(r)\hat{e}_\theta \quad (3.5)$$

where  $\hat{e}_x$  and  $\hat{e}_\theta$  are unit vectors for the axial and tangential directions. The gradient operator , $\nabla$  in cylindrical coordinates, is

$$\vec{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \frac{1}{r} \hat{e}_\theta \frac{\partial}{\partial \theta} + \frac{\partial}{\partial z} \hat{e}_z = 0 \quad (3.6)$$

To close the problem and to write in terms of pressure, the thermodynamic relation for the speed of sound is used

$$A^2 = \left. \frac{\partial p}{\partial \rho} \right|_s \quad (3.7)$$

Utilizing the equation of state in differential form and with material derivatives



$$\frac{Dp}{Dt} = A^2 \frac{D\rho}{Dt} + \left. \frac{\partial p}{\partial s} \right|_{\rho} \frac{Ds}{Dt} \quad (3.8)$$

The conervation of energy can be rewritten in terms of pressure, by using 3.7 and 3.8

$$\frac{Dp}{Dt} = A^2 \frac{D\rho}{Dt}. \quad (3.9)$$

Using the 3.1 in non-conservative form and the definition  $A^2 = \gamma p / \rho$  (See Appendix for derivation)

$$\frac{Dp}{Dt} + \gamma p (\nabla \cdot \vec{V}) = 0. \quad (3.10)$$

Expanding equations ( 3.1, 3.2, 3.10 ) with the corresponding cylindrical expressions become,

$$\frac{\partial \rho}{\partial t} + v_r \frac{\partial \rho}{\partial r} + \frac{v_\theta}{r} \frac{\partial \rho}{\partial \theta} + v_x \frac{\partial \rho}{\partial x} + \rho \left( \frac{1}{r} \frac{\partial(rv_r)}{\partial r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_x}{\partial x} \right) = 0 \quad (3.11)$$

$$\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta^2}{r} + v_x \frac{\partial v_r}{\partial x} = -\frac{1}{\rho} \frac{\partial p}{\partial r} \quad (3.12)$$

$$\frac{\partial v_\theta}{\partial t} + v_r \frac{\partial v_\theta}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{v_r v_\theta}{r} + v_x \frac{\partial v_\theta}{\partial x} = -\frac{1}{\rho r} \frac{\partial p}{\partial \theta} \quad (3.13)$$

$$\frac{\partial v_x}{\partial t} + v_r \frac{\partial v_x}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_x}{\partial \theta} + v_x \frac{\partial v_x}{\partial x} = -\frac{1}{\rho} \frac{\partial p}{\partial x} \quad (3.14)$$

$$\frac{\partial p}{\partial t} + v_r \frac{\partial p}{\partial r} + \frac{v_\theta}{r} \frac{\partial p}{\partial \theta} + v_x \frac{\partial p}{\partial x} + \gamma p \left( \frac{1}{r} \frac{\partial(rv_r)}{\partial r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_x}{\partial x} \right) = 0 \quad (3.15)$$

### 3.3 Nonuniformities from swirling mean flow

If the mean flow contains a swirling component, i.e. a velocity vector in the tangential direction, the mean quantities, pressure , density are non-uniform, thus also changing the speed of sound. By integrating the radial momentum equation, an expression for the speed of sound was established to account for the resulting

nonuniformities due to rotations in the flow.

$$p = \int_{r_{min}}^{r_{max}} \frac{\rho v_{\theta}^2}{r} dr \quad (3.16)$$

where  $r_{min}$  and  $r_{max}$  are the bounds of the radius. Since the flow is isentropic, the pressure is related to the speed of sound through  $\nabla p = A^2 \nabla \rho$ ; which is used to compute  $\rho$ . With the relationship  $A^2 = \gamma p / \rho$ , the speed of sound is found to be,

$$\tilde{A}(\tilde{r}) = \exp \left[ \left( \frac{1-\gamma}{2} \right) \int_{\tilde{r}}^1 \frac{M_{\theta}}{\tilde{r}} \partial \tilde{r} \right] \quad (3.17)$$

The appendix shows how the speed of sound was extracted. For special cases of swirling flow, the relation to between the speed of sound and the tangential velocity can be found. Expressions can be derived for free vortex , and/or solid body swirl. The non-dimesionalization is shown in the next section.

### 3.4 Linearizing the Governing Equations

To linearize the Euler equations, we substitute each flow variable with its equivalent mean and perturbation components. Note that the mean term is only a function of space whereas the perturbation component is a dependent on both space and time (functional dependence is not explicitly written with each variable). Assuming that we can divide the variable into a known laminar flow solution to the governing equations and a small amplitude perturbation solution,

$$v_r = V_r(x) + v'_r \quad (3.18)$$

$$v_\theta = V_\theta + v'_\theta \quad (3.19)$$

$$v_x = V_x + v'_x \quad (3.20)$$

$$p = \bar{p} + p' \quad (3.21)$$

$$\rho = \bar{\rho} + \rho' \quad (3.22)$$

One key assumption is that the perturbation quantities,  $\tilde{p}$ ,  $\tilde{v}_r, \tilde{v}_\theta$ , and  $\tilde{v}_x$ , are all exponential and that they are solely a function of radius,

$$v'_r = v_r(r)e^{i(k_x x + m\theta - \omega t)} \quad (3.23)$$

$$v'_\theta = v_\theta(r)e^{i(k_x x + m\theta - \omega t)} \quad (3.24)$$

$$v'_x = v_x(r)e^{i(k_x x + m\theta - \omega t)} \quad (3.25)$$

$$p' = p(r)e^{i(k_x x + m\theta - \omega t)} \quad (3.26)$$

There are a few important assumptions that will be utilized,

- The small disturbances are infinitesimal (thus linearized)
- Neglect second order terms.
- The continuity equation is comprised of mean velocity components. This is subtracted off in each of the governing equations

The following relationships were utilized to simplify the linearized equations,

$$\frac{\partial P}{\partial r} = \frac{\bar{\rho} V_\theta^2}{r}$$

$$\gamma P = \bar{\rho} A^2$$

$$\rho' = \frac{1}{A^2} p'$$

Note that the momentum equation in the  $\theta$  and  $x$  directions remain unchanged.

