# pyGEMS - 1D: A 1D Python Port of the General Mesh and Equations Solver

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**PLEASE NOTE**: THIS DOCUMENTATION IS NOT UP-TO-DATE. It is not reflective of the state of the code. Please check back in a couple days for completed documentation.

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# 1 Introduction

This code is intended to be a sort of low-fidelity Python port of the General Mesh and Equations Solver (GEMS) [?], originally written by Guoping Xia at Purdue University, and since expanded upon over the decades by researchers from Purdue University, the University of Michigan, Ann Arbor, and the Air Force Research Laboratory. Although this port is "low-fidelity" in the sense that the code lacks much of the functionality of the original GEMS solver (e.g. robustness controls, a wide variety of flow physics and reaction models, complex numerical solver algorithms), the hope is that this might serve as a useful code for reduced-order model (ROM) practitioners to develop and test new methods on simple 1D reacting flow problems, ideally with a low barrier to implementation and application. Additional functionality may be added over time to equip this code with tools found in GEMS.

# 2 Physics

### 2.1 Governing Equations

The equations of motion for the 1D flame are:

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} - \frac{\partial \mathbf{E}_v}{\partial x} = \mathbf{H},\tag{1}$$

where Q is the conservative variables,

$$\mathbf{Q} = \begin{pmatrix} \rho & \rho u & \rho h^0 - p & \rho Y_l \end{pmatrix}^\top, \tag{2}$$

E and  $E_v$  are the inviscid and viscous flux vectors, respectively:

$$\mathbf{E} = \begin{pmatrix} \rho u & \rho u^2 + p & \rho u h^0 & \rho u Y_l \end{pmatrix}^\top, \tag{3}$$

$$\mathbf{E}_{\mathbf{v}} = \begin{pmatrix} 0 & \tau & u\tau - q & -\rho V_{x,l} Y_l, \end{pmatrix}^{\top}, \tag{4}$$

where,  $\tau = \frac{4}{3}\mu_{ref}\frac{\partial u}{\partial x}$  is the shear stress, and q is the heat flux in the x direction:

$$q = -K\frac{\partial T}{\partial x} + \rho \sum_{l} V_{x,l} Y_{l} h_{l}. \tag{5}$$

Here, K is the mixture thermal conductivity:

$$K = \frac{1}{2} \left[ \sum_{l=1}^{N} X_l K_l + \left( \sum_{l=1}^{N} \frac{X_l}{K_l} \right)^{-1} \right], \tag{6}$$

and  $K_l = \frac{\mu_{ref,l}c_{p,l}}{Pr_l}$  is the thermal conductivity of the  $l^{th}$  species, obtained by the reference viscosity  $(\mu_{ref})$ , specific heat at constant pressure  $(c_p)$ , and the Prandtl number (Pr) of the  $l^{th}$  species. In the above formulation,  $X_l = Y_l(\frac{W}{(MW)_l})$  is the mole fraction, where W is the molecular weight of the mixture and  $(MW)_l$  is the molecular weight of the  $l^{th}$  species. The diffusion velocity  $V_{x,l}$  of species l in the x direction is obtained by:

$$Y_l V_{x,l} = -D_l \nabla Y_l, \tag{7}$$

where  $D_l = \frac{\mu_{ref,l}}{\rho Sc_l}$  is the species mass diffusivity, and  $Sc_l$  is the Schmidt number of the  $l^{th}$  species. Finally,  $\mathbf{H}$  is the chemical reaction source term,

$$\mathbf{H} = \begin{pmatrix} 0 & 0 & 0 & \dot{\omega}_l \end{pmatrix}^{\mathsf{T}} \tag{8}$$

The 1D code solves the vector of primitive variables,

$$\mathbf{Q}_p = \begin{pmatrix} p & u & T & Y_l \end{pmatrix}^\top. \tag{9}$$

With the dual-time scheme introduced for pseudo iteration,

$$\Gamma_{p} \frac{\partial \mathbf{Q}_{p}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{E}}{\partial x} - \frac{\partial \mathbf{E}_{v}}{\partial x} = \mathbf{H}, \tag{10}$$

where the transformation Jacobian,  $\Gamma_p = \frac{\partial \mathbf{Q}}{\partial \mathbf{Q}_p}$ , is,

$$\Gamma_{p} = \begin{pmatrix}
\rho_{P} & 0 & \rho_{T} & \rho_{Y_{l}} \\
u\rho_{P} & \rho & u\rho_{T} & u\rho_{Y_{l}} \\
\rho_{P}h^{0} + \rho h_{P} - 1 & \rho u & \rho_{T}h^{0} + \rho h_{T} & \rho_{Y_{l}}h^{0} + \rho h_{Y_{l}} \\
Y_{l}\rho_{P} & 0 & Y_{l}\rho_{T} & \rho + Y_{l}\rho_{Y_{l}}
\end{pmatrix}$$
(11)

