

# **Cgcns** Reference Manual: An Overture Solver for the Compressible Navier–Stokes Equations on Composite Overlapping Grids

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## **Abstract:**

**Cgcns** can be used to solve the compressible Navier-Stokes equations, the reactive Euler equations, multi-fluid and multi-phase equations on moving overlapping grids with adaptive mesh refinement. This document is a reference manual for Cgcns and describes the governing equations, equations of state, reactions, and boundary conditions. Also included are the results from a collection of computations that demonstrate the capabilities of Cgcns.

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# 1 Introduction

Cgcns solves the compressible Navier-Stokes equations and reactive Euler (i.e. inviscid) equations (and variations thereof, see below) on overlapping grids and is built upon the **Overture** framework [1],[3],[2].

Cgcns can be used to solve problems in complex geometry and moving and deforming geometry. Cgcns uses adaptive mesh refinement (AMR).

Cgcns can be used to solve the

1. Euler equations.
2. reactive Euler equations with
  - (a) one-step reaction 3.1
  - (b) ignition and growth reaction for explosives modeling 3.3.
3. compressible Navier-Stokes.
4. multi-fluid Euler equations 2.4.
5. multi-phase Euler equations 2.5.

Here are some papers that describe the algorithms

## References

Here are some papers that use Cgcns to solve problems

## 2 The Equations

### 2.1 The compressible Euler equations

### 2.2 The compressible Navier-Stokes equations

The compressible Navier-Stokes equations can be written in conservation form

$$\mathbf{u}_t + \frac{\partial \mathbf{F}}{\partial x_1} + \frac{\partial \mathbf{G}}{\partial x_2} + \frac{\partial \mathbf{H}}{\partial x_3} = 0.$$

The vector of conserved variables  $\mathbf{u}$  is

$$\mathbf{u} = \begin{bmatrix} \rho \\ E \\ \rho v_1 \\ \rho v_2 \\ \rho v_3 \end{bmatrix},$$

where  $\rho$ ,  $E$  and  $\mathbf{v} = [v_1, v_2, v_3]^T$  denote the density, energy and velocity vector with components parallel to the  $x_1$ ,  $x_2$ , and  $x_3$  axes, respectively. The fluxes

$$\begin{bmatrix} \mathbf{F} \\ \mathbf{G} \\ \mathbf{H} \end{bmatrix} = \begin{bmatrix} \mathbf{F}^C \\ \mathbf{G}^C \\ \mathbf{H}^C \end{bmatrix} - \begin{bmatrix} \mathbf{F}^V \\ \mathbf{G}^V \\ \mathbf{H}^V \end{bmatrix}$$

are a combination of *convective* fluxes  $[\mathbf{F}^C, \mathbf{G}^C, \mathbf{H}^C]^T$  and *viscous* fluxes  $[\mathbf{F}^V, \mathbf{G}^V, \mathbf{H}^V]^T$ . The convective (or Euler) fluxes are given by

$$\mathbf{F}^C = \begin{bmatrix} \rho v_1 \\ v_1(E + p) \\ \rho v_1^2 + p \\ \rho v_2 v_1 \\ \rho v_3 v_1 \end{bmatrix}, \quad \mathbf{G}^C = \begin{bmatrix} \rho v_2 \\ v_2(E + p) \\ \rho v_1 v_2 \\ \rho v_2^2 + p \\ \rho v_3 v_2 \end{bmatrix}, \quad \mathbf{H}^C = \begin{bmatrix} \rho v_3 \\ v_3(E + p) \\ \rho v_1 v_3 \\ \rho v_2 v_3 \\ \rho v_3^2 + p \end{bmatrix},$$

and the viscous fluxes are

$$\mathbf{F}^V = \begin{bmatrix} 0 \\ \sum_n v_n \tau_{1n} - q_1 \\ \tau_{11} \\ \tau_{12} \\ \tau_{13} \end{bmatrix}, \quad \mathbf{G}^V = \begin{bmatrix} 0 \\ \sum_n v_n \tau_{2n} - q_2 \\ \tau_{21} \\ \tau_{22} \\ \tau_{23} \end{bmatrix}, \quad \mathbf{H}^V = \begin{bmatrix} 0 \\ \sum_n v_n \tau_{3n} - q_3 \\ \tau_{31} \\ \tau_{32} \\ \tau_{33} \end{bmatrix}.$$

