

# 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.

# 2 Methods

The SWIRL code requires two mean flow parameters as a function of radius,  $M_x$ , and  $M_\theta$ . 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.

## 2.1 Theory

To relate the speed of sound to a given flow, the radial momentum equation is used. If the flow contains a swirling component, then the primitive variables are nonuniform through the flow, and mean flow assumptions are not valid.

To account for this, the radial momentum is simplified by assuming the flow is steady, the flow has no radial component. In addition, the viscous and body forces are neglected.

The radial pressure derivative term is set equal to the dynamic pressure term and separation of variables is applied.

$$\frac{v_\theta^2}{r} = \frac{1}{\rho} \frac{\partial P}{\partial r}$$
$$P = \int_r^{r_{max}} \frac{\rho V_\theta^2}{\partial r}$$

Since  $\tilde{r} = r/r_{max}$ ,

$$r = \tilde{r}r_{max}.$$

Taking total derivatives (i.e. applying chain rule),

$$dr = d(\tilde{r}r_{max}) = d(\tilde{r})r_{max}$$

Substituting these back in and evaluating the right hand side,

$$\int_{\tilde{r}}^1 \frac{\bar{\rho} v_{\theta}^2}{\tilde{r}} \partial \tilde{r} = P(1) - P(\tilde{r})$$

For reference the minimum value of  $\tilde{r}$  is

$$\sigma = \frac{r_{max}}{r_{min}}$$

For the radial derivative, the definition of the speed of sound is utilized,

$$\frac{\partial A^2}{\partial r} = \frac{\partial}{\partial r} \left( \frac{\gamma P}{\rho} \right).$$

Using the quotient rule, we can extract the definition of the speed of sound.

$$\begin{aligned} &= \frac{\partial P}{\partial r} \frac{\gamma \bar{\rho}}{\bar{\rho}^2} - \left( \frac{\gamma P}{\bar{\rho}^2} \right) \frac{\partial \bar{\rho}}{\partial r} \\ &= \frac{\partial P}{\partial r} \frac{\gamma}{\bar{\rho}} - \left( \frac{A^2}{\bar{\rho}} \right) \frac{\partial \bar{\rho}}{\partial r} \end{aligned}$$

Using isentropic condition  $\partial P/A^2 = \partial \rho$ ,

$$\begin{aligned}
&= \frac{\partial P}{\partial r} \frac{\gamma}{\bar{\rho}} - \left( \frac{1}{\bar{\rho}} \right) \frac{\partial P}{\partial r} \\
\frac{\partial A^2}{\partial r} &= \frac{\partial P}{\partial r} \frac{\gamma - 1}{\bar{\rho}}
\end{aligned}$$

$$\frac{\bar{\rho}}{\gamma - 1} \frac{\partial A^2}{\partial r} = \frac{\partial P}{\partial r}$$

Going back to the radial momentum equation, and rearranging the

$$\begin{aligned}
\frac{\bar{\rho} v_\theta^2}{r} &= \frac{\partial P}{\partial r} \\
\frac{\bar{\rho} v_\theta^2}{r} &= \frac{\bar{\rho}}{\gamma - 1} \frac{\partial A^2}{\partial r} \\
\frac{v_\theta^2}{r} (\gamma - 1) &= \frac{\partial A^2}{\partial r}
\end{aligned}$$

To start the nondimensionalization, we define,

$$\begin{aligned}
M_\theta &= \frac{V_\theta}{A} \\
\tilde{r} &= \frac{r}{r_{max}} \\
\tilde{A} &= \frac{A}{A_{r,max}} \\
A &= \tilde{A}A_{r,max} \\
r &= \tilde{r}r_{max} \\
\frac{\partial}{\partial r} &= \frac{\partial \tilde{r}}{\partial r} \frac{\partial}{\partial \tilde{r}} \\
&= \frac{1}{r_{max}} \frac{\partial}{\partial \tilde{r}}
\end{aligned}$$

Dividing by  $A$ ,

$$\frac{M_\theta^2}{r} (\gamma - 1) = \frac{\partial A^2}{\partial r} \frac{1}{A^2}$$

At this point we can either find the derivative of  $\bar{A}$  or the integral of  $M_\theta$  with respect to  $r$

1.