The Jacobian for the inviscid flux  $\mathbf{E}$ ,  $A_p = \frac{\partial \mathbf{E}}{\partial \mathbf{Q}_p}$  is:

$$A_{p} = \begin{pmatrix} u\rho_{P} & \rho & u\rho_{T} & u\rho_{Y_{l}} \\ u^{2}\rho_{P} + 1 & 2\rho u & u^{2}\rho_{T} & u^{2}\rho_{Y_{l}} \\ \rho_{P}uh^{0} + \rho uh_{P} & \rho h^{0} + \rho u^{2} & u(\rho_{T}h^{0} + \rho h_{T}) & u(\rho_{Y_{l}}h^{0} + \rho h_{Y_{l}}) \\ uY_{l}\rho_{P} & \rho Y_{l} & uY_{l}\rho_{T} & u(\rho + Y_{l}\rho_{Y_{l}}) \end{pmatrix}$$

$$(12)$$

and the Jacobian for the viscous flux  $\mathbf{E}_v$ ,  $A_{p,v} = \frac{\partial \mathbf{E}_v}{\partial \mathbf{Q}_p}$  is:

$$A_{p,v} = \begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & \frac{4}{3}\mu_{ref} & 0 & 0\\ 0 & \frac{4}{3}\mu_{ref}u & K & \frac{\mu_{ref}}{Sc}h\\ 0 & 0 & 0 & \frac{\mu_{ref}}{Sc} \end{pmatrix},$$
(13)

where,  $h = \sum_{l} Y_{l} h_{l}$ , and  $h_{l}$  is the enthalpy of the  $l^{th}$  species.

## 2.2 Equation of State and Thermodynamic Properties

Th ideal gas law is used,

$$\rho = \frac{p}{RT} \tag{14}$$

where  $R = R_u/MW$  with  $R_u$  as the universal gas constant and  $MW = 1/\left(\sum_l \frac{Y_l}{(MW)_l}\right)$ . Here,  $Y_l$  and  $(MW)_l$  are the mass fraction and molecular weight of the  $l^{\text{th}}$  species, and the mass fraction of the last species is computed by the mass fractions of the rest of the species:

$$Y_N = 1 - \sum_{l=1}^{N-1} Y_l. (15)$$

Therefore,  $\rho_p=1/(RT)$ ,  $\rho_T=-p/(RT^2)$  and  $\rho_{Y_k}=-p/(R^2T)\frac{\partial R}{\partial Y_k}=-pR_u/(MW_lR^2T)$ . The stagnation enthalpy of the mixture reads:

$$h^0 = \sum_{l} Y_l h_l + \frac{u^2}{2},\tag{16}$$

where, the enthalpy of the  $l^{th}$  species is computed by its reference enthalpy and the reference temperature:

$$h_l = h_{ref,l} + c_{p,l}(T - T_{ref}),$$
 (17)

and  $c_{p,l}$  is the specific heat of the  $l^{th}$  species at constant pressure. Thus, the derivatives of the stagnation enthalpy are  $h_p = 0$ ,  $h_u = u$ ,  $h_T = \sum_l Y_l c_{p,l}$ , and  $h_{Y_l} = h_l - h_N$ .

Species	MW (g/mol)	$c_p$ (kJ/kg/K)	Pr	Sc	$\mu_{ref}$ (kg/m/s)	$h_{ref}$ (kJ/kg)
Reactant	21.32	1.538	0.713	0.62	$7.35 \times 10^{-4}$	-7,432
Product	21.32	1.538	0.713	0.62	$7.35 \times 10^{-4}$	-10,800

Table 1: Properties of species reactant and product.

### 2.3 Reaction Model

The 1D problem was calculated with simplified single-step, two-species reaction,

Reactant 
$$\rightarrow$$
 Product. (18)

where both the reactant and product species are formulated as calorically perfect gases (CPG).