The pressure,  $p$ , and temperature,  $T$ , are given by the relations

$$p = (\gamma - 1) \left[ E - \frac{1}{2} \rho (v_1^2 + v_2^2 + v_3^2) \right],$$

$$T = \frac{p}{\rho R_g},$$

where  $R_g$  is the gas constant. The viscous stress terms,  $\tau_{mn}$ , and heat flux,  $q_n$ , are given by

$$\tau_{mn} = \mu \left( \frac{\partial v_n}{\partial x_m} + \frac{\partial v_m}{\partial x_n} \right) - \frac{2}{3} \mu (\nabla \cdot \mathbf{v}) \delta_{mn},$$

$$q_n = -k \frac{\partial T}{\partial x_n} = -\frac{k}{R_g} \frac{\partial}{\partial x_n} \left( \frac{p}{\rho} \right) := -\tilde{k} \frac{\partial}{\partial x_n} \left( \frac{p}{\rho} \right),$$

where  $\delta_{mn}$  is the Kronecker delta and  $\tilde{k} = k/R_g$  is a scaled thermal conductivity.

## 2.3 The reactive Euler Equations

## 2.4 The multi-fluid equations

## 2.5 The compressible multi-phase equations

# 3 Reactions

The species equation is

$$(\rho \mathbf{Y})_t + \nabla \cdot (\rho \mathbf{u} \mathbf{Y}) = R$$

## 3.1 One-step Reaction

For the one-step reaction

$$R = (1 - Y) \sigma \exp(\epsilon^{-1} (1 - 1/T))$$

where

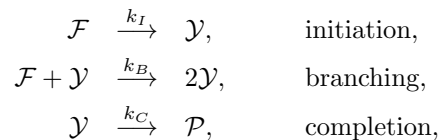
$$\sigma = \frac{\tilde{\sigma} \epsilon}{(\gamma - 1) |Q|}$$

$\tilde{\sigma}$  = rate constant  
 $\epsilon$  = reciprocal activation energy  
 $Q$  = heat release

The parameters  $\tilde{\sigma}$ ,  $Q$  and  $\epsilon$  are assigned in the command file.

## 3.2 Chain-branching reaction

The chain-branching reaction is a three-step reaction given by



where  $\mathcal{F}$ ,  $\mathcal{Y}$  and  $\mathcal{P}$  denote fuel, radical and product species, respectively, and  $k_I$ ,  $k_B$  and  $k_C$  are the rates of the initiation, branching and completion reactions, respectively (see [5]). The initiation and branching rates are assumed to have state-sensitive Arrhenius forms

$$k_i = \exp \left[ \frac{1}{\epsilon_i} \left( \frac{1}{T_i} - \frac{1}{T} \right) \right], \quad i = I \text{ or } B, \quad (1)$$

where  $\epsilon_I$  and  $\epsilon_B$  are reciprocal activation energies and  $T_I$  and  $T_B$  are cross-over temperatures. The completion reaction rate is taken to be  $k_C = 1$  which specifies the time scale. For this case,  $\mathbf{Y} = [\beta_1, \beta_2]^T$ , where  $\beta_1$  is the fraction of product and  $\beta_2$  is the fraction of radical (the fraction of fuel is  $1 - \beta_1 - \beta_2$ ). Laws of mass action give

$$\mathbf{R} = \begin{bmatrix} \beta_2 k_C \\ (1 - \beta_1 - \beta_2)(k_I + \beta_2 k_B) - \beta_2 k_C \end{bmatrix}, \quad (2)$$

and the contribution to the total energy is

$$q = \beta_1 Q_1 + \beta_2 Q_2.$$

Here,  $Q_1 < 0$  is the total chemical energy available in the unreacted mixture and  $Q_2 > 0$  is the amount of energy absorbed by the initiation and branching reactions to convert fuel to (energetic) radical.

### 3.3 Ignition and growth reaction

Finish me.

### 3.4 Ignition and growth with desensitization

Finish me.

### 3.5 One equation mixture fraction

Finish me.

### 3.6 Two equation mixture fraction and extent of reaction

Finish me.

### 3.7 One step pressure law

Finish me.

## 4 Axisymmetric Equations (Cylindrical Coordinates)

The equations for axisymmetric flow are derived from the full Navier-Stokes equations written in cylindrical coordinates  $(x, r, \theta)$ . Let  $\mathbf{v} = u\hat{\mathbf{x}} + v\hat{\mathbf{r}} + w\hat{\boldsymbol{\theta}}$  denote the components of the velocity in cylindrical coordinates (i.e.  $u = V^x$ ,  $v = V^r$  and  $w = V^\theta$ ). The Euler equations in conservation form in cylindrical coordinates are (\*CHECK ME\*) (finish me for Navier-Stokes)