$$\begin{aligned}
\text{Integrating both sides } \int_r^{r_{max}} \frac{M_\theta}{r} (\gamma - 1) \partial r &= \int_{A^2(r)}^{A^2(r_{max})} \frac{1}{A^2} \partial A^2 \\
\int_r^{r_{max}} \frac{M_\theta^2}{r} (\gamma - 1) \partial r &= \ln(A^2(r_{max})) - \ln(A^2(r)) \\
\int_r^{r_{max}} \frac{M_\theta^2}{r} (\gamma - 1) \partial r &= \ln \left( \frac{A^2(r_{max})}{A^2(r)} \right)
\end{aligned}$$

Defining non dimensional speed of sound  $\tilde{A} = \frac{A(r)}{A(r_{max})}$

$$\int_r^{r_{max}} \frac{M_\theta}{r} (\gamma - 1) \partial r = \ln \left( \frac{1}{\tilde{A}^2} \right)$$

$$= -2\ln(\tilde{A})$$

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

replacing r with  $\tilde{r} \rightarrow \tilde{A}(r) = \exp \left[ - \int_r^{r_{max}} \frac{M_\theta}{r} \frac{(\gamma - 1)}{2} \partial r \right]$

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

2. Or we can differentiate

Solving for  $M_\theta$  ,

$$M_\theta^2 = \frac{\partial A^2}{\partial r} \frac{r}{A^2 (\gamma - 1)}$$

Nondimensionalizing:

Plugging in,

$$M_\theta^2 \frac{(\gamma - 1)}{\tilde{r} r_{max}} = \frac{1}{(\tilde{A} A_{r,max})^2} \frac{A_{r,max}^2}{r_{max}} \frac{\partial \tilde{A}^2}{\partial \tilde{r}}$$

$$M_\theta^2 \frac{(\gamma - 1)}{\tilde{r}} = \frac{1}{\tilde{A}^2} \frac{\partial \tilde{A}^2}{\partial \tilde{r}}$$

$$M_\theta = \sqrt{\frac{\tilde{r}}{(\gamma - 1) \tilde{A}^2} \frac{\partial \tilde{A}^2}{\partial \tilde{r}}} \quad (1)$$

3.1 Guidelines for Creating Manufactured Solutions states:

1. The manufactured solutions should be composed of smooth analytic functions
2. The manufactured solutions should exercise every term in the governing equation that is being tested,
3. The solution should have non trivial derivatives.
4. The solution derivatives should be bounded by a small constant. In this case this constant should prevent the function from becoming greater than one.
5. The solution should not prevent the code from running
6. The solution should be defined on a connected subset of two- or three-dimensional space to allow flexibility in choosing the domain of the PDE. Section 3.3.1 provides more information about this.
7. The solution should coincide with the differential operators of the PDE. For example, the flux term in Fourier's law of conduction requires  $T$  to be differentiable.

With these guidelines, a function is specified for the speed of sound to conduct a method of manufactured solutions on SWIRL's speed of sound numerical integration. This is checked by observing the tangential mach number produced from the speed of sound and comparing that to the tangential mach number that has been analytically defined (See Equation 1).

## 2.2 Procedure

To test the integration code,  $M_\theta$  is defined as a result of differentiating the speed of sound. This is done opposed to integrating  $M_\theta$  as a preference, but a function can be defined for  $M_\theta$ , and then integrate 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 1,

$$M_\theta = \sqrt{\frac{\tilde{r}}{(\gamma - 1)\tilde{A}^2} \frac{\partial \tilde{A}^2}{\partial \tilde{r}}}$$

This time we define the speed of sound with the subscript *Analytic* to indicate that this is the analytical function of choice and has no physical relevance to the actual problem

$$\tilde{A}_{Analytic} = \cos(k(\tilde{r} - \widetilde{r_{max}}))$$

Taking the derivative with respect to  $\tilde{r}$ ,

$$\begin{aligned} \frac{\partial \tilde{A}_{Analytic}}{\partial \tilde{r}} &= \frac{\partial}{\partial \tilde{r}} (\cos(k(\tilde{r} - \widetilde{r_{max}}))) \\ \frac{\partial \tilde{A}_{Analytic}}{\partial \tilde{r}} &= -k \sin(k(\tilde{r} - \widetilde{r_{max}})) \end{aligned}$$



Now we substitute this into the expression for  $M_\theta$  in Equation 1,

$$M_\theta = \sqrt{2} \sqrt{-\frac{k r \sin(k(r - r_{\max}))}{(\gamma - 1) \cos(k(r - r_{\max}))}}$$

### 2.3 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 id 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. The error for each grid is expressed as

$$\epsilon_{M_\theta}(\Delta r) = |M_{\theta,Analytic} - M_{\theta,calc}|$$

where  $M_{\theta,Analytic}$  is the tangential mach number that is defined from the speed of sound we also defined and the  $M_{\theta,calc}$  is the result from SWIRL. The  $\Delta r$  is to indicate that this is a discretization error for a specific grid spacing. Applying the same concept to to the speed of sound,

