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

SWIRL is a linearized Euler equations of motion code that calculates the axial wavenumber and radial mode shapes from small unsteady disturbances in a mean flow. The mean flow varies along the axial and tangetial directons as a function of radius. The flow domain can either be a circular or annular duct, with or without acoustic liner. SWIRL was originally written by Kousen [insert ref].

The SWIRL code requires two mean flow parameters as a function of radius, M_x , and M_θ. Afterwards, the speed of sound, $\widetilde{A}$ is calculated by integrating M_θ with respect to r. To verify that SWIRL is handling and returning the accompanying mean flow parameters, the error between the

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mean flow input and output variables are computed. Since the trapezoidal rule is used to numerically integrate M_θ, 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.

$$\frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} - \frac{v_\theta^2}{r} v_x \frac{\partial v_r}{\partial x} = \frac{1}{\rho} \frac{\partial P}{\partial r}$$

To account to 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. Then the radial pressure derivative term is set equal to the dynamic pressure term. Seperation of variables is applied.

$$\frac{v_\theta^2}{r} = \frac{1}{\rho}\frac{\partial P}{\partial r}$$

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

To show the work, we will start with the dimensional form of the equation and differentiate both sides. Applying separation of variables,

$$\int_r^{r_{max}} \frac{\bar{\rho} v_\theta^2}{r}\partial r = -\int_{P(r)}^{P(r_{max})}\partial p.$$

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, the definition of the speed of sound is extracted,

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

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

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

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

Going back to the radial momentum equation, and rearranging the terms will simplify the expression. The following terms are defined to start the nondimensionalization.

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$$M_\theta = \frac{V_\theta}{A}$$

$$\widetilde{r} = \frac{r}{r_{max}}$$

$$\widetilde{A} = \frac{A}{A_{r,max}}$$

$$A = \widetilde{A}A_{r,max}$$

$$r = \widetilde{r}r_{max}$$

$$\frac{\partial}{\partial r} = \frac{\partial \widetilde{r}}{\partial r}\frac{\partial}{\partial \widetilde{r}}$$

$$= \frac{1}{r_{max}}\frac{\partial}{\partial \widetilde{r}}$$

Dividing by A,

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

Now there is two options, either find the derivative of $\bar{A}$ or the integral of M_θ with respect to r.

1. 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_θ ,

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

Nondimensionalizing and substituting,

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

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

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

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2.2   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 is 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 than demonstrates the strength of using tanh functions. One additonal 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_θ is defined as a result of differentiating the speed of sound, A. This is done opposed to integrating

M_θ analytically. However, an analytical function can be defined for M_θ, which can then be integrated to find what $\widetilde{A}$ should be. Instead, the procedure of choice is to back calculate what the appropriate M_θ is for a given expression for $\widetilde{A}$. Since it is easier to take derivatives , we will solve for M_θ using Equation 1 ,

2.3 Tanh Summaion Formulation

The goal is generate an MS with a number of "stairs" that is bounded between zero and one. Here's what my focus group ideas are,

$$1 = R + L$$

where, 1 is a constraint, and R and L are the two waves when summed need to cancel if it were the exact same amplitude & opposite sign

so ,

$$R + L = \tanh(x) + -\tanh(x) = 0$$

or in our case,

$$R + L = \tanh(x) + -\tanh(x) = 1$$

We can tweak this by adding knobs by adding "knobs" A and B. If we dont want the total to not exceed one then, $A_j + A_{j+1} \cdots A_{last} = 1$. B_1 changes the steepnes of the kink that we want. In order to generalize this,

$$\bar{A} = \sum_{j=1}^{n} R_{ij} + \sum_{j=1}^{n} L_{ij}$$

where,

$$R_{ij} = A_j \tanh(B_j(x_i - x_j))$$

$$L_{ij} = A_j \tanh(B_j(x_j - x_n))$$

Letting $n = 3\ldots$

$$\bar{A} = S_{vert} + \sum_{j=1}^{3} R_{ij} + \sum_{j=1}^{3} L_{ij}$$

$$\bar{A} = A_1 \tanh(B_1(x_i - x_1)) + A_2 \tanh(B_2(x_i - x_2)) + A_3 \tanh(B_3(x_i - x_3)) +$$

$$A_1 \tanh(B_1(x_1 - x_n)) + A_2 \tanh(B_2(x_2 - x_n)) + A_3 \tanh(B_3(x_3 - x_n))$$

and,

$$A_1 = A_2 = A_3 = k_1$$

$$B_1 = B_2 = B_3 = k_2$$

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.