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v) + \frac{1}{r} \frac{\partial}{\partial \theta}(\rho w) = 0 \quad (3)$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v u) + \frac{1}{r} \frac{\partial}{\partial \theta}(\rho w u) + \frac{\partial p}{\partial x} = 0 \quad (4)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho u v) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v v) + \frac{1}{r} \frac{\partial}{\partial \theta}(\rho w v) + \frac{\partial p}{\partial r} = 0 \quad (5)$$

$$\frac{\partial}{\partial t}(\rho w) + \frac{\partial}{\partial x}(\rho u w) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v w) + \frac{1}{r} \frac{\partial}{\partial \theta}(\rho w w) + \frac{1}{r} \frac{\partial p}{\partial \theta} = 0 \quad (6)$$

$$\frac{\partial}{\partial t}(E) + \frac{\partial}{\partial x}(u(E + p)) + \frac{1}{r} \frac{\partial}{\partial r}(r v(E + p)) + \frac{1}{r} \frac{\partial}{\partial \theta}(w(E + p)) = 0 \quad (7)$$

In the case where there is no variation in the angular direction  $\theta$  direction we have the equations for two-dimensional axisymmetric flow,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v) = 0 \quad (8)$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u u) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v u) + \frac{\partial p}{\partial x} = 0 \quad (9)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho u v) + \frac{1}{r} \frac{\partial}{\partial r}(r \rho v v) + \frac{\partial p}{\partial r} = 0 \quad (10)$$

$$\frac{\partial}{\partial t}(E) + \frac{\partial}{\partial x}(u(E + p)) + \frac{1}{r} \frac{\partial}{\partial r}(r v(E + p)) = 0 \quad (11)$$

The two-dimensional axisymmetric equations can be written in the form of the two-dimensional Cartesian equations plus source terms

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial r}(\rho v) + \frac{\rho v}{r} = 0 \quad (12)$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u u) + \frac{\partial}{\partial r}(\rho v u) + \frac{\rho v u}{r} + \frac{\partial p}{\partial x} = 0 \quad (13)$$

$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(\rho u v) + \frac{\partial}{\partial r}(\rho v v) + \frac{\rho v v}{r} + \frac{\partial p}{\partial r} = 0 \quad (14)$$

$$\frac{\partial}{\partial t}(E) + \frac{\partial}{\partial x}(u(E + p)) + \frac{\partial}{\partial r}(v(E + p)) + \frac{v(E + p)}{r} = 0 \quad (15)$$

Note that on the axis  $r = 0$ ,  $v = 0$  and thus

$$\frac{\rho v}{r} = \frac{\partial}{\partial r}(\rho v) = \rho \frac{\partial v}{\partial r}, \quad \text{on } r = 0 \quad (16)$$

$$\frac{\rho u v}{r} = \frac{\partial}{\partial r}(\rho u v) = \rho u \frac{\partial v}{\partial r}, \quad \text{on } r = 0 \quad (17)$$

$$\text{etc.} \quad (18)$$

When using Cgns to compute axisymmetric flow, the  $r$  direction corresponds to the  $y$ -axis and the axis of symmetry is  $y = 0$ .

## 5 Discretization

Finish me ...

## 6 Cgns Boundary Conditions

Here is a description of the boundary conditions for Cgns.

**Note:** Normally the boundary conditions assign the primitive variables:

$$\mathbf{r} = \rho, \quad (\text{density}) \quad (19)$$

$$\mathbf{u} = u, \quad (\text{x-component of the velocity}) \quad (20)$$

$$\mathbf{v} = v, \quad (\text{y-component of the velocity}) \quad (21)$$

$$\mathbf{w} = w, \quad (\text{z-component of the velocity}) \quad (22)$$

$$\mathbf{T} = T, \quad (\text{Temperature}) \quad (23)$$

$$\mathbf{s} = s, \quad (\text{species component}) \quad (24)$$

**NOTE:** For the Godunov scheme  $\mathbf{T}$  is defined to be  $p/\rho = R_g T$ , i.e. the Godunov scheme works with  $R_g T$  instead of  $T$ .