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 L2 norm of the error will decrease by a factor of 4 for every halving of the grid cell size. Since the input variables should remain unchanged (except from minor changes from the Akima interpolation), the error for the axial and tangential mach number should be zero. As for the speed of sound, since we are using an analytic expression for the tangential mach number, we know what the theoretical result would be from the numerical integration technique as shown above. Similarly we define the discretization error for the speed of sound.

$$\epsilon_A(\Delta r) = |A_{Analytic} - A_{calc}|$$

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.

We expect the error at each grid point  $j$  to satisfy the following,

$$0 = |A_{Analytic}(r_j) - A_{calc}(r_j)|$$

$$\tilde{A}_{Analytic}(r_j) = \tilde{A}_{calc}(r_j) + (\Delta r)^\alpha \beta(r_j) + H.O.T$$

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  $A_{Analytic}$  from both sides gives

$$\begin{aligned} A_{calc}(r_j) - A_{Analytic}(r_j) &= A_{Analytic}(r_j) - A_{Analytic}(r_j) + \beta(r_j)(\Delta r)^\alpha \\ \epsilon_A(r_j)(\Delta r) &= \beta(r_j)(\Delta r)^\alpha \end{aligned}$$

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  $\hat{\epsilon}_A$

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

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

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,

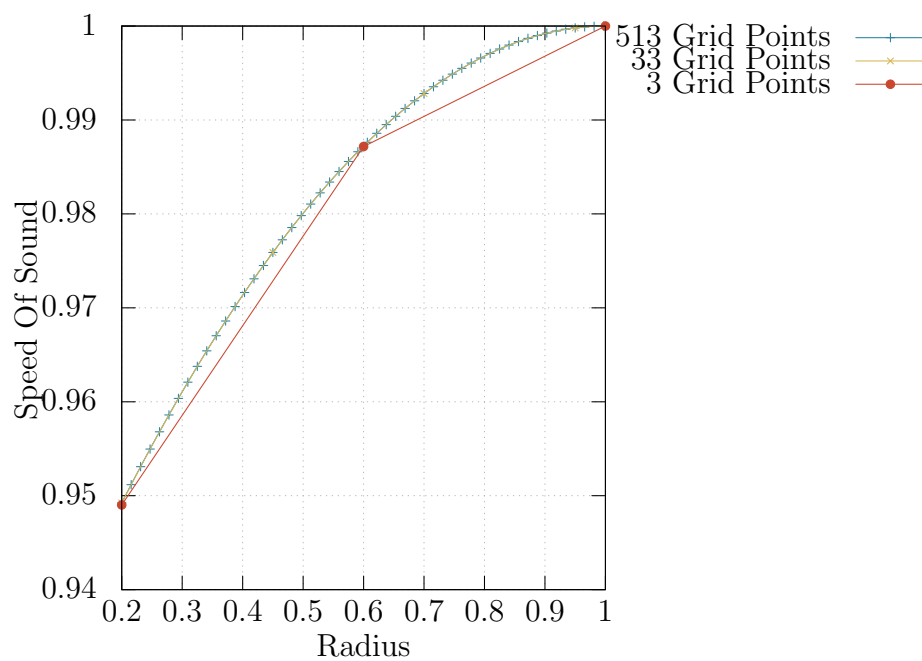
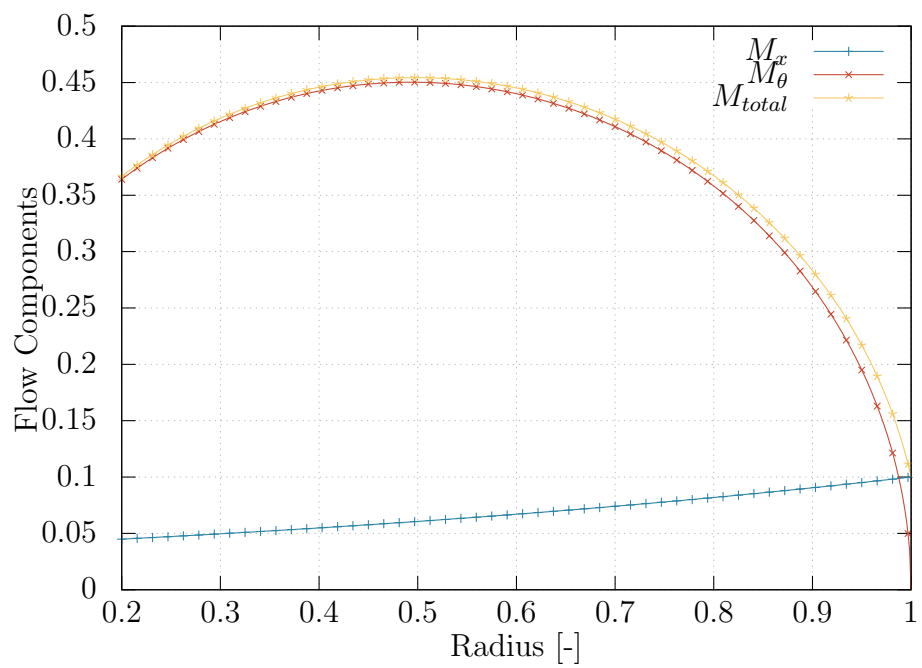
$$\begin{aligned}
\frac{\hat{\epsilon}_{grid2}}{\hat{\epsilon}_{grid1}} &= \frac{\hat{\beta}(\Delta r)^\alpha}{\hat{\beta}(\Delta r)^\alpha} \sigma^\alpha \\
&= \sigma^\alpha
\end{aligned}$$