The expression for the chemical reaction source term for the reactant follows the Arrhenius form,

$$\dot{\omega}_{\text{Reactant}} = -MW_{\text{Reactant}} \cdot A \exp\left(\frac{-E_A/R_u}{T}\right) \left[\frac{\rho Y_{\text{Reactant}}}{MW_{\text{Reactant}}}\right]^a \tag{19}$$

where the pre-exponential factor  $A = 2 \times 10^{10}$ , the activation energy  $E_A/R_u = 24358$  and the concentration exponent has been set to unity, a = 1.0.

Therefore the Jacobian for the source term,  $D_p = \frac{\partial \mathbf{H}}{\partial \mathbf{Q}_p}$ , is,

where (will check the derivations below),

$$\frac{\partial \dot{\omega}_{\text{Reactant}}}{\partial p} = -\rho_{p} M W_{\text{Reactant}} \cdot A \exp\left(\frac{-E_{A}/R_{u}}{T}\right) \left(\frac{Y_{\text{Reactant}}}{M W_{\text{Reactant}}}\right) \tag{21}$$

$$\frac{\partial \dot{\omega}_{\text{Reactant}}}{\partial T} = -\rho_{T} M W_{\text{Reactant}} \cdot A \exp\left(\frac{-E_{A}/R_{u}}{T}\right) \left(\frac{Y_{\text{Reactant}}}{M W_{\text{Reactant}}}\right) + M W_{\text{Reactant}} \frac{-E_{A}/R_{u}}{T^{2}} \cdot A \exp\left(\frac{-E_{A}/R_{u}}{T}\right) \left(\frac{\rho Y_{\text{Reactant}}}{M W_{\text{Reactant}}}\right)$$

$$\frac{\partial \dot{\omega}_{\text{Reactant}}}{\partial Y_{\text{Reactant}}} = -\rho_{Y_{\text{Reactant}}} M W_{\text{Reactant}} \cdot A \exp\left(\frac{-E_{A}/R_{u}}{T}\right) \left(\frac{Y_{\text{Reactant}}}{M W_{\text{Reactant}}}\right) - M W_{\text{Reactant}} \cdot A \exp\left(\frac{-E_{A}/R_{u}}{T}\right) \left(\frac{\rho}{M W_{\text{Reactant}}}\right)$$

$$(23)$$

#### **Numerics** 3

#### 3.1 **Spatial Discretization**

The finite volume formulation of Eq. 10 is (assuming constant area computation domain),

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \Gamma_p \frac{\partial \mathbf{Q}_p}{\partial \tau} dx + \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \mathbf{Q}}{\partial t} dx + \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \mathbf{E}}{\partial x} dx - \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \mathbf{E}_v}{\partial x} dx = \int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{H} dx$$
 (24)

where,

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \mathbf{E}}{\partial x} dx = \mathbf{E}_{i+1/2} - \mathbf{E}_{i-1/2}$$
(25)

Then Eq. 24 becomes,

$$\Gamma_{p} \frac{\partial \mathbf{Q}_{p,i}}{\partial \tau} + \frac{\partial \mathbf{Q}_{i}}{\partial t} + \frac{\mathbf{E}_{i+1/2} - \mathbf{E}_{i-1/2}}{x_{i+1/2} - x_{i-1/2}} - \frac{\mathbf{E}_{v,i+1/2} - \mathbf{E}_{v,i-1/2}}{x_{i+1/2} - x_{i-1/2}} = \mathbf{H}_{i}$$
 (26)

where  $Q_{p,i}$  is the solution variables at  $i_{th}$  cell center.

### **Roe Flux Difference Splitting**

The flux at  $i + 1/2^{th}$  face of  $i^{th}$  cell can be written as

$$\mathbf{E}_{i+1/2} = \frac{1}{2} \left[ \mathbf{E}_i + \mathbf{E}_{i+1} \right] - \frac{1}{2} \left[ \left| \frac{\partial \mathbf{E}}{\partial Q_p} \frac{\partial Q_p}{\partial Q} \right| \frac{\partial Q}{\partial Q_p} \delta Q_{p,i+1/2} \right]$$
(27)

where the dissipation can be recognized as the last term. Writing this in terms of the Jacobian  $\Gamma$ ,