### 6.1 superSonicInflow

At a supersonic inflow all variables are given (since all characteristics are entering the domain):

$$\begin{bmatrix} \rho \\ \mathbf{u} \\ T \\ \mathbf{s} \end{bmatrix} = \begin{bmatrix} \rho_0(\mathbf{x}, t) \\ \mathbf{u}_0(\mathbf{x}, t) \\ T_0(\mathbf{x}, t) \\ \mathbf{s}_0(\mathbf{x}, t) \end{bmatrix}. \quad (25)$$

Examples:

1. Set the density ( $\mathbf{r}$ ),  $\mathbf{u}$  component of velocity and total energy,  $\mathbf{e}$ , ( $\mathbf{e} = \rho e + \frac{1}{2}\rho|\mathbf{u}|^2$ ) to a uniform value on inflow:

```
backGround(0,0)=superSonicInflow uniform(r=2.6667,u=1.25,e=10.119)
```

2. Set the density ( $\mathbf{r}$ ),  $\mathbf{u}$  component of velocity and total energy, temperature, and a species component ( $\mathbf{s}$ ) to a uniform value on inflow:

```
channel(1,0)=superSonicInflow uniform(r=1.0,u=-3.2,T=9.325417e-01,s=2.033854e-02)
```

### 6.2 superSonicOutflow

At a supersonic outflow all variables are extrapolated (since all characteristics are exiting the domain) and thus nothing needs to be set.

Example:

1. Assign superSonicOutflow:

```
backGround(0,1)=superSonicOutflow
```

### 6.3 slipWall

At a slip wall the normal component of the velocity is specified (normally zero for a non-moving wall),

$$\mathbf{n} \cdot \mathbf{u} = g(\mathbf{x}, t) \quad (26)$$

Example:

1. Assign a slipWall boundary condition,

```
annulus(0,1)=slipWall
```

There are different implementations of the slip wall BC. These are chosen using the following option:

```
OBPDE:slip wall boundary condition option [0|1|2|3|4]
```

```
(** finish me**)
```

## 6.4 subSonicInflow

At a subsonic inflow there is one characteristic leaving the domain so that all variables except one are specified. There are different possible options that one could apply for subsonic inflow. Here we set the incoming velocity and apply mixed conditions on the density and temperature (\*\*check me\*\*)

$$\text{subSonicInflow: } \begin{bmatrix} \alpha_\rho \rho + \beta_\rho \rho_n = g_\rho(\mathbf{x}, t), \\ \mathbf{u} \\ \alpha_T T + \beta_T T_n = g_T(\mathbf{x}, t), \\ \mathbf{s} \end{bmatrix} = \begin{bmatrix} \rho_0(\mathbf{x}, t) \\ \mathbf{u}_0(\mathbf{x}, t) \\ T_0(\mathbf{x}, t) \\ \mathbf{s}_0(\mathbf{x}, t) \end{bmatrix}. \quad (27)$$

By default  $(\alpha_\rho, \beta_\rho) = (1, 1)$  and  $(\alpha_T, \beta_T) = (1, 1)$ . The mixed derivative condition ( $\beta > 0$ ) is a softer condition that allows waves to exit the domain with fewer reflections. Note that if the flow is nearly uniform at inflow then  $\rho_n \approx 0$  and  $T_n \approx 0$  and the condition reduces to a dirichlet condition.

Examples:

1. Set the velocity  $(u, v, w) = (1, 0, 0)$ ,  $\rho + \rho_n = 1$  and  $T + T_n = 300$ :

```
square(0,0)=subSonicInflow uniform(r=1.,u=1,v=0,w=0,T=300.)
```

## 6.5 subSonicOutflow

At a subsonic outflow there is one characteristic entering the domain and thus one variable should be set and all others can be extrapolated. At a subsonic outflow we set the temperature (i.e.  $p/\rho$  for the Godunov scheme) at outflow or a mixed derivative on the temperature

$$\alpha T + \beta T_n = g(\mathbf{x}, t). \quad (28)$$

The mixed derivative condition ( $\beta > 0$ ) is a softer condition that allows waves to exit the domain with fewer reflections. Note that if the flow is nearly uniform at outflow then  $T_n \approx 0$  and the condition reduces to a dirichlet condition. Normally one might set  $\alpha = 1$  and  $\beta$  a small value, e.g.  $\beta = .1$  (but note that  $\beta$  dimensional quantity and thus should scale with the domain size)

$$T + \beta T_n = T_0(\mathbf{x}, t). \quad (29)$$

Equation (29) will thus approximate  $T \approx T_0(\mathbf{x}, t)$  if  $\beta T_n$  is small.

Example:

1. Set  $T \approx 300$  and outflow:

```
square(1,0)=subSonicOutflow mixedDerivative(1.*t+.1*t.n=300.)
```

## 6.6 Axisymmetric

The axisymmetric boundary condition is used to specify an axisymmetric boundary for two-dimensional axisymmetric computations (see Section 4), The conditions on an axisymmetric boundary  $y = 0$  are (\*\*CHECK ME\*\*)

$$\rho_y(x, 0) = 0, \quad (30)$$

$$u_y(x, 0) = 0, \quad (31)$$

$$v(x, 0) = 0, \quad (32)$$

$$T_y(x, 0) = 0 \quad (33)$$

Example:

1. Assign superSonicOutflow:

```
bcNumber3=axisymmetric
```



## 7 Equations of State

There are a number of equations of state available.