The term  $\frac{\partial(rv'_r)}{\partial r} = \frac{\partial(r)}{\partial r}v'_r + \frac{\partial v'_r}{\partial r}r$  in the Energy equation

$$\begin{aligned} \frac{1}{\bar{\rho} A^2} \left( \frac{\partial p'}{\partial t} + \frac{V_\theta}{r} \frac{\partial p'}{\partial \theta} + V_x \frac{\partial p'}{\partial x} \right) + \frac{V_\theta^2}{A^2 r} v'_r + \frac{\partial v'_r}{\partial r} + \frac{v'_r}{r} + \frac{1}{r} \frac{\partial v'_\theta}{\partial \theta} + \frac{\partial v'_x}{\partial x} &= 0 \\ \frac{\partial v'_r}{\partial t} + \frac{V_\theta}{r} \frac{\partial v'_r}{\partial \theta} - \frac{2V_\theta v'_\theta}{r} + V_x \frac{\partial v'_r}{\partial x} &= \frac{1}{\bar{\rho}} \frac{\partial p'}{\partial r} + \frac{V_\theta}{\bar{\rho} r A^2} p' \\ \frac{\partial v'_\theta}{\partial t} + v'_r \frac{\partial V_\theta}{\partial r} + \frac{V_\theta}{r} \frac{\partial v'_\theta}{\partial \theta} + \frac{v'_r V_\theta}{r} + V_x \frac{\partial v'_\theta}{\partial x} &= -\frac{1}{\bar{\rho} r} \frac{\partial p'}{\partial \theta} \\ \frac{\partial v'_x}{\partial t} + v'_r \frac{\partial V_x}{\partial r} + \frac{V_\theta}{r} \frac{\partial v'_x}{\partial \theta} + V_x \frac{\partial v'_x}{\partial x} &= -\frac{1}{\bar{\rho}} \frac{\partial p'}{\partial x} \end{aligned}$$

Substituting Equation (3.26) into the linearized equations will give us the final governing equations.

$$\begin{aligned} i \left( -\omega + \frac{m}{r} + k_x V_x \right) v_r - \frac{2\bar{v}_\theta}{r} v_\theta &= -\frac{1}{\bar{\rho}} \frac{\partial P}{\partial r} + \frac{V_\theta^2}{A^2} \frac{1}{\bar{\rho} r} p \\ i \left( -\omega + \frac{m}{r} + k_x V_x \right) v_\theta + \left( \frac{V_\theta}{r} + \frac{\partial V_\theta}{\partial r} \right) v_\theta &= -\frac{m}{\bar{\rho} r} p \\ i \left( -\omega + \frac{m V_\theta}{r} + k_x V_x \right) v_x + \frac{\partial V_x}{\partial r} v_r &= -\frac{i k_x}{\bar{\rho}} p \\ \frac{1}{\bar{\rho} A^2} \left( -i\omega + \frac{i m V_\theta}{r} + i k_x V_x \right) p(r) + \frac{V_\theta^2}{A^2 r} v_r + \frac{v_r}{r} + \frac{\partial v_r(r)}{\partial r} + \frac{i m}{r} v_\theta(r) + i k_x v_x(r) &= 0 \end{aligned}$$

### 3.5 Non-Dimensionalization

Defining

$$r_T = r_{max}$$

$$A_T = A(r_{max})$$

$$k = \frac{\omega r_T}{A_T}$$

$$\bar{\gamma} = k_x r_T$$

$$\tilde{r} = \frac{r}{r_T}$$

$$\frac{\partial}{\partial r} = \frac{\partial \tilde{r}}{\partial r} \frac{\partial}{\partial \tilde{r}} = \frac{1}{r_T} \frac{\partial}{\partial \tilde{r}}$$

$$V_\theta = M_\theta A$$

$$V_x = M_x A$$

$$\tilde{A} = \frac{A}{A_T}$$

$$v_x = \tilde{v}_x A$$

$$v_r = \tilde{v}_r A$$

$$v_\theta = \tilde{v}_\theta A$$

$$p = \tilde{p} \bar{\rho} A^2$$

Substituting in yields ,

$$i \left[ -\frac{k}{\tilde{A}} + \frac{m M_\theta}{\tilde{r}} + \bar{\gamma} M_x \right] \tilde{v}_r - \frac{2 M_\theta \tilde{v}_\theta}{\tilde{r}} = -\frac{\partial \tilde{p}}{\partial \tilde{r}} - (\gamma - 1) \frac{\gamma M_\theta}{\tilde{r}} \tilde{p} \quad (3.27)$$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{m M_\theta}{\tilde{r}} + \bar{\gamma} M_x \right] \tilde{v}_\theta + \left( \frac{M_\theta}{\tilde{r}} + \frac{1}{A} \frac{\partial M_\theta A}{\partial \tilde{r}} \right) \tilde{v}_r = \frac{im}{\tilde{r}} \tilde{p} \quad (3.28)$$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{m M_\theta}{\tilde{r}} + \bar{\gamma} M_x \right] \tilde{v}_x + \frac{1}{A} \frac{\partial M_x A}{\partial \tilde{r}} \tilde{v}_r = -i \bar{\gamma} \tilde{p} \quad (3.29)$$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{m M_\theta}{\tilde{r}} + \bar{\gamma} M_x \right] \tilde{p} + \frac{M_\theta^2}{\tilde{r}} \tilde{v}_r + \frac{\partial \tilde{v}_r}{\partial \tilde{r}} + \frac{1}{A} \frac{\partial A}{\partial \tilde{r}} v_r + \frac{\tilde{v}_r}{\tilde{r}} + \frac{im}{\tilde{r}} \tilde{v}_\theta + i \bar{\gamma} \tilde{v}_x = 0 \quad (3.30)$$