$$\mathbf{E}_{i+1/2} = \frac{1}{2} \left[ \mathbf{E}_i + \mathbf{E}_{i+1} \right] - \frac{1}{2} \left( \left[ |A_p \Gamma_p^{-1}| \Gamma_p \right] \right)_{i+1/2} \delta Q_{i+1/2}$$
 (28)

using the relation |CB|A = A|BC|,

$$\mathbf{E}_{i+1/2} = \frac{1}{2} \left[ \mathbf{E}_i + \mathbf{E}_{i+1} \right] - \frac{1}{2} \left( \left[ \Gamma_p | \Gamma_p^{-1} A_p | \right] \right)_{i+1/2} \delta Q_{i+1/2}$$
 (29)

where the matrix  $\lceil \Gamma^{-1} A \rceil$  can be written using the eigenvalue and right eigenvector matrix as,

$$\left(|\Gamma_p^{-1} A_p|\right)_{i+1/2} = \left[R|\Lambda|R^{-1}\right]_{i+1/2} \tag{30}$$

In order to conserve the fluxes while using the direction of the fluxes in determining the dissipation, appropriate average values need to be used. This is accomplished following the averaging procedure due to Roe, which for the density, velocity and enthalpy is given as:

$$\rho_{i+1/2} = \sqrt{\rho_i \rho_{i+1}} \tag{31}$$

$$u_{i+1/2} = \frac{u_i \sqrt{\rho_i} + u_{i+1} \sqrt{\rho_{i+1}}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}$$
(31)

$$h_{i+1/2} = \frac{h_i \sqrt{\rho_i} + h_{i+1} \sqrt{\rho_{i+1}}}{\sqrt{\rho_i} + \sqrt{\rho_{i+1}}}$$
(33)

(34)

The remaining variables follow the same averaging procedure as velocity and enthalpy.

### 3.3 Face Reconstruction

The viscous flux is evaluated at the cell faces. Therefore, variables are defined on the face of each cell using Taylor series:

$$\mathbf{Q}_{p,L} \approx \mathbf{Q}_p - \phi \nabla \mathbf{Q}_p(\frac{\Delta x}{2}), \tag{35}$$

$$\mathbf{Q}_{p,R} \approx \mathbf{Q}_p + \phi \nabla \mathbf{Q}_p(\frac{\Delta x}{2}),$$
 (36)

where,  $\Delta x = x_{i+1} - x_i$ , and  $\mathbf{Q}_{p,L}$  and  $\mathbf{Q}_{p,R}$  are the vectors of primitive variables evaluated at the left and right cell faces, respectively. The gradient  $\nabla \mathbf{Q}_p$  is evaluated at the cell centers using a first-order difference scheme (i.e., second-order central difference with respect to the cell face):

$$\nabla \mathbf{Q}_{p,i} = \frac{\mathbf{Q}_{p,i} - \mathbf{Q}_{p,i-1}}{\Delta x},\tag{37}$$

Here,  $\phi$  is the cell limiter that is introduced to enhance stability:

$$\phi = \min(\phi_L, \phi_R),\tag{38}$$

and,

$$\phi_L = \begin{cases} min(1, \frac{\mathbf{Q}_{p,max} - \mathbf{Q}_p}{\mathbf{Q}_{p,L} - \mathbf{Q}_p}) & \mathbf{Q}_{p,L} - \mathbf{Q}_p < 0, \\ min(1, \frac{\mathbf{Q}_{p,min} - \mathbf{Q}_p}{\mathbf{Q}_{p,L} - \mathbf{Q}_p}) & \mathbf{Q}_{p,L} - \mathbf{Q}_p > 0, \end{cases}$$
(39)

$$\phi_R = \begin{cases} min(1, \frac{\mathbf{Q}_{p,max} - \mathbf{Q}_p}{\mathbf{Q}_{p,R} - \mathbf{Q}_p}) & \mathbf{Q}_{p,R} - \mathbf{Q}_p < 0, \\ min(1, \frac{\mathbf{Q}_{p,min} - \mathbf{Q}_p}{\mathbf{Q}_{n,R} - \mathbf{Q}_p}) & \mathbf{Q}_{p,R} - \mathbf{Q}_p > 0, \end{cases}$$
(40)

where,  $\mathbf{Q}_{p,L}$  and  $\mathbf{Q}_{p,R}$  are initially evaluated without the limiter (i.e., using  $\phi = 1$ ), and  $\mathbf{Q}_{p,max}$  and  $\mathbf{Q}_{p,min}$  indicate the maximum and minimum values at the neighboring cells. Finally, the values computed at the cell faces by equations 35 and 36 are Roe-averaged and used to evaluate the viscous flux.