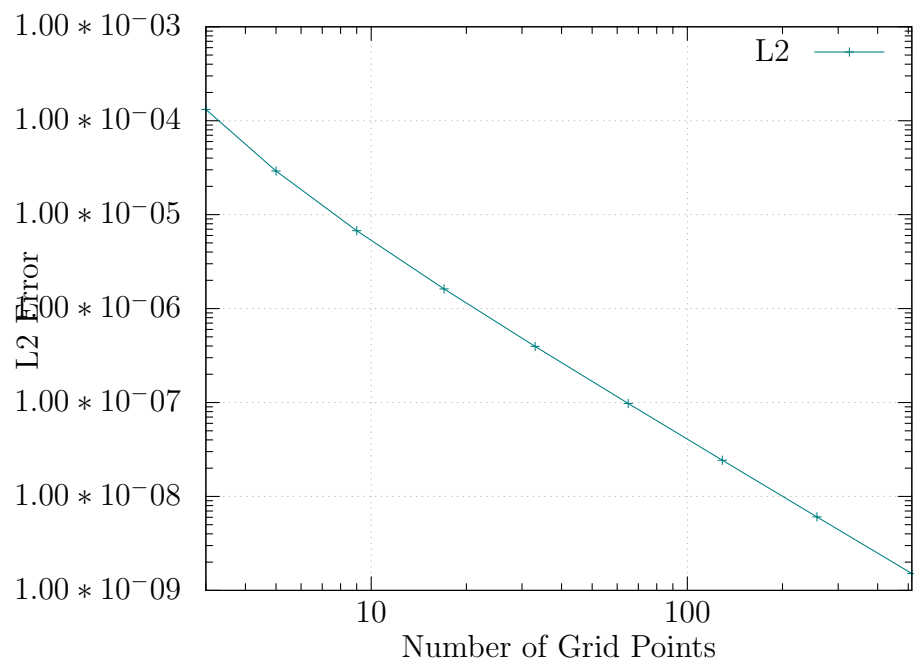
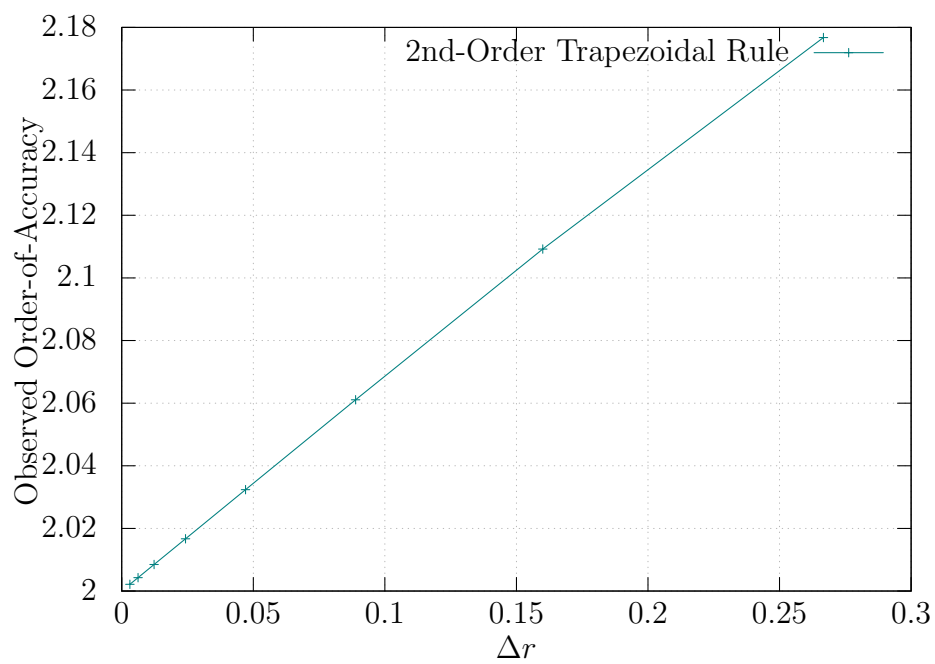
Thus,  $\alpha$ , the asymptotic rate of convergence is computed as follows