The mean flow derivatives  $\partial A / \partial r$  and  $\partial(\bar{\rho} A^2) / \partial r$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{mM_\theta}{\tilde{r}} + \bar{\gamma}M_x \right] \tilde{v}_r - \frac{2M_\theta \tilde{v}_\theta}{\tilde{r}} = -\frac{\partial \tilde{p}}{\partial \tilde{r}} - (\gamma - 1) \frac{\gamma M_\theta}{\tilde{r}} \tilde{p} \quad (3.31)$$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{mM_\theta}{\tilde{r}} + \bar{\gamma}M_x \right] \tilde{v}_\theta + \left( \frac{M_\theta}{\tilde{r}} + \frac{1}{A} \frac{\partial M_\theta A}{\partial \tilde{r}} \right) \tilde{v}_r = \frac{im}{\tilde{r}} \tilde{p} \quad (3.32)$$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{mM_\theta}{\tilde{r}} + \bar{\gamma}M_x \right] \tilde{v}_x + \frac{1}{A} \frac{\partial M_x A}{\partial \tilde{r}} \tilde{v}_r = -i\bar{\gamma} \tilde{p} \quad (3.33)$$

$$i \left[ -\frac{k}{\tilde{A}} + \frac{mM_\theta}{\tilde{r}} + \bar{\gamma}M_x \right] \tilde{p} + \frac{M_\theta^2}{\tilde{r}} \tilde{v}_r + \frac{\partial \tilde{v}_r}{\partial \tilde{r}} + \frac{1}{A} \frac{\partial A}{\partial \tilde{r}} \tilde{v}_r + \frac{\tilde{v}_r}{\tilde{r}} + \frac{im}{\tilde{r}} \tilde{v}_\theta + i\bar{\gamma} \tilde{v}_x = 0 \quad (3.34)$$

Defining,  $\lambda = -i\bar{\gamma}$

and defining

$$\{\bar{x}\} = \begin{Bmatrix} \tilde{v}_r \\ \tilde{v}_\theta \\ \tilde{v}_x \\ \tilde{p} \end{Bmatrix}$$

The governing equations can be written in the form of  $[A]x - \lambda[B]x$

$$\begin{bmatrix} -i \left( \frac{k}{\tilde{A}} - \frac{mM_\theta}{\tilde{r}} \right) - \lambda M_x & -\frac{2M_\theta}{\tilde{r}} & 0 & \frac{\partial}{\partial \tilde{r}} + \frac{\gamma-1}{\tilde{r}} \\ \frac{M_\theta}{\tilde{r}} + \frac{\partial M_\theta}{\partial \tilde{r}} + \left( \frac{\gamma-1}{2} \right) \frac{M_\theta^2}{\tilde{r}} & -i \left( \frac{k}{\tilde{A}} - \frac{mM_\theta}{\tilde{r}} \right) - \lambda M_x & 0 & \frac{im}{\tilde{r}} \\ \frac{\partial M_x}{\partial \tilde{r}} + \left( \frac{\gamma-1}{2} \right) \frac{M_x M_\theta^2}{\tilde{r}} & 0 & -i \left( \frac{k}{\tilde{A}} - \frac{mM_\theta}{\tilde{r}} \right) - \lambda M_x & -\lambda \\ \frac{\partial}{\partial \tilde{r}} + \frac{\gamma+1}{2} \frac{M_\theta^2}{\tilde{r}} + \frac{1}{\tilde{r}} & \frac{im}{\tilde{r}} & -\lambda & -i \left( \frac{k}{\tilde{A}} - \frac{mM_\theta}{\tilde{r}} \right) - \lambda M_x \end{bmatrix} \bar{x} = 0$$

(place holder for analytics)

# Chapter 4

## Verification and Validation Techniques for Numerical Approximations

### 4.1 Introduction

The Method of Manufactured Solutions (MMS) is a process for generating an analytical solution for a code that provides the numerical solution for a given domain. The goal of MMS is to establish a manufactured solution that can be used to establish the accuracy of the code within question. For this study, SWIRL, a code used to calculate the radial modes within an infinitely long duct is being validated through code verification. SWIRL accepts a given mean flow and uses numerical integration to obtain the speed of sound. The integration technique is found to be the composite trapezoidal rule through asymptotic error analysis.

For SWIRL, the absolute bare minimum requirement is to define the corresponding flow components for the domain of interest. SWIRL assumes no flow in the radial direction, leaving only two other components, axial and tangential for a 3D cylindrical domain. Since SWIRL is also non dimensionalized, the mean flow components are



defined using the Mach number. SWIRL uses the tangential mach number to obtain the speed of sound using numerical integration. The speed of sound is then used to find the rest of the primitive variables for the given flow.

### 4.1.1 Examining Convergence Using Multiple Grids

When repeating the simulation while increasing the number of grid points is standard practice when conducting a numerical approximation. The discretization errors that initially arise should asymptotically approach zero, excluding computer round-off error.

Although it is desirable to know the error band for the results obtained from a fine grid, the study may require a coarse grid due to time constraints for design iteration. Furthermore, as the grid gets finer, the computational time required increases. So it is desirable to compute the discretization on grids with fewer points to get a sense of where the asymptotic range is located. The approach for generating the series of grids is to generate a grid with what the user would consider small or fine grid spacing, reaching the upper limit of one's tolerance for generating a grid. Otherwise, the finest grid that requires the least amount of computation on that grid to converge should be chosen. Then coarser grids can be obtained by removing every other grid point. Finally, the number of iterations can be increased to create additional levels of coarse grids. For example, in generating the fine grid, one can choose the number of coarser grids by satisfying the following relation,

$$N = (2^n)m + 1 \tag{4.1}$$

where,  $N$  is the number of grid points,  $n$  is the iteration level, and  $m$  is an arbitrary integer. The base 2 has the effect of doubling grid points. However  $m$  can change between iterations which will allow for grids which are fractions of double.

One can use the finest grid that was run to determine how to iterate from a coarser grid up to a finer one. Note that the number of grid points does not to be doubled each time, however the grid refinement should be such that the ratio between grid spacing it is less than 0.91 since it is easier to determine which errors occur from

discretization as opposed to computer round-off error or iterative convergence errors.