## 3.4 Temporal Discretization

Two types of discretization in time to approximate physical time derivative can be used. The one with first-order accuracy is shown in Eq. 41

$$\frac{\partial \mathbf{Q}}{\partial t} = \frac{\mathbf{Q}^{n+1} - \mathbf{Q}^n}{\Delta t},\tag{41}$$

and the second-order one is shown in Eq. 42

$$\frac{\partial \mathbf{Q}}{\partial t} = \frac{3\mathbf{Q}^{n+1} - 4\mathbf{Q}^n + \mathbf{Q}^{n-1}}{2\Delta t}.$$
(42)

As mentioned in previous section, finite volume methods and flux scheme are used to discretize the spatial derivative and the resulting algebraic system is then solved by introducing a pseudo-time derivative into Eq. 1 as an iterative variable that can be marched from a selected initial condition to a converged final result. Because  $\frac{\partial \mathbf{Q_p}}{\partial \tau}$  vanishes as the pseudo time goes to infinity and so have no impact on the final solution it can be expressed in non-conservative form,

$$\Gamma_{p} \frac{\partial \mathbf{Q}_{p,i}}{\partial \tau} + \frac{\partial \mathbf{Q}_{i}}{\partial t} + (\mathbf{E}_{i+1/2} - \mathbf{E}_{i-1/2}) - (\mathbf{E}_{v,i+1/2} - \mathbf{E}_{v,i-1/2}) = \mathbf{H}_{i}$$
(43)

The pseudo time derivative introduced in Eq. 45 is approximated using time discretization of first order accuracy,

$$\frac{\partial \mathbf{Q}_p}{\partial \tau} = \frac{\mathbf{Q}_p^{n+1} - \mathbf{Q}_p^n}{\Delta \tau} \tag{44}$$

During the advancement from time n to time step k + 1,

$$\Gamma_{p,i}^{k} \frac{\mathbf{Q}_{p,i}^{k+1} - \mathbf{Q}_{p,i}^{k}}{\Delta \tau} + \frac{3}{2} \frac{\mathbf{Q}_{i}^{k+1} - \mathbf{Q}_{i}^{k}}{\Delta t} = -\mathbf{S}_{i}^{k} - \frac{\mathbf{E}_{i+1/2}^{k+1} - \mathbf{E}_{i-1/2}^{k+1}}{x_{i+1/2} - x_{i-1/2}} + \frac{\mathbf{E}_{v,i+1/2}^{k+1} - \mathbf{E}_{v,i-1/2}^{k+1}}{x_{i+1/2} - x_{i-1/2}} + \mathbf{H}_{i}^{k+1}$$
(45)

where,

$$\mathbf{S}^k = \frac{3\mathbf{Q}^k - 4\mathbf{Q}^n + \mathbf{Q}^{n-1}}{2\Delta t} \tag{46}$$

and,

$$\mathbf{E}^{k+1} = \mathbf{E}^k + \mathbf{A}_p^k \left( \mathbf{Q}_p^{k+1} - \mathbf{Q}_p^k \right) \tag{47}$$

$$\mathbf{E}_{v}^{k+1} = \mathbf{E}_{v}^{k} + \mathbf{A}_{p,v}^{k} \left( \mathbf{Q}_{p}^{k+1} - \mathbf{Q}_{p}^{k} \right)$$

$$\tag{48}$$

Therefore the final discretized ODE format of the governing equations becomes,

$$\left(\frac{\Gamma_p^k}{\Delta \tau} + \frac{3}{2} \frac{\Gamma_p^k}{\Delta t} - D^k + \left(\tilde{A}_p^k - \tilde{A}_{p,v}^k\right)_R - \left(\tilde{A}_p^k - \tilde{A}_{p,v}^k\right)_L\right) \left(\mathbf{Q}_p^{k+1} - \mathbf{Q}_p^k\right) =$$

$$-\mathbf{S}^k - \frac{\mathbf{E}_R^k - \mathbf{E}_L^k}{x_R - x_L} + \frac{\mathbf{E}_{v,R}^k - \mathbf{E}_{v,L}^k}{x_R - x_L} + \mathbf{H}^k$$
(49)

where

$$\mathbf{Q}_{p}^{k} = \begin{pmatrix} \mathbf{Q}_{p,1}^{k} & \mathbf{Q}_{p,2}^{k} & \cdots & \mathbf{Q}_{p,NI-1}^{k} & \mathbf{Q}_{p,NI}^{k} \end{pmatrix}^{\top}.$$
 (50)

and  $D^k$  is the chemical source term Jacobian,  $D = \frac{\partial \mathbf{H}}{\partial \mathbf{Q}_p}$  and the flux Jacobians,  $\tilde{A}_p^k$  and  $\tilde{A}_{p,v}^k$  are evaluated for each cell face.