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

Defining for a doubling of grid points ,

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





### **3 Results And Discussion**

The data in Figure 1 indicates the two flow components of the velocity vector used for the MMS. This test was intended to have a large swirling component to put emphasis on the integration technique used to determine the speed of sound. Figure 2 shows the resulting speed of sound which was calculated with the composite trapezoidal rule as the numerical integration scheme. The results, as seen in Figure 2, show the improvement in calculation as the number of grid points are increased. Note that not all grid points are shown in Figure 2. Figure 3 shows the L2 Error for the calculated speed of sound as it compared to the expected speed of sound. The L2 norm suggest that the Figure 4 shows the asymptotic rate of convergence for the composite trapezoidal rule.

### **4 Conclusion**

### **5 Appendix**

#### **5.1 Error Analysis**

Reference: A. Ralston, A first course in numerical analysis 2nd edition

##### **5.1.1 Exact Polynomial Approximation**

Say we have some discrete data,

$$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$$

We want to find a polynomial of the LEAST degree that fits these points exactly. Such a polynomial is called a Lagrange Polynomial. If in addition you supply a function, or derivative value, you can use Hermite interpolation to help the desired fitted polynomial handle sudden changes (?)

For Lagrange Polynomials, the general form is,

$$p(x_i) = \sum_{j=1}^n l_j(x_i) f(x_j) + \underbrace{\frac{f^{(n)}(c)}{n!} p_n(x_i)}_{\text{Error at } x_i},$$

where,

$$p_n(x_i) = \prod_{j=1}^n (x_i - x_j)$$

$$p_n(x_i) = (x_i - x_1)(x_i - x_2) \dots (x_i - x_n)$$

So if we have two data points  $x_i$  and  $x_{i+1}$ , the function of least degree that fits the data *exactly* for a Lagrange interpolation is,

$$p(x_i) = l_i(x_i) f(x_i) + l_{i+1}(x_{i+1}) f(x_{i+1}) + [\text{Error at } x_i]$$

Note that I said *exactly*! So I will drop the error term...