For this work, the number of grid points will be computed using the following

#### 4.1.2 Calculation of Observed Order-of-Accuracy

The numerical scheme used to perform the integration of the tangential velocity will have a theoretical order-of-accuracy. To find the theoretical order-of-accuracy, the discretization error must first be defined. The error,  $\epsilon$ , is a function of grid spacing,  $\Delta r$

$$\epsilon = \epsilon(\Delta r)$$

The discretization error in the solution should be proportional to  $(\Delta r)^\alpha$  where  $\alpha > 0$  is the theoretical order for the computational method. An error between two quantities can expressed as

$$\epsilon(\Delta r) = |f_{analytic} - f_{calc}|$$

where  $f_{analytic}$  is the function value of an analytic solution and  $f_{calc}$  represents some calculated value. The  $\Delta r$  is to indicate that this is a discretization error for a specific grid spacing.

If we define this error on various grid sizes and compute  $\epsilon$  for each grid, the observed order of accuracy can be estimated and compared to the theoretical order of accuracy. For instance, if the numerical solution is second-order accurate and the error is converging to a value, the  $L_2$  norm of the error will decrease by a factor of 4 for every halving of the grid cell size.

For a perfect answer, we expect  $\epsilon$  to be zero. Since a Taylor series can be used to derive the numerical schemes, we know that the truncation of higher order terms is what indicates the error we expect from using a scheme that is constructed with

such truncated Taylor series.

The error at each grid point  $j$  is expected to satisfy the following,

$$0 = |f_{analytic}(r_j) - f_{calc}(r_j)|$$

$$f_{analytic}(r_j) = f_{calc}(r_j) + (\Delta r)^\alpha \beta(r_j) + H.O.T$$

where the value of  $\beta(r_j)$  does not change with grid spacing, and  $\alpha$  is the asymptotic order of accuracy of the method. It is important to note that the numerical method recovers the original equations as the grid spacing approached zero. It is important to note that  $\beta$  represents the first derivative of the Taylor Series. Subtracting  $f_{analytic}$  from both sides gives,

$$f_{calc}(r_j) - f_{analytic}(r_j) = f_{analytic}(r_j) - f_{analytic}(r_j) + \beta(r_j)(\Delta r)^\alpha$$

$$\epsilon(r_j)(\Delta r) = \beta(r_j)(\Delta r)^\alpha$$

To estimate the order of accuracy of the accuracy, we define the global errors by calculating the L2 Norm of the error which is denoted as  $\hat{\epsilon}$

$$\hat{\epsilon} = \sqrt{\frac{1}{N} \sum_{j=1}^N \epsilon(r_j)^2}$$

$$\hat{\beta}(r_j) = \sqrt{\frac{1}{N} \sum_{j=1}^N \beta(r_j)^2}$$

As the grid density increases,  $\hat{\beta}$  should asymptote to a constant value. Given two

grid densities,  $\Delta r$  and  $\sigma\Delta r$ , and assuming that the leading error term is much larger than any other error term,

$$\begin{aligned}\hat{\epsilon}_{grid1} &= \hat{\epsilon}(\Delta r) = \hat{\beta}(\Delta r)^\alpha \\ \hat{\epsilon}_{grid2} &= \hat{\epsilon}(\sigma\Delta r) = \hat{\beta}(\sigma\Delta r)^\alpha \\ &= \hat{\beta}(\Delta r)^\alpha \sigma^\alpha\end{aligned}$$

The ratio of two errors is given by,

$$\begin{aligned}\frac{\hat{\epsilon}_{grid2}}{\hat{\epsilon}_{grid1}} &= \frac{\hat{\beta}(\Delta r)^\alpha}{\hat{\beta}(\Delta r)^\alpha} \sigma^\alpha \\ &= \sigma^\alpha\end{aligned}$$

Thus,  $\alpha$ , the asymptotic rate of convergence is computed as follows

$$\alpha = \frac{\ln \frac{\hat{\epsilon}_{grid2}}{\hat{\epsilon}_{grid1}}}{\ln(\sigma)}$$

Defining for a doubling of grid points ,

$$\alpha = \frac{\ln(\hat{\epsilon}(\frac{1}{2}\Delta r)) - \ln(\hat{\epsilon}(\Delta r))}{\ln(\frac{1}{2})}$$

## 4.2 Methods

The SWIRL code requires two mean flow parameters as a function of radius,  $M_x$ , and  $M_\theta$ . Afterwards, the speed of sound,  $\tilde{A}$  is calculated by integrating  $M_\theta$  with respect to  $r$ . To verify that SWIRL is handling and returning the accompanying mean flow parameters, the error between the mean flow input and output variables are computed. Since the trapezoidal rule is used to numerically integrate  $M_\theta$ , the discretization error and order of accuracy is computed. Since finite differencing schemes are to be used on the result of this integration, it is crucial to accompany the integration with methods of equal or less order of accuracy. This will be determined by applying another MMS on the eigenproblem which will also have an order of accuracy.

### 4.2.1 Procedure

There are a few constraints and conditions that must be followed in order for the analytical function to work with SWIRL,

- The mean flow and speed of sound must be real and positive. This will occur if a speed of sound is chosen such that the tangential mach number is imaginary
- The derivative of the speed of sound must be positive
- Any bounding constants used with the mean flow should not allow the total Mach number to exceed one.
- the speed of sound should be one at the outer radius of the cylinder

Given these constraints,  $\tanh(r)$  is chosen as a function since it can be modified to meet the conditions above. Literature (The tanh method: A tool for solving certain classes of nonlinear evolution and wave equations) is a paper that demonstrates the strength of using tanh functions. One additional benefit of  $\tanh(r)$  is that it is bounded between one and negative one, i.e.