# 3.5 Boundary Conditions

# 3.6 Linearized Equations

Linearization of the flux in equation (28) yields:

$$\mathbf{E}_{i+1/2} = \frac{1}{2} \left[ \bar{\mathbf{E}}_{i} + \frac{\overline{\partial \mathbf{E}_{i}}}{\partial \mathbf{Q}_{i}} \mathbf{Q}_{i}' + \bar{\mathbf{E}}_{i+1} + \frac{\overline{\partial \mathbf{E}_{i+1}}}{\partial \mathbf{Q}_{i+1}} \mathbf{Q}_{i+1}' \right] - \frac{1}{2} \left( \left[ |A_{p} \Gamma_{p}^{-1}| \Gamma_{p} \right] \right)_{i+1/2} (\bar{\mathbf{Q}}_{i+1} + \mathbf{Q}_{i+1}' - \bar{\mathbf{Q}}_{i} - \mathbf{Q}_{i}').$$
(51)

Similarly,

$$\mathbf{E}_{i-1/2} = \frac{1}{2} \left[ \bar{\mathbf{E}}_{i-1} + \frac{\overline{\partial \mathbf{E}_{i-1}}}{\partial \mathbf{Q}_{i-1}} \mathbf{Q}'_{i-1} + \bar{\mathbf{E}}_i + \frac{\overline{\partial \mathbf{E}_i}}{\partial \mathbf{Q}_i} \mathbf{Q}'_i \right] - \frac{1}{2} \left( \left[ |A_p \Gamma_p^{-1}| \Gamma_p \right] \right)_{i-1/2} (\bar{\mathbf{Q}}_i + \mathbf{Q}'_i - \bar{\mathbf{Q}}_{i-1} - \mathbf{Q}'_{i-1}),$$
(52)

and the linearized source term is:

$$\mathbf{H}_{i} = \mathbf{\bar{H}}_{i} + \frac{\overline{\partial \mathbf{H}_{i}}}{\partial \mathbf{Q}_{i}} \mathbf{Q}_{i}^{\prime}. \tag{53}$$

where  $\frac{\partial \mathbf{E}}{\partial \mathbf{Q}} = \frac{\partial \mathbf{E}}{\partial \mathbf{Q}_p} \frac{\partial \mathbf{Q}_p}{\partial \mathbf{Q}} = A_p \Gamma_p^{-1}$ , and  $\frac{\partial \mathbf{H}}{\partial \mathbf{Q}} = \frac{\partial \mathbf{H}}{\partial \mathbf{Q}_p} \frac{\partial \mathbf{Q}_p}{\partial \mathbf{Q}} = D_p \Gamma_p^{-1}$ . The viscous flux is linearized in a similar manner. Substituting the linearized fluxes and source term in the semi-discretized form of equation (1), and denoting  $\mathbf{F} = \mathbf{E} - \mathbf{E}_v$ , we get the following ODE for the state perturbation:

$$\frac{d\mathbf{Q}_{i}'}{dt} = -\frac{1}{2\Delta x} \left[ \frac{\overline{\partial \mathbf{F}_{i}}}{\partial \mathbf{Q}_{i}} \mathbf{Q}_{i}' + \frac{\overline{\partial \mathbf{F}_{i+1}}}{\partial \mathbf{Q}_{i+1}} \mathbf{Q}_{i+1}' \right] + \frac{1}{2\Delta x} \left( \left[ \overline{|A_{p}\Gamma_{p}^{-1}|\Gamma_{p}} \right] \right)_{i+1/2} (\mathbf{Q}_{i+1}' - \mathbf{Q}_{i}') 
+ \frac{1}{2\Delta x} \left[ \frac{\overline{\partial \mathbf{F}_{i-1}}}{\partial \mathbf{Q}_{i-1}} \mathbf{Q}_{i-1}' + \frac{\overline{\partial \mathbf{F}_{i}}}{\partial \mathbf{Q}_{i}} \mathbf{Q}_{i}' \right] - \frac{1}{2\Delta x} \left( \left[ \overline{|A_{p}\Gamma_{p}^{-1}|\Gamma_{p}} \right] \right)_{i-1/2} (\mathbf{Q}_{i}' - \mathbf{Q}_{i-1}') 
+ \frac{\overline{\partial \mathbf{H}_{i}}}{\partial \mathbf{Q}_{i}} \mathbf{Q}_{i}'.$$
(54)