Then we *claim* that

$$p(x_i) = l_i(x_i) f_i(x_i) + l_{i+1}(x_{i+1}) f_{i+1}(x_{i+1})$$

which means that we also claim that

$$l_i(x) = \frac{x - x_{i+1}}{x_i - x_{i+1}}$$

$$l_{i+1}(x) = \frac{x - x_i}{x_{i+1} - x_i}$$

if  $x = x_i$ ,

$$l_i(x_i) = \frac{x_i - x_{i+1}}{x_i - x_{i+1}} = 1$$

,

$$l_{i+1}(x_i) = \frac{x_i - x_i}{x_{i+1} - x_i} = 0$$

and if  $x = x_{i+1}$ ,

$$l_i(x_{i+1}) = \frac{x_{i+1} - x_{i+1}}{x_i - x_{i+1}} = 0$$

,

$$l_{i+1}(x_{i+1}) = \frac{x_{i+1} - x_i}{x_{i+1} - x_i} = 1$$

let's see if  $p(x)$  passes through these points exactly,

$$p(x_i) = 1f_i(x_i) + 0f(x_i) = f(x_i)$$

$$p(x_{i+1}) = 1f_{i+1}(x_{i+1}) + 0f(x_{i+1}) = f(x_{i+1})$$

Defining,

$$\Delta x^+ = x_{i+1} - x_i$$

$$\hat{x} = x - x_i$$

Using this on the Lagrange polynomial for two points gives

$$\begin{aligned} & \left( \frac{(x - x_{i+1})}{(x_i - x_{i+1})} f_i + \frac{(x - x_i)}{(x_{i+1} - x_i)} f_{i+1} \right) \\ & \left( \frac{(x - (x_{i+1}))}{(x_i - x_{i+1})} f_i + \frac{(x + (-x_i))}{((x_{i+1}) + (-x_i))} f_{i+1} \right) \\ & \left( \frac{(x - (\Delta x^+ + x_i))}{x_i - (\Delta x^+ + x_i)} f_i + \frac{(x + (\hat{x} - x))}{((\Delta x^+ + x_i) + (-x_i))} f_{i+1} \right) \\ & \left( \frac{((x - x_i) - \Delta x^+)}{-\Delta x^+} f_i + \frac{(\hat{x})}{((\Delta x^+ + x_i) + (-x_i))} f_{i+1} \right) \\ & \frac{\hat{x} - \Delta x^+}{-\Delta x^+} f_i + \frac{\hat{x}}{\Delta x^+} f_{i+1} \end{aligned}$$

The Lagrange polynomial is

$$\tilde{f}(\hat{x}) = \left( \frac{\hat{x}}{\Delta x^+} f_{i+1} + \frac{\Delta x^+ - \hat{x}}{\Delta x^+} f_i \right)$$

## 5.2 Integration

Recall that

$$\hat{x} = x - x_i$$

Now we prepare to integrate,

$$\begin{aligned} \int_{x_1}^{x_2} \tilde{f} dx &= \int_{x_1 - x_i}^{x_2 - x_i} \tilde{f} \frac{\partial x}{\partial \hat{x}} d\hat{x} \\ &= \int_{x_1 - x_i}^{x_2 - x_i} \tilde{f} d\hat{x} \end{aligned}$$

In the interior of the domain  $i = 1, iMax - 1$ , the function is integrated from  $\hat{x} = 0$  to  $\hat{x} = \Delta x^+$ . In other words, the integration covers the complete range of the polynomial. Note that we are only integrating over a single interval.

$$\begin{aligned}
\int_0^{\Delta x^+} \tilde{f} d\hat{x} &= \int_0^{\Delta x^+} \left( \frac{\hat{x}}{\Delta x^+} f_{i+1} + \frac{\Delta x^+ - \hat{x}}{\Delta x^+} f_i \right) \\
&= \frac{1}{\Delta x^+} f_{i+1} \int_0^{\Delta x^+} (\hat{x}) d\hat{x} + \frac{1}{\Delta x^+} f_i \left( \int_0^{\Delta x^+} (\Delta x^+) d\hat{x} - \int_0^{\Delta x^+} (\hat{x}) d\hat{x} \right) \\
&= \frac{1}{\Delta x^+} \left( f_{i+1} \left[ \frac{(\Delta x^+)^2}{2} - 0 \right]_0^{\Delta x^+} + f_i \left[ \frac{(\Delta x^+)^2}{2} - 0 \right]_0^{\Delta x^+} \right) \\
&= \frac{(\Delta x^+)^2}{2\Delta x^+} [f_{i+1} + f_i] \\
&= \frac{\Delta x^+}{2} [f_{i+1} + f_i]
\end{aligned}$$

Which is the trapezoidal rule!

### 5.3 Taylor Series Error Analysis

Here we try to determine the order of accuracy of the trapezoidal rule. The Taylor series for the integral  $F$  and for the function  $f$  are:

$$\begin{aligned}
f_{i+1} &= f_i + \Delta x \frac{\partial f}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 f}{\partial x^2} \Big|_i + \mathcal{O}(\Delta x^3) \\
f_i &= f_i
\end{aligned}$$

Summing the two gives,

$$f_i + f_{i+1} = 2f_i + \Delta x \frac{\partial f}{\partial x} + \mathcal{O}(\Delta x^2)$$

Multiplying by  $\Delta x/2$

$$\frac{\Delta x}{2}(f_i + f_{i+1}) = f_i \Delta x + \frac{\Delta x^2}{2} \frac{\partial f}{\partial x} + \mathcal{O}(\Delta x^3)$$

## 5.4 Composite Trapezoidal Rule

To account for the entire domain, we express our trapezoidal rule as the sum of sub intervals for a uniform grid, to do so we redefine the grid spacing,

$$\Delta x^+ = \frac{\Delta \tilde{x}^+}{n-1}$$

where  $\tilde{x}^+$  is the length of the domain and  $n$  is the total number of grid points.