Notes to developers: To add a new equation of state change the files

1. CnsParameters.{h,C} : add EOS enums and names, change getDerivedFunction to define p for plotting.
2. setupPde.C - change EOS menu
3. eosdat.h - define EOS for fortran
4. dudr2d.f - change getp2d
5. consPrim.bf - define conservative to primitive conversion
6. Cgcns.C - output EOS name for info.

### 7.1 Ideal Gas law

The ideal gas law is

$$\rho e = C_v T = p/(\gamma - 1) \quad (\text{caloric EOS}) \quad (34)$$

$$p = \rho R_g T \quad (\text{thermal EOS}) \quad (35)$$

For a non-reactive flow, the temperature only appears in the boundary conditions, since the boundary conditions are applied to the primitive variables  $(\rho, \mathbf{u}, T)$ .

The Godunov solver needs to know some derivatives of  $p = P(\rho, \rho e)$  :

$$\left. \frac{\partial p}{\partial \rho} \right|_{\rho e = K} = 0, \quad \left. \frac{\partial p}{\partial \rho e} \right|_{\rho = K} = \gamma - 1 \quad (36)$$

### 7.2 JWL Equation of State

This section needs to be written. See the paper ??.

### 7.3 Stiffened Gas Equation of State

The stiffened gas law is

$$\rho e = (p + \gamma p_\infty)/(\gamma - 1) \quad (\text{caloric EOS}) \quad (37)$$

$$p = \rho R_g T \quad (\text{thermal EOS}) \quad (38)$$

Here  $p_\infty$  is a constant. The second equation (38) can be thought of as the definition for  $T$ .

The Godunov solver needs to know some derivatives of  $p = P(\rho, \rho e)$  :

$$\left. \frac{\partial p}{\partial \rho} \right|_{\rho e = K} = 0, \quad \left. \frac{\partial p}{\partial \rho e} \right|_{\rho = K} = \gamma - 1 \quad (39)$$

The stiffened gas law is sometimes used to model shocks in water, which is less compressible than air. Water might be modeled using  $p_\infty = 4921.15$  bar and  $\gamma = 5.5$ .

### 7.4 Tait Equation of State

The Tait equation of state is

$$\frac{p + B}{P_0 + B} = \left( \frac{\rho}{\rho_0} \right)^n \quad (40)$$

$$e = C_v(T - T_0) + e_0 \quad (\text{is this right?}) \quad (41)$$

$$T \equiv p/(R_g T) \quad (\text{is this right?}) \quad (42)$$

Here  $n$ ,  $B$ ,  $P_0$ ,  $e_0$  and  $\rho_0$  are constants.

Since  $p$  only depends on  $\rho$ , the energy equation is decoupled from the equations for  $(\rho, \rho \mathbf{u})$ .  
The Godunov solver needs to know some derivatives of  $p = P(\rho, \rho e)$  :

$$\left. \frac{\partial p}{\partial \rho} \right|_{\rho e=K} = \frac{n \rho^{n-1}}{\rho_0^n} (P_0 + B), \quad \left. \frac{\partial p}{\partial \rho e} \right|_{\rho=K} = 0 \quad (43)$$

The Tait equation of state is used to model shocks in water with  $n=?$ , ...

## 7.5 Mie-Gruneisen Equation of State

The Mie-Gruneisen Equation of State refers to a general class of equations of state that are applicable to high temperature solids, see for example, Lemons and Lund[4].

The form of the Mie-Gruneisen EOS taken here is

$$e = C_v T + \frac{1}{\rho} E_c(\rho) \quad (\text{caloric EOS}) \quad (44)$$

$$p = \rho \kappa R_g T + F(\rho) \quad (\text{thermal EOS}) \quad (45)$$

where  $F(\rho)$  and  $E_c(\rho)$  are some given functions of the density. The ideal gas law would correspond to  $F = 0$  and  $E_c = 0$ . Here we have assumed that  $C_p$  and  $C_v$  are constant and related by  $C_p = C_v + \kappa R_g$ , for some constant,  $\kappa$ ,

$$\begin{aligned} C_p &= C_v + \kappa R_g \\ \gamma &= \frac{C_p}{C_v} \\ R_g &= \frac{\gamma - 1}{\kappa} C_v \end{aligned}$$