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

where,

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

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

$$\frac{\partial \widetilde{A}_{analytic}}{\partial \widetilde{r}} = \left(1 - \tanh^2\left((r - r_{max})\, k_2\right)\right) k_1 k_2,$$

$$= \frac{k_1 k_2}{\cosh^2\left((r - r_{max})\, k_2\right)}.$$

Substitute this into the expression for M_θ in Equation 1,

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

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

2.4 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, ϵ, is a function of id spacing, Δr

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

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 Δr 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 ϵ for each grid, the observed order of accuracy can be estimated and compared to the theoretical order of accuracy. For instance, if the numerical soution 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 ϵ 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,

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

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

where the value of $\beta(r_j)$ does not change with grid spacing, and α 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 β represents the first derivative of the Taylor Series. Subtracting $A_{analytic}$ from both sides gives,

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

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

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 $\hat{\epsilon}_A$

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

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

As the grid density increases, $\hat{\beta}$ should asymptote to a constant value. Given two grid densities, Δr and $\sigma\Delta r$, and assuming that the leading error term is much larger than any other error term,

$$\hat{\epsilon}_{grid1} = \hat{\epsilon}(\Delta r) = \hat{\beta}(\Delta r)^{\alpha}$$

$$\hat{\epsilon}_{grid2} = \hat{\epsilon}(\sigma\Delta r) = \hat{\beta}(\sigma\Delta r)^{\alpha}$$

$$= \hat{\beta}(\Delta r)^{\alpha}\sigma^{\alpha}$$

The ratio of two errors is given by,

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

$$= \sigma^{\alpha}$$

Thus, α,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 , Similarly for the eigenvalue problem,

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

3   Code Documentation

placeholder

4   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.

5 Conclusion

6 Appendix

6.1 Error Analysis

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

6.1.1 Exact Polynomial Approximation

Let there be discrete data,

$$(x_i, y_2), (x_2, y_2), \ldots, (x_n, y_n)$$

The goal is to find a polynomial of the LEAST degree that fits these points exactly. Such a polynomial is called a Lagrange Polynomial. If in addition ,a function, or derivative value, is supplied, Hermitie intepolation can help the desired fitted polynomial handle sudden changes [insert ref]

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,

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

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$$p_n(x_i) = (x_i - x_j)(x_i - x_{i+1})(x_i - x_{i+2})(x_i - x_{i+3})\ldots(x_i - x_n)$$

For two data points, x_i and x_{i+1}, the function of least degree that fits the data *exactly* for a Langrange 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 the polynomial fits *exactly*! So the error term is dropped. The next *claim* is,

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

which means that,

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

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,

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

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

Defining,

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

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

Using this on the Lagrange polynomial for two points gives

$$\left(\frac{(x - x_{i+1})}{(x_i - x_{i+1})} f_i + \frac{(x - x_i)}{(x_{i+1} - x_i)} f_{i+1} \right)$$

$$\left(\frac{(x - (x_{i+1}))}{(x_i - x_{i+1})} f_i + \frac{(x + (-x_i))}{((x_{i+1}) + (-x_i))} f_{i+1} \right)$$

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

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

$$\frac{\hat{x} - \Delta x^+}{-\Delta x^+} f_i + \frac{\hat{x}}{\Delta x^+} f_{i+1}$$