where,  $\Delta x = x_{i+1/2} - x_{i-1/2}$ , and the equation is further simplified as below:

$$\frac{d\mathbf{Q}_{i}'}{dt} = -\frac{1}{2\Delta x} \left[ \frac{\overline{\partial \mathbf{F}_{i+1}}}{\partial \mathbf{Q}_{i+1}} \mathbf{Q}_{i+1}' - \left( \left[ \overline{|A_{p}\Gamma_{p}^{-1}|\Gamma_{p}} \right] \right)_{i+1/2} (\mathbf{Q}_{i+1}' - \mathbf{Q}_{i}') \right] 
+ \frac{1}{2\Delta x} \left[ \frac{\overline{\partial \mathbf{F}_{i-1}}}{\partial \mathbf{Q}_{i-1}} \mathbf{Q}_{i-1}' - \left( \left[ \overline{|A_{p}\Gamma_{p}^{-1}|\Gamma_{p}} \right] \right)_{i-1/2} (\mathbf{Q}_{i}' - \mathbf{Q}_{i-1}') \right] + \frac{\overline{\partial \mathbf{H}_{i}}}{\partial \mathbf{Q}_{i}} \mathbf{Q}_{i}'.$$
(55)

### 3.7 Linearized Boundary Conditions

Boundary conditions are implemented at the ghost points. In the linearized equations, only the perturbation variables are calculated at the boundaries. Thus, for the mean flow non-reflective boundary conditions at the inlet we have:

$$P_0' = -\frac{w_3'(\overline{\rho c})}{2},\tag{56}$$

$$u_0' = -\frac{P_0'}{\overline{\rho c}},\tag{57}$$

$$T_0' = \frac{P_0'}{\rho C_p},\tag{58}$$

$$Y'_{k,0} = 0, (59)$$

where the zero index corresponds to the ghost cell, c is the speed of sound, and variables with over-line are evaluated by the mean flow.  $w_3'$  is the characteristic variable corresponding to the outgoing characteristic line:

$$w_3' = u' - \frac{P'}{\rho c},\tag{60}$$

which is extrapolated from the first interior cell.

Similarly, for the mean flow non-reflective boundary conditions at the outlet we have:

$$P'_{N+1} = \frac{w_2' \overline{\rho c} + P_b}{2},\tag{61}$$

$$u'_{N+1} = \frac{P'_{N+1} - P_b}{\overline{\rho c}},\tag{62}$$

$$T'_{N+1} = w'_1 + \frac{P'_{N+1}}{\overline{\rho C_p}},\tag{63}$$

$$Y'_{N+1} = w'_4, (64)$$

where N+1 is the index of the ghost cell, and  $P_b$  is pressure perturbation.  $w_1'$ ,  $w_2'$ , and  $w_4'$  are the characteristic variables corresponding to the outgoing characteristic lines:

$$w_1' = T' - \frac{P'}{\overline{\rho C_p}},\tag{65}$$

$$w_2' = u' + \frac{P'}{\overline{\rho c}},\tag{66}$$

$$w_4' = Y_k', (67)$$

that are extrapolated from the last interior cell.

# 4 Projection-based Reduced-Order Modeling

- 4.1 Galerkin Projection
- 4.2 Least-Squares Petrov-Galerkin Projection
- 4.3 Structure-Preserving Least-squares with Variable Transformation
- 4.4 Linear Subspace Methods
- 4.4.1 Proper Orthogonal Decomposition
- 4.5 Nonlinear Manifold Methods via Convolutional Autoencoders
- 4.5.1 An Encoder Projection Approximation

- 5 Utilities
- **5.1** Mean-flow Boundary Parameter Calculations
- **5.2 POD Basis Generation**
- **5.3** Projection Error Calculations