which

The functions  $F$  and  $E_c$  are taken as

$$F(\rho) = \alpha(v - 1) + \beta(v - 1)^2 \quad (46)$$

$$= \alpha \frac{(1 - \tilde{\rho})}{\tilde{\rho}} + \beta \frac{(1 - \tilde{\rho})^2}{\tilde{\rho}^2} \quad (47)$$

$$E_c(\rho) = -\left( \frac{\alpha}{2} \frac{(v - 1)^2}{v} + \frac{\beta}{3} \frac{(v - 1)^3}{v} \right) \quad (48)$$

$$= -\left( \frac{\alpha}{2} \frac{(1 - \tilde{\rho})^2}{\tilde{\rho}} + \frac{\beta}{3} \frac{(1 - \tilde{\rho})^3}{\tilde{\rho}^2} \right) \quad (49)$$

$$v := \rho_0 / \rho = V / V_0 \quad (50)$$

$$V = 1 / \rho \quad (51)$$

$$\tilde{\rho} := \rho / \rho_0 \quad (52)$$

where  $\rho_0 = 1/V_0$  is some reference state for the density (or specific volume  $V = 1/\rho$ ).

Note that for high temperatures  $C_v$  is almost constant,  $C_v \approx 3R_g$ .

Since  $C_v = \kappa R_g / (\gamma - 1)$  it follows from (44) and (45) that the pressure is given by

$$p = \mathcal{P}(\rho, e) := (\gamma - 1) \left( \rho e - E_c(\rho) \right) + F(\rho)$$

or using  $E = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2$  implies

$$p = \mathcal{P}(\rho, \mathbf{u}, E) := (\gamma - 1) \left( E - \frac{1}{2} \rho |\mathbf{u}|^2 - E_c(\rho) \right) + F(\rho)$$

It follows that

$$e = \frac{1}{(\gamma - 1)\rho} \left( p - F(\rho) \right) + \frac{1}{\rho} E_c(\rho) \quad (53)$$

The enthalpy  $h = e + p/\rho$  can be written as a function of  $p$  and  $\rho$ ,

$$h = \mathcal{H}(\rho, p) = \frac{\gamma}{(\gamma - 1)} \frac{p}{\rho} - \frac{1}{(\gamma - 1)\rho} F(\rho) + \frac{E_c(\rho)}{\rho}, \quad (\text{enthalpy, Mie-Gruneisen}). \quad (54)$$

$$= \frac{\gamma}{(\gamma - 1)} \frac{p}{\rho} + G(\rho) \quad (55)$$

$$G(\rho) := -\frac{1}{(\gamma - 1)\rho} F(\rho) + \frac{E_c(\rho)}{\rho} \quad (56)$$

**Speed of sound** Given a caloric EOS for the enthalpy of the form  $h = \mathcal{H}(p, \rho)$  the speed of sound is (see Toro [6])

$$a^2 = -\frac{\partial_p \mathcal{H}}{\partial_p \mathcal{H} - \rho^{-1}}$$

and thus

$$a^2 = \frac{\frac{\gamma}{(\gamma-1)} \frac{p}{\rho^2} + G'(\rho)}{\frac{\gamma}{(\gamma-1)\rho} - \rho^{-1}}$$

$$a^2 = \frac{\gamma p}{\rho} + \rho(\gamma-1)G'(\rho)$$

## 7.6 User defined equation of state

New equations of state can be created by changing the file `cg/cns/src/userDefinedEOS.C`.

\*\*\*FINISH ME\*\*\*

## 8 Shock Jump Conditions

For the one-dimensional Euler equations, the jump conditions at a shock travelling with speed  $U$  are (see for example Whitham [7])

$$[\rho v] = 0$$

$$[p + \rho v^2] = 0$$

$$[h + \frac{1}{2}v^2] = 0$$

here  $v = U - u$  is the speed relative to the shock and  $h = e + p/\rho$  is the enthalpy.

Written out in terms of the states on either side of the shock:

$$\rho_2 v_2 = \rho_1 v_1$$

$$p_2 + \rho_2 v_2^2 = p_1 + \rho_1 v_1^2$$

$$h_1 + \frac{1}{2}v_1^2 = h_2 + \frac{1}{2}v_2^2$$

Given state 1,  $[\rho_1 \ v_1 \ h_1 \ p_1]$ , state 2 can be determined by writing  $v_2, p_2$  as functions of  $\rho_2$

$$v_2 = (\rho_1 v_1)/\rho_2$$

$$p_2 = P(\rho_2) = (p_1 + \rho_1 v_1^2) - (\rho_1 v_1)^2/\rho_2$$

If  $h = e + p/\rho$  can be written, using the equations of state, as a function of  $\rho$  and  $p$ ,  $h = \mathcal{H}(\rho, p)$  then we can form an equation

$$\mathcal{H}(\rho_2, P(\rho_2)) + \frac{1}{2}(\rho_1 v_1)^2/\rho_2^2 = h_1^2 + \frac{1}{2}v_1^2$$

which defines a single equation of  $\rho_2$  in terms of the known values of state 1. Thus this last equation can be hopefully solved for  $\rho_2$ . Given  $\rho_2$  the other state 2 variables are easily computed from the relations given above.