$$\begin{aligned}
\int_{x_1}^{x_n} \tilde{f} d\hat{x} &= \frac{\Delta x^+}{2} \sum_{i=1}^n (f_i + f_{i+1}) \\
&= \frac{\Delta x^+}{2} [(f_1 + f_2) + (f_2 + f_3) + \cdots + (f_{n-2} + f_{n-1}) + (f_{n-1} + f_n)] \\
&= \frac{\Delta x^+}{2} [(f_1 + 2f_2 + 2f_3 + \cdots + 2f_{n-2} + 2f_{n-1} + f_n)] \\
&= \frac{\Delta x^+}{2} \left[ f_1 + f_n + 2 \sum_{i=2}^{n-1} f_i \right] \\
&= \frac{\Delta x^+}{2} [f_1 + f_n] + \Delta x^+ \sum_{i=2}^{n-1} f_i
\end{aligned}$$

Noe we can use A taylor series expansion on the composite trapezoidal rule to get an order of accuracy

the summation will be expanded Around  $i\Delta x$  in order to interpret the sum as a Riemann sum

$$\begin{aligned}
&f_1 = f_1 \\
&i\Delta x \frac{\partial f}{\partial x} + \frac{(i\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{(i\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} + \cdots
\end{aligned}$$

Let's further simplify the Taylor series at the last grid point,

$$\begin{aligned}
f_n &= f_1 + \Delta \tilde{x}^+ \frac{\partial f}{\partial x} + \frac{(\Delta \tilde{x}^+)^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{(\Delta \tilde{x}^+)^3}{3!} \frac{\partial^3 f}{\partial x^3} + \cdots \\
&= f_1 + (n-1) \Delta x^+ \frac{\partial f}{\partial x} + \frac{(n-1)^2}{2} \Delta x^+ \frac{\partial^2 f}{\partial x^2} + \frac{(n-1)^3}{3} \Delta x^+ \frac{\partial^3 f}{\partial x^3}
\end{aligned}$$

Okay this is a bit tricky, lets distribute the summation on the Taylor

series expanded around each grid point. Since this Taylor Series expansion involves the 1st grid point we re-adjust our summation to show this.

$$\begin{aligned}
\sum_{i=2}^{n-1} f_i &= \sum_{i=1}^{n-2} \left( f_1 + i\Delta x \frac{\partial f}{\partial x} + \frac{(i\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{(i\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} + \dots \right) \\
&= \sum_{i=1}^{n-2} (f_1) + \sum_{i=1}^{n-2} \left( i\Delta x \frac{\partial f}{\partial x} \right) + \sum_{i=1}^{n-2} \left( \frac{(i\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} \right) + \sum_{i=1}^{n-2} \left( \frac{(i\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} \right) + \dots \\
&= \sum_{i=1}^{n-2} (f_1) + \Delta x \frac{\partial f}{\partial x} \sum_{i=1}^{n-2} (i) + \frac{(\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} \sum_{i=1}^{n-2} (i^2) + \frac{(\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} \sum_{i=1}^{n-2} (i^3)
\end{aligned}$$

Now we can substitute this into the composite trapezoidal rule and gather the coefficients

$$\frac{\Delta x^+}{2} [f_1 + f_n] + \Delta x^+ \sum_{i=1}^{n-2} f_i$$

Let's look at one common term at a time, starting with  $f_1$ , note the two halves summing to one,

$$\begin{aligned}
&\frac{\Delta x^+}{2} \left[ f_1 + f_1 + \sum_{i=1}^{n-2} f_1 \right] \\
&\Delta x^+ f_1 \left[ 1 + \sum_{i=1}^{n-2} 1 \right]
\end{aligned}$$

Now for the rest of the terms, we factor out  $\Delta x^+$

$$\begin{aligned}
& (\Delta x^+)^2 \frac{\partial f}{\partial x} \left( \sum_{i=1}^{n-2} (i) + \frac{n-1}{2} \right) + \\
& \frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left( \sum_{i=1}^{n-2} (i)^2 + \frac{(n-1)^2}{2} \right) + \\
& \frac{(\Delta x^+)^4}{3!} \frac{\partial^3 f}{\partial x^3} \left( \sum_{i=1}^{n-2} (i)^3 + \frac{(n-1)^3}{2} \right) \dots
\end{aligned}$$

Using the following summation rules we can further simplify the problem

$$\begin{aligned}
\sum_{i=1}^n c &= cn \\
\sum_{i=1}^n i &= \frac{n(n-1)}{2} \\
\sum_{i=1}^n i^2 &= \frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6} \\
\sum_{i=1}^n i^3 &= \frac{n^4}{4} + \frac{n^3}{2} + \frac{n^2}{4}
\end{aligned}$$