The Lagrange polynomial is

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

6.2 Integration

Recall that

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

Preparing to integrate,

$$\int_{x_1}^{x_2} \widetilde{f} dx = \int_{x_1 - x_i}^{x_2 - x_i} \widetilde{f} \frac{\partial x}{\partial \hat{x}} d\hat{x}$$

$$= \int_{x_1 - x_i}^{x_2 - x_i} \widetilde{f} d\hat{x}$$

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 the integration is over a single interval.

$$\int_0^{\Delta x^+} \widetilde{f} d\hat{x} = \int_0^{\Delta x^+} \left(\frac{\hat{x}}{\Delta x^+} f_{i+1} + \frac{\Delta x^+ - \hat{x}}{\Delta x^+} f_i \right)$$

$$= \frac{1}{\Delta x^+} f_{i+1} \int_0^{\Delta x^+} (\hat{x}) d\hat{x} + \frac{1}{\Delta x^+} f_i \left(\int_0^{\Delta x^+} (\Delta x^+) d\hat{x} - \int_0^{\Delta x^+} (\hat{x}) d\hat{x} \right)$$

$$= \frac{1}{\Delta x^+} \left(f_{i+1} \left[\frac{(\Delta x^+)^2}{2} - 0 \right]_0^{\Delta x^+} + f_i \left[\frac{(\Delta x^+)^2}{2} - 0 \right]_0^{\Delta x^+} \right)$$

$$= \frac{(\Delta x^+)^2}{2 \Delta x^+} [f_{i+1} + f_i]$$

$$= \frac{\Delta x^+}{2} [f_{i+1} + f_i]$$

Which is the trapezoidal rule!

6.3 Taylor Series Error Analysis

The goal is to determine the order of accuracy of the trapezoidal rule. The Taylor series for the integral F and for the function f are:

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

$$f_i = f_i$$

Summing the two gives,

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

Multiplying by $\Delta x/2$,

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

6.4   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,

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

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

$$\int_{x_1}^{x_n} \widetilde{f} d\hat{x} = \frac{\Delta x^+}{2} \sum_{i=1}^{n} (f_i + f_{i+1})$$

$$= \frac{\Delta x^+}{2} [(f_1 + f_2) + (f_2 + f_3) + \cdots + (f_{n-2} + f_{n-1}) + (f_{n-1} + f_n)]$$

$$= \frac{\Delta x^+}{2} [(f_1 + 2f_2 + 2f_3 + \cdots + 2f_{n-2} + 2f_{n-1} + f_n)]$$

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

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

A taylor series expansion on the composite trapezoidal rule gives an order of accuracy. The summation will be expanded around $i\Delta x$ in order to interpret the sum as a Riemann sum.

$$f_1 = f_1$$

$$i\Delta x \frac{\partial f}{\partial x} + \frac{(i\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{(i\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} + \cdots$$

Further simplifing the Taylor series at the last grid point,

$$f_n = f_1 + \Delta \widetilde{x}^+ \frac{\partial f}{\partial x} + \frac{(\Delta \widetilde{x}^+)^2}{2!} \frac{\partial^2 f}{\partial x^2} + \frac{(\Delta \widetilde{x}^+)^3}{3!} \frac{\partial^3 f}{\partial x^3} + \cdots$$

$$= f_1 + (n-1) \Delta x^+ \frac{\partial f}{\partial x} + \frac{(n-1)^2}{2} \Delta x^+ \frac{\partial^2 f}{\partial x^2} + \frac{(n-1)^3}{3} \Delta x^+ \frac{\partial^3 f}{\partial x^3}$$

Distribute the summation of the Taylor series expanded around each grid point. Since this Taylor Series expanison involves the 1st grid point the summation is re-adjusted to show the following,

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

$$= \sum_{i=1}^{n-2} (f_1) + \sum_{i=1}^{n-2} \left(i\Delta x \frac{\partial f}{\partial x} \right) + \sum_{i=1}^{n-2} \left(\frac{(i\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} \right) + \sum_{i=1}^{n-2} \left(\frac{(i\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} \right) + \cdots$$

$$= \sum_{i=1}^{n-2} (f_1) + \Delta x \frac{\partial f}{\partial x} \sum_{i=1}^{n-2} (i) + \frac{(\Delta x)^2}{2!} \frac{\partial^2 f}{\partial x^2} \sum_{i=1}^{n-2} (i^2) + \frac{(\Delta x)^3}{3!} \frac{\partial^3 f}{\partial x^3} \sum_{i=1}^{n-2} (i^3)$$