For the Mie-Gruneisen equation of state the enthalpy  $h = \mathcal{H}(\rho, p)$  is given by equation (54).

$\rho_2 \approx 3.4058$ ,  $u_2 \approx 1.4128$ ,  $p_2 \approx 3.4089$  and  $E_2 \approx 14.1614$ .

## 9 Travelling Wave profiles for Reacting flow

Suppose that we look for a steady travelling wave profile of the form  $f(x - Ut)$  then the Euler equations for a one-dimensional reacting flow become

$$\begin{aligned} -U\rho_x + (\rho u)_x &= 0 \\ -U(\rho u)_x + (\rho u^2 + p)_x &= 0 \\ -UE_x + (uE + pu)_x &= 0 \\ -U(\rho Y)_x + (\rho uY)_x &= \rho R \end{aligned}$$

where

$$\begin{aligned} e &= \frac{1}{(\gamma - 1)\rho}(p - F(\rho)) + \frac{1}{\rho}E_c \\ h &= \frac{\gamma}{(\gamma - 1)\rho}p - \frac{1}{(\gamma - 1)\rho}(pF(\rho)) + \frac{1}{\rho}E_c \\ E &= \frac{1}{(\gamma - 1)}(p - F) + E_c + \rho QY \\ T &= (p - F)/(\kappa\rho R_g) \end{aligned}$$

Letting  $v = u - U$  it follows that

$$\begin{aligned} (\rho v)_x &= 0 \\ (\rho v^2 + p)_x &= 0 \\ (e + p/\rho + \frac{1}{2}v^2 + QY)_x &= 0 \\ (\rho vY)_x &= \rho R \end{aligned}$$

Let  $\rho_0, u_0, p_0$ , etc. denote the solution values in the unreacted state and letting  $m = \rho v$  (constant) then

$$\begin{aligned} p - p_0 &= m^2(\rho_0^{-1} - \rho^{-1}) \quad (\text{Rayleigh line}) \\ &= m(v_0 - v) \\ v - v_0 &= m(\rho_0^{-1} + \rho^{-1}) \\ v^2 - v_0^2 &= -(p - p_0)(\rho_0^{-1} + \rho^{-1}) \\ \frac{\gamma}{(\gamma - 1)}(p/\rho - p_0/\rho_0) + \frac{1}{2}(v^2 - v_0^2) + Q(Y - Y_0) + G(\rho) - G(\rho_0) &= 0 \\ G(\rho) &\equiv -\frac{1}{(\gamma - 1)\rho}(F(\rho)) + \frac{1}{\rho}E_c \end{aligned}$$

and thus the Hugoniot for this system is

$$\mathcal{H}(p, \rho, Y) \equiv \frac{\gamma}{(\gamma - 1)}(p/\rho - p_0/\rho_0) - \frac{1}{2}(p + p_0)(\rho_0^{-1} + \rho^{-1}) + Q(Y - Y_0) + G(\rho) - G(\rho_0) = 0$$

The Hugoniot only depends on the thermodynamic quantities and not the velocity.

For each fixed value of  $Y$ ,  $0 \leq Y \leq 1$  the intersection of the Rayleigh line and the Hugoniot will determine a value of  $\rho$ :

$$\begin{aligned} p - p_0 &= m^2(\rho_0^{-1} - \rho^{-1}) \quad (\text{Rayleigh line}) \\ \frac{\gamma}{(\gamma - 1)}(p/\rho - p_0/\rho_0) - \frac{1}{2}(p - p_0)(\rho_0^{-1} + \rho^{-1}) + Q(Y - Y_0) + G(\rho) - G(\rho_0) &= 0 \quad (\text{Hugoniot}) \end{aligned}$$

or in terms of  $V = 1/\rho$ ,

$$\begin{aligned} p &= p_0 + m^2(V_0 - V) \quad (\text{Rayleigh line}) \\ p &= \frac{p_0[\Gamma V_0 - V] - 2[Q(Y - Y_0) + G(\rho) - G(\rho_0)]}{\Gamma V - V_0} \quad (\text{Hugoniot}) \\ \Gamma &= \frac{\gamma + 1}{\gamma - 1} \end{aligned}$$