- As  $r \rightarrow \infty$   $\tanh(r) \rightarrow 1$
- As  $-r \rightarrow -\infty$   $\tanh(r) \rightarrow -1$

To test the numerical integration method,  $M_\theta$  is defined as a result of differentiating the speed of sound,  $A$ . This is done opposed to integrating  $M_\theta$  analytically. However, an analytical function can be defined for  $M_\theta$ , which can then be integrated to find what  $\tilde{A}$  should be. Instead, the procedure of choice is to back calculate what the appropriate  $M_\theta$  is for a given expression for  $\tilde{A}$ . Since it is easier to take derivatives, we will solve for  $M_\theta$  using Equation ?? ,

### 4.2.2 Tanh Summation Formulation

Knupp’s Code Verification by the Method of Manufactured Solution (MMS) provides “guidelines” for creating a manufactured solution (MS) such that the observed order of accuracy will approach a theoretical order of accuracy as the number of grid points are reduced from one iteration to the next. While these guidelines offer a road map, there are choices that are left to the investigator that would benefit from additional examples. The first guideline gives the user a free choice of the MS as long as it is smooth. The benefit of the tanh summation method (TSM) reduces the difficulty in defining a sufficient MS by providing a general summation formulation that allows the user to Vary the number of terms in the MS, and the MS behavior without manually changing terms in the MS symbolic expression.

The general form of the MS will be a summation of *tanh* bounded between zero and one. A MS created with the TSM can provide a significant result for a numerical differencing/integration technique by having inflection points of each *tanh* at various locations along the domain, giving a stair like slope. While the TSM can add a layer of complexity to the MS that may not be needed, writing the formulation in a summation lends itself to iterative loops that can be coded, thus reducing the need for manual adjust of the MS, which can be an initial hurdle when performing MMS.

## 4.3 General form of a Hyperbolic Tangent

$$R = A \tanh(B(x - C)) \tag{4.2}$$

$$L = A \tanh(B(C - E)) \tag{4.3}$$

$$y = R + L + D \tag{4.4}$$



where

- $R \equiv$  The value of the hyperbolic tangent. The variable  $R$  represents a “right” facing hyperbolic tangent kink.
- $A \equiv$  magnitude factor that increases or decreases the asymptotic limits  $\lim_{x \rightarrow -\infty} = -1$   $\lim_{x \rightarrow \infty} = 1$
- $B \equiv$  “steepness” of the hyperbolic tangent
- $C \equiv$  The shift in inflection point of the hyperbolic tangent along the  $x$  axis
- $D \equiv$  The shift in inflection point of the hyperbolic tangent along the  $y$  axis
- $E \equiv x_{i=imax}$
- $x$  The domain.  $x_i$  is used to indicate grid point indices.

The idea is to sum up an arbitrary amount of tangents that will be bounded by zero and one.

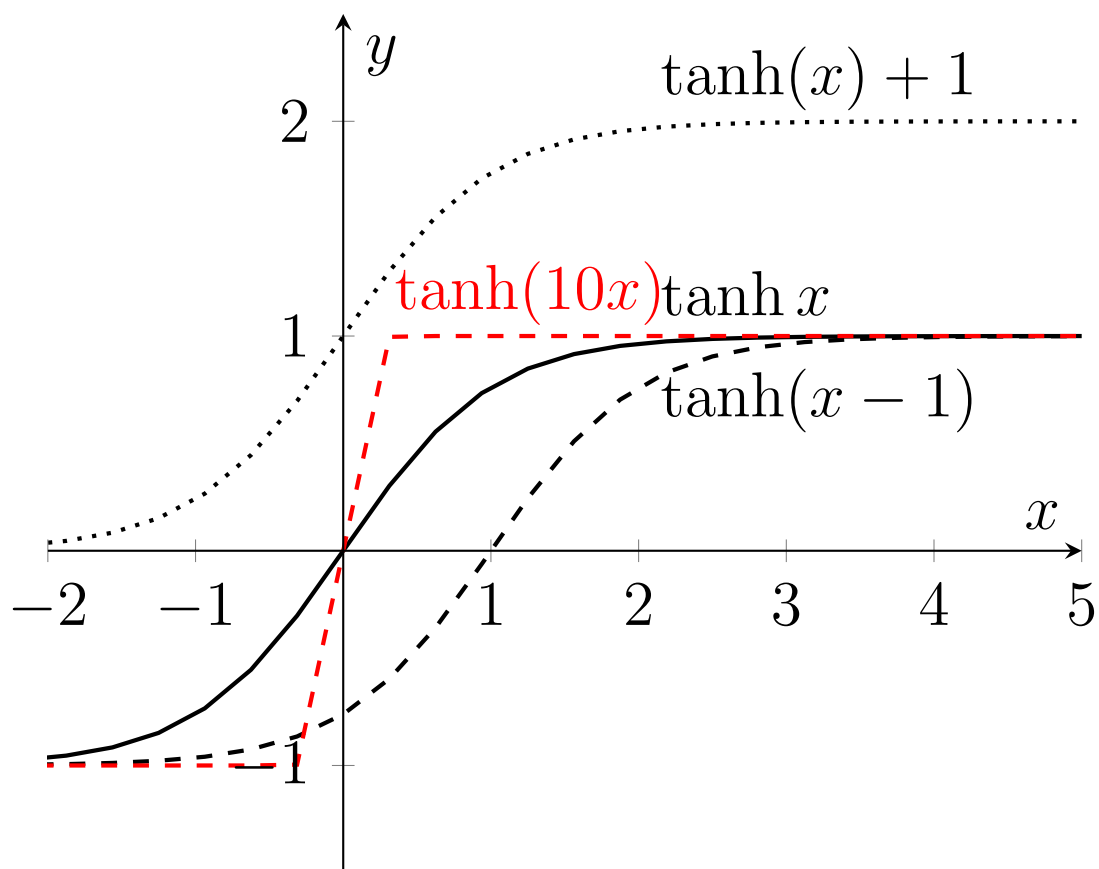
Now the goal is to generalize this formulation such that we can add up terms.  $A$  is determined by setting a maximum amplitude for each  $\tanh$  function by  $A = A_{max}/n$ . Note that amplitude can be different for each term but is chosen to be the same. A parameter  $\hat{x} = (x - x_{min})/(x_{max} - x_{min})$  scales the domain to be between the minimum and maximum bounds.

$$R_{ij} = A \tanh(B(x_i - C_j)) \quad (4.5)$$

$$L_j = A \tanh(B(C_j - E)) \quad (4.6)$$

$$y = \sum_{j=1}^n R_{ij} + \sum_{j=1}^n L_j + D \quad (4.7)$$

The function `TanhMethod` does this procedure.