Now substitute this into the composite trapezoial rule and gather the coefficients,

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

Looking at one common term at a time, starting with f_1. (Note the two halfs summing to one),

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

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

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Now for the rest of the terms, factor out Δx^+,

$$(\Delta x^+)^2 \frac{\partial f}{\partial x} \left(\sum_{i=1}^{n-2} (i) + \frac{n-1}{2} \right) +$$

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

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

Using the following summation rules the problem can further simplified,

$$\sum_{i=1}^{n} c = cn$$

$$\sum_{i=1}^{n} i = \frac{n(n-1)}{2}$$

$$\sum_{i=1}^{n} i^2 = \frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6}$$

$$\sum_{i=1}^{n} i^3 = \frac{n^4}{4} + \frac{n^3}{2} + \frac{n^2}{4}$$

Putting the terms back together, and then simplifing with the closed form

expressions for the summations,

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

$$(\Delta x^+)^2 \frac{\partial f}{\partial x} \left(\sum_{i=1}^{n-2} (i) + \frac{n-1}{2} \right) +$$

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

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

$$\Delta x^+ f_1 \left[1 + (n-2) \right] +$$

$$(\Delta x^+)^2 \frac{\partial f}{\partial x} \left(\frac{(n-2)[(n-2)-1]}{2} + \frac{n-1}{2} \right) +$$

$$\frac{(\Delta x^+)^3}{2!} \frac{\partial^2 f}{\partial x^2} \left(\frac{(n-2)^3}{3} + \frac{(n-2)^2}{2} + \frac{(n-2)}{6} + \frac{(n-1)^2}{2} \right) +$$

$$\frac{(\Delta x^+)^4}{3!} \frac{\partial^3 f}{\partial x^3} \left(\frac{(n-2)^4}{4} + \frac{(n-2)^3}{2} + \frac{(n-2)^2}{4} + \frac{(n-1)^3}{2} \right) \dots$$

$$\Delta x^+ f_1\left[(n-1)\right]+$$

$$(\Delta x^+)^2 \frac{\partial f}{\partial x}\left(\frac{(n-2)\,(n-1)}{2}+\frac{n-1}{2}\right)+$$

$$\frac{(\Delta x^+)^3}{2!}\frac{\partial^2 f}{\partial x^2}\left(\frac{(n-2)^3}{3}+\frac{(n-2)^2}{2}+\frac{(n-2)}{6}+\frac{(n-1)^2}{2}\right)+$$

$$\frac{(\Delta x^+)^4}{3!}\frac{\partial^3 f}{\partial x^3}\left(\frac{(n-2)^4}{4}+\frac{(n-2)^3}{2}+\frac{(n-2)^2}{4}+\frac{(n-1)^3}{2}\right)\cdots$$

$$f_1\left[\Delta \widetilde{x}^+\right]+$$

$$(\Delta x^+)^2 \frac{\partial f}{\partial x}\left(\frac{(n-2)\,(n-1)}{2}+\frac{n-1}{2}\right)+$$

$$\frac{(\Delta x^+)^3}{2!}\frac{\partial^2 f}{\partial x^2}\left(\frac{(n-2)^3}{3}+\frac{(n-2)^2}{2}+\frac{(n-2)}{6}+\frac{(n-1)^2}{2}\right)+$$

Side note:

$$\frac{(n-2)(n-1)}{2}+\frac{(n-1)}{2}$$

$$\frac{(n-2)(n-1)+(n-1)}{2}$$

Factor out $(n-1)$

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

Using this for the coefficient of the second term,

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

The third term is expected 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. In addition, the leading coefficient is expected to have 1/6 as well. Multiplying by 3 and setting the result equal $(n-1)j^3$ gives,

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

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

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