Let's put the terms back together, and then simplify with the closed form



expressions for the summations,

$$\begin{aligned}
& \Delta x^+ f_1 \left[ 1 + \sum_{i=1}^{n-2} 1 \right] + \\
& (\Delta x^+)^2 \frac{\partial f}{\partial x} \left( \sum_{i=1}^{n-2} (i) + \frac{n-1}{2} \right) + \\
& \frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left( \sum_{i=1}^{n-2} (i)^2 + \frac{(n-1)^2}{2} \right) + \\
& \frac{(\Delta x^+)^4}{3!} \frac{\partial^3 f}{\partial x^3} \left( \sum_{i=1}^{n-2} (i)^3 + \frac{(n-1)^3}{2} \right) \dots
\end{aligned}$$

$$\begin{aligned}
& \Delta x^+ f_1 [1 + (n-2)] + \\
& (\Delta x^+)^2 \frac{\partial f}{\partial x} \left( \frac{(n-2)[(n-2)-1]}{2} + \frac{n-1}{2} \right) + \\
& \frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left( \frac{(n-2)^3}{3} + \frac{(n-2)^2}{2} + \frac{(n-2)}{6} + \frac{(n-1)^2}{2} \right) + \\
& \frac{(\Delta x^+)^4}{3!} \frac{\partial^3 f}{\partial x^3} \left( \frac{(n-2)^4}{4} + \frac{(n-2)^3}{2} + \frac{(n-2)^2}{4} + \frac{(n-1)^3}{2} \right) \dots
\end{aligned}$$

$$\begin{aligned}
& \Delta x^+ f_1 [(n-1)] + \\
& (\Delta x^+)^2 \frac{\partial f}{\partial x} \left( \frac{(n-2)(n-1)}{2} + \frac{n-1}{2} \right) + \\
& \frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left( \frac{(n-2)^3}{3} + \frac{(n-2)^2}{2} + \frac{(n-2)}{6} + \frac{(n-1)^2}{2} \right) + \\
& \frac{(\Delta x^+)^4}{3!} \frac{\partial^3 f}{\partial x^3} \left( \frac{(n-2)^4}{4} + \frac{(n-2)^3}{2} + \frac{(n-2)^2}{4} + \frac{(n-1)^3}{2} \right) \dots
\end{aligned}$$

$$\begin{aligned}
& f_1 [\Delta \tilde{x}^+] + \\
& (\Delta x^+)^2 \frac{\partial f}{\partial x} \left( \frac{(n-2)(n-1)}{2} + \frac{n-1}{2} \right) + \\
& \frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left( \frac{(n-2)^3}{3} + \frac{(n-2)^2}{2} + \frac{(n-2)}{6} + \frac{(n-1)^2}{2} \right) +
\end{aligned}$$

Side note:

$$\begin{aligned}
& \frac{(n-2)(n-1)}{2} + \frac{(n-1)}{2} \\
& \frac{(n-2)(n-1) + (n-1)}{2}
\end{aligned}$$

Factor out  $(n - 1)$

$$\frac{\frac{[(n - 2) + 1 (n - 1)]}{2}}{\frac{(n - 1) (n - 1)}{2}} = \frac{(n - 1)^2}{2}$$

Using this for the coefficient of the second term,

$$\begin{aligned} & f_1 [\Delta \tilde{x}^+] + \\ & (\Delta x^+)^2 \frac{\partial f}{\partial x} \left( \frac{(n - 1)^2}{2} \right) + \\ & \frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left( \frac{(n - 2)^3}{3} + \frac{(n - 2)^2}{2} + \frac{(n - 2)}{6} + \frac{(n - 1)^2}{2} \right) + \end{aligned}$$

Since we expect the third term to have a  $(n - 1)^3$  if this pattern of the Taylor series being expanded around L, the coefficient of the third term is going to be set equal to  $(n - 1)^3$  and simplified,

We also expect the leading coefficient to have 1/6 as well. Multiplying by 3 and setting the result equal  $(n - 1)^3$  gives,

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

$$\frac{n - 1}{2}$$

Plugging this back in, along with the definition of  $\Delta\tilde{x}^+$  for the rest of the terms gives,

$$f_1 [\Delta\tilde{x}^+] + \frac{(\Delta\tilde{x}^+)^2}{2} \frac{\partial f}{\partial x} + \frac{(\Delta x)^3}{3!} \frac{\partial^2 f}{\partial x^2} \frac{\Delta\tilde{x}^+}{2\Delta x}$$