Setting  $A = 1/16$  and  $C_1 = 0$  ,  $C_2 = 0.75$  ,  $C_3 = 1$  ,  $D = 1$ ,  $E = 1$  and  $B = 10$

$$\sum_{j=1}^3 R_{ij} = 1/16 \tanh(10(\hat{x}_i)) + 1/16 \tanh(10(\hat{x}_i - 0.75)) + 1/16 \tanh(10(\hat{x}_i - 1)) \quad (4.8)$$

$$\sum_{j=1}^3 L_j = 1/16 \tanh(10(-1)) + 1/16 \tanh(10(0.75 - 1)) + 1/16 \tanh(10(1 - 1)) \quad (4.9)$$

The simplified expression becomes,

$$y = \frac{1}{16} \tanh\left(\frac{100}{9}r - \frac{100}{9}\right) + \frac{1}{16} \tanh\left(\frac{100}{9}r - \frac{55}{9}\right) + \frac{1}{16} \tanh\left(\frac{100}{9}r - \frac{10}{9}\right) + \frac{7}{8} \quad (4.10)$$

A tanh summation method was constructed to make a manufactured solution with strong changes in slope. This ensures that the numerical approximation will not give trivial answers. then for some functions we need to impose boundary conditions. We will demonstrate how the careless implementation of a boundary condition can lead to close approximations on the interior. The speed of sound is defined with the subscript *analytic* to indicate that this is the analytical function of choice and has no physical relevance to the actual problem.

$$\tilde{A}_{analytic} = \Lambda + k_1 \tanh(k_2(\tilde{r} - \tilde{r}_{max})),$$

where,

$$\Lambda = 1 - k_1 \tanh(k_2(1 - \tilde{r}_{max})),$$

When,  $\tilde{r} = \tilde{r}_{max}$  ,  $\tilde{A}_{analytic} = 1$ . Taking the derivative with respect to  $\tilde{r}$ ,

$$\begin{aligned}\frac{\partial \tilde{A}_{analytic}}{\partial \tilde{r}} &= (1 - \tanh^2((r - r_{max})k_2))k_1k_2, \\ &= \frac{k_1k_2}{\cosh^2((r - r_{max})k_2)}.\end{aligned}$$

Substitute this into the expression for  $M_\theta$  in Equation ??,

$$M_\theta = \sqrt{2} \sqrt{\frac{rk_1k_2}{(\kappa - 1)(\tanh((r - r_{max})k_2)k_1 + \tanh((r_{max} - 1)k_2)k_1 + 1)\cosh^2((r - r_{max})k_2)}}$$

Now that the mean flow is defined, the integration method used to obtain the speed of sound

Initially the source terms were defined without mention of the indices of the matrices they make up. In other words, there was no fore sight on the fact that these source terms are sums of the elements within A,B, and X. To investigate the source terms in greater detail, the FORTRAN code that calls the source terms will output the terms within the source term and then sum them, instead

of just their sum. i  $[A]x = \lambda[B]x$

which can be rearranged as,

$$[A]x - \lambda[B]x = 0$$

Here,  $x$  is an eigenvector composed of the perturbation variables,  $v_r, v_\theta, v_x, p$  and  $\lambda$  is the associated eigenvalue, (Note:  $\lambda = -i\bar{\gamma}$ )

Writing this out we obtain  $\dots$ .

Linear System of Equations:

$$-i \left( \frac{k}{A} - \frac{m}{r} M_\theta \right) v_r - \frac{2}{r} M_\theta v_\theta + \frac{dp}{dr} + \frac{(\kappa - 1)}{r} M_\theta^2 p - \lambda M_x v_r = S_1 \quad (4.11)$$

Using matrix notation,

$$A_{11}x_1 - A_{12}x_2 + A_{14}x_4 - \lambda B_{11}x_1 = S_1 \quad (4.12)$$

But  $A_{14}$  and  $A_{41}$  in Kousen's paper only has the derivative operator. Since I am currntly writing the matrix out term by term and not doing the matrix math to obtain the symbolic expressions, I will define  $A_{14}$  with  $dp/dr$  and  $A_{41}$  with  $dv_r/dr$ . Similarly,

$$A_{21}x_1 - A_{22}x_2 + A_{24}x_4 - \lambda B_{22}x_2 = S_2 \quad (4.13)$$

$$A_{31}x_1 - A_{33}x_3 - \lambda(B_{33}x_3 + B_{34}x_4) = S_3 \quad (4.14)$$

$$A_{41}x_1 + A_{42}x_2 + A_{44}x_4 - \lambda(B_{33}x_3 + B_{44}x_4) = S_4 \quad (4.15)$$

Now we can begin looking at the source terms, term by term. They each should also converge at a known rate

Goal: How can we modify a manufactured solution such that the endpoints are suitable for comparison against a codes boundary condition implementation

## 4.4 Setting Boundary Condition Values Using a Fairing Function

### 4.4.1 Using $\beta$ as a scaling parameter

Defining the nondimensional radius in the same way that SWIRL does:

$$\tilde{r} = \frac{r}{r_T}$$

where  $r_T$  is the outer radius of the annulus.

The hub-to-tip ratio is defined as:

$$\sigma = \frac{r_H}{r_T} = \tilde{r}_H$$

where  $\tilde{r}_H$  is the inner radius of the annular duct. The hub-to-tip ratio can also be zero indicating the duct is hollow.

A useful and similar parameter is introduced,  $\beta$ , where  $0 \leq \beta \leq 1$

$$\beta = \frac{r - r_H}{r_T - r_H}$$

Dividing By  $r_T$

$$\begin{aligned}\beta &= \frac{\frac{r}{r_T} - \frac{r_H}{r_T}}{\frac{r_T}{r_T} - \frac{r_H}{r_T}} \\ &= \frac{\tilde{r} - \tilde{r}_H}{1 - \sigma}\end{aligned}$$

Suppose a manufactured solution  $f_{MS}$  with boundaries  $f_{MS}(r = \sigma)$  and  $f_{MS}(\tilde{r} = 1)$  is the specified analytical solution. The goal is to change the boundary conditions of the manufactured solution in such way that allows us to adequately check the boundary conditions imposed on SWIRL. Defining the manufactured solution,  $f_{MS}(\tilde{r})$ , where  $\sigma \leq \tilde{r} \leq 1$  and there are desired values of  $f$  at the boundaries desired values are going to be denoted as  $f_{minBC}$  and  $f_{maxBC}$ . The desired changes in  $f$  are defined as:

$$\Delta f_{minBC} = f_{minBC} - f_{MS}(\tilde{r} = \sigma)$$

$$\Delta f_{maxBC} = f_{maxBC} - f_{MS}(\tilde{r} = 1)$$

We'd like to impose these changes smoothly on the manufactured solution function.

To do this, the fairing functions,  $A_{min}(\tilde{r})$  and  $A_{max}(\tilde{r})$  where:

$$f_{BCsImposed}(\tilde{r}) = f_{MS}(\tilde{r}) + A_{min}(\tilde{r})\Delta f_{minBC} + A_{max}(\tilde{r})\Delta f_{maxBC}$$

Then, in order to set the condition at the appropriate boundary, the following conditions are set,

$$A_{min}(\tilde{r} = \sigma) = 1$$

$$A_{min}(\tilde{r} = 1) = 0$$

$$A_{max}(\tilde{r} = 1) = 1$$

$$A_{max}(\tilde{r} = \sigma) = 0$$

If  $A_{min}(\tilde{r})$  is defined as a function of  $A_{max}(\tilde{r})$  then only  $A_{max}(\tilde{r})$  needs to be defined, therefore

$$A_{min}(\tilde{r}) = 1 - A_{max}(\tilde{r})$$

It is also desirable to set the derivatives for the fairing function at the boundaries incase there are boundary conditions imposed on the derivatives of the fairing function.

$$\begin{aligned}\frac{\partial A_{max}}{\partial \tilde{r}}|_{\tilde{r}=\sigma} &= 0 \\ \frac{\partial A_{max}}{\partial \tilde{r}}|_{\tilde{r}=1} &= 0\end{aligned}$$

$$\begin{aligned}\frac{\partial A_{min}}{\partial \tilde{r}}|_{\tilde{r}=\sigma} &= 0 \\ \frac{\partial A_{min}}{\partial \tilde{r}}|_{\tilde{r}=1} &= 0\end{aligned}$$

#### 4.4.2 Minimum Boundary Fairing Function

Looking at  $A_{min}$  first, the polynomial is:



$$A_{min}(\beta) = a + b\beta + c\beta^2 + d\beta^3$$

$$A_{min}(\tilde{r}) = a + b\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right) + c\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right)^2 + d\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right)^3$$

Taking the derivative,

$$A'_{min}(\tilde{r}) = b\left(\frac{1}{1 - \sigma}\right) + 2c\left(\frac{1}{1 - \sigma}\right)\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right) + 3d\left(\frac{1}{1 - \sigma}\right)\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right)^2$$

$$A'_{min}(\beta) = \left(\frac{1}{1 - \sigma}\right)[b + 2c\beta + 3d\beta^2]$$

Now we will use the conditons mentioned earlier as constraints to this system of equations Using the possible values of  $\tilde{r}$ ,

$$A_{min}(\sigma) = a \qquad \qquad \qquad = 1$$

$$A_{min}(1) = a + b + c + d \qquad \qquad \qquad = 0$$

$$A'_{min}(\sigma) = b \qquad \qquad \qquad = 0$$

$$A'_{min}(1) = b + 2c + 3d \qquad \qquad \qquad = 0$$

which has the solution,

$$a = 1$$

$$b = 0$$

$$c = -3$$

$$d = 2$$

giving the polynomial as:

$$A_{min}(\tilde{r}) = 1 - 3 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 + 2 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3$$

#### 4.4.3 Max boundary polynomial

Following the same procedure for  $A_{max}$  gives

$$A_{min}(\tilde{r}) = 3 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 - 2 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3$$

#### 4.4.4 Corrected function

The corrected function is then,

$$\begin{aligned} f_{BCsImposed}(\tilde{r}) &= f_{MS}(\tilde{r}) + A_{min}\Delta f_{minBC} + A_{max}\Delta f_{maxBC} \\ &= f_{MS}(\tilde{r}) + \left( 1 - 3 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 + 2 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3 \right) [\Delta f_{minBC}] \\ &\quad + \left( 3 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 - 2 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3 \right) [\Delta f_{maxBC}] \\ f_{BCsImposed}(\beta) &= f_{MS}(\beta) + \Delta f_{minBC} + (3\beta^2 - 2\beta^3) [\Delta f_{maxBC} - \Delta f_{minBC}] \end{aligned}$$

Note that we're carrying the correction throughout the domain, as opposed to limiting the correction at a certain distance away from the boundary. The application of this correction ensures that there is no discontinuous derivatives inside the domain; as suggested in Roach's MMS guidelines (insert ref)

What is meant by "just because  $A_{min}$  and its first derivative go to zero doesn't mean that the second derivatives"

#### 4.4.5 Symbolic Sanity Checks

We want to ensure that  $f_{BCsImposed}$  has the desired boundary conditions,  $f_{minBC/maxBC}$  instead of the original boundary values that come along for the ride in the manufactured solutions,  $f_{MS}(\tilde{r} = \sigma/1)$ . In another iteration of this method, we will be changing the derivative values, so let's check the values of  $\frac{\partial f_{BCsImposed}}{\partial \tilde{r}}$  to make sure those aren't effected unintentionally.

##### Symbolic Sanity Check 1

The modified manufactured solution,  $f_{BCsImposed}$  with the fairing functions  $A_{min}$  and  $A_{max}$  substituted in is,

$$f_{BCsImposed}(\tilde{r}) = \left( 3 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 - 2 \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3 \right) [\Delta f_{maxBC}].$$

Further simplification yields,

$$\begin{aligned} f_{BCsImposed}(\tilde{r} = \sigma) &= \left( f_{MS}(\tilde{r} = \sigma) + \Delta f_{minBC} + \left( 3 \left( \frac{\sigma - \sigma}{1 - \sigma} \right)^2 - 2 \left( \frac{\sigma - \sigma}{1 - \sigma} \right)^3 \right) [\Delta f_{maxBC} - \Delta f_{minBC}] \right) \\ &= f_{MS}(\tilde{r} = \sigma) + \Delta f_{minBC} \\ &= f_{MS}(\tilde{r} = \sigma) + (f_{minBC} - f_{MS}(\tilde{r} = \sigma)) \\ &= f_{minBC} \end{aligned}$$

$$\begin{aligned}
f_{BCsImposed}(\tilde{r} = 1) &= \left( f_{MS}(\tilde{r} = 1) + \Delta f_{minBC} + \left( 3 \left( \frac{1-\sigma}{1-\sigma} \right)^2 - 2 \left( \frac{1-\sigma}{1-\sigma} \right)^3 - \right) [\Delta f_{maxBC} - \Delta f_{minBC}] \right) \\
&= f_{MS}(\tilde{r} = 1) + \Delta f_{maxBC} \\
&= f_{MS}(\tilde{r} = 1) + (f_{maxBC} - f_{MS}(\tilde{r} = 1)) \\
&= f_{maxBC}
\end{aligned}$$

$$\begin{aligned}
&\frac{\partial}{\partial \tilde{r}} \left( f_{BCsImposed}(\tilde{r}) = \left( 3 \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^2 - 2 \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^3 \right) [\Delta f_{maxBC}] \right) \\
&\frac{\partial f_{MS}}{\partial \tilde{r}} + \left( \frac{6}{1-\sigma} \right) \left( \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right) - \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^2 \right) (\Delta f_{maxBC} - \Delta f_{minBC})
\end{aligned}$$

At  $\tilde{r} = \sigma$ , the derivative is:

$$\begin{aligned}
&\frac{\partial f_{MS}}{\partial \tilde{r}}|_{\sigma} \\
&\frac{\partial f_{MS}}{\partial \tilde{r}}|_1
\end{aligned}$$

#### 4.4.6 Min boundary derivative polynomial

The polynomial is of the form:

$$\begin{aligned}
B_{min}(\beta) &= a + b\beta + c\beta^2 + d\beta^3 \\
B_{min}(\tilde{r}) &= a + b \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right) + c \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^2 + d \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^3
\end{aligned}$$

Taking the derivative,

$$B'_{min}(\tilde{r}) = b \left( \frac{1}{1-\sigma} \right) + 2c \left( \frac{1}{1-\sigma} \right) \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right) + 3d \left( \frac{1}{1-\sigma} \right) \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^2$$

$$B'_{min}(\beta) = \left( \frac{1}{1-\sigma} \right) [b + 2c\beta + 3d\beta^2]$$

Applying the four constraints gives:

$$a = 0$$

$$b = (1 - \sigma)$$

$$a + b + c + d = 0$$

$$2 + 2c + 3d = 0$$

$$c + d = -b$$

$$2c + 3d = -b$$

$$c = -2b$$

$$d = b$$

and the min boundary derivative polynomial is:

$$B_{min}(\tilde{r}) = b \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right) - 2b \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^2 + b \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^3$$

$$= (1 - \sigma) \left( \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right) - 2 \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^2 + \left( \frac{\tilde{r}-\sigma}{1-\sigma} \right)^3 \right)$$

#### 4.4.7 Polynomial function, max boundary derivative

The polynomial is of the form:

The polynomial is of the form:

$$B_{max}(\beta) = a + b\beta + c\beta^2 + d\beta^3$$

$$B_{max}(\tilde{r}) = a + b\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right) + c\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right)^2 + d\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right)^3$$

which has the derivative,

$$B'_{max}(\tilde{r}) = b\left(\frac{1}{1 - \sigma}\right) + 2c\left(\frac{1}{1 - \sigma}\right)\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right) + 3d\left(\frac{1}{1 - \sigma}\right)\left(\frac{\tilde{r} - \sigma}{1 - \sigma}\right)^2$$

$$B'_{max}(\beta) = \left(\frac{1}{1 - \sigma}\right)[b + 2c\beta + 3d\beta^2]$$

Applying the four constraints gives:

$$a = 0$$

$$b = 0$$

$$a + b + c + d = 0$$

$$b + 2c + 3d = (1 - \sigma)$$

working this out:

$$c + d = 0$$

$$2c + 3d = (1 - \sigma)$$

gives

$$c = -(1 - \sigma) d = (1 - \sigma)$$

and the max boundary derivative polynomial is:

$$B_{max}(\tilde{r}) = (1 - \sigma) \left( - \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 + \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3 \right)$$

#### 4.4.8 Putting it together

The corrected function is then:

$$\begin{aligned} f_{BCsImposed}(\tilde{r}) &= f_{MS} + B_{min}(\tilde{r}) \Delta f'_{minBC} + B_{max}(\tilde{r}) \Delta f'_{maxBC} \\ &= f_{MS} + \\ &\quad (1 - \sigma) \left( \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right) - \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 \right) \Delta f'_{minBC} + \\ &\quad (1 - \sigma) \left( - \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^2 + \left( \frac{\tilde{r} - \sigma}{1 - \sigma} \right)^3 \right) (\Delta f'_{minBC} + \Delta f'_{maxBC}) \end{aligned}$$

# Chapter 5

## Results and Discussion

### 5.1 Verification of Numerical Schemes using the Method of Manufactured Solution



# References