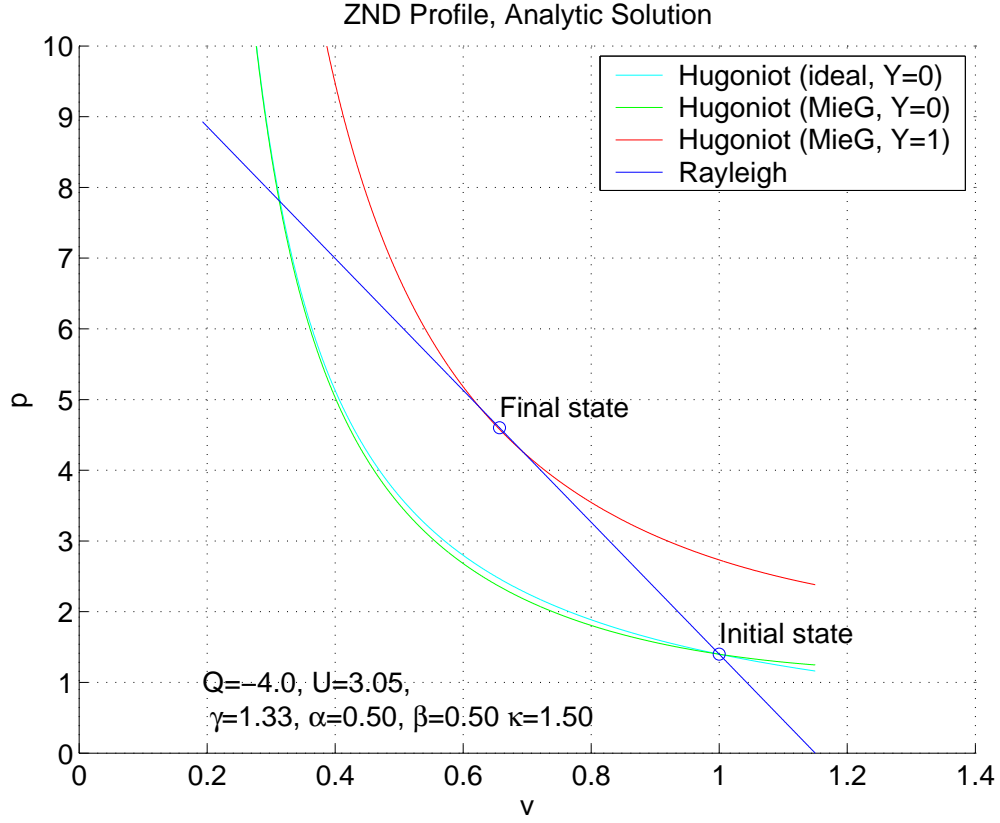


Figure 1: Hugoniot curves and Rayleigh line for the 1D reacting flow problem. The solution must always remain on the Rayleigh line. The Hugoniot curve moves upward to the right as  $Y$  increases. The final state is found at the intersection of the Rayleigh line and the Hugoniot curve for  $Y = 1$ . The Chapman-Jouguet detonation occurs when the Hugoniot curve for  $Y = 1$  is tangent to the Rayleigh line.

We can thus determine  $\rho$  as a function of  $Y$ . It follows that we also know  $v$ ,  $p$ ,  $T$  etc. as a function of  $Y$  since these are known as functions of  $\rho$ ,

For the one-step reaction

$$R = (1 - Y)\sigma \exp(\epsilon^{-1}(1 - 1/T))$$

and thus

$$\begin{aligned} Y_x &= \frac{\rho}{m} (1 - Y)\sigma \exp(\epsilon^{-1}(1 - 1/T)) \\ &\equiv \mathcal{R}(Y) \end{aligned}$$

This last equation can be integrated as an initial value problem to give  $Y = Y(x)$ . Alternatively since  $Y$  is a monotone function we can instead solve

$$\frac{dx}{dY} = 1/\mathcal{R}(Y)$$

by quadrature from some known point  $Y(x_a) = Y_a$ , to give  $x$  as a single valued function of  $Y$

$$x(Y) - x_a = \int_{Y_a}^Y 1/\mathcal{R}(\xi) d\xi$$

The condition for a Chapman-Jouget detonation is that the Rayleigh-line be tangent to the Hugoniot which implies

$$V_{CJ} = V_0/\Gamma \pm \frac{1}{\Gamma m} \left[ V_0(p_0\Gamma^2 - 1) - 2\frac{\Gamma}{V_0}(Q + G(V_{CG})) \right]^{1/2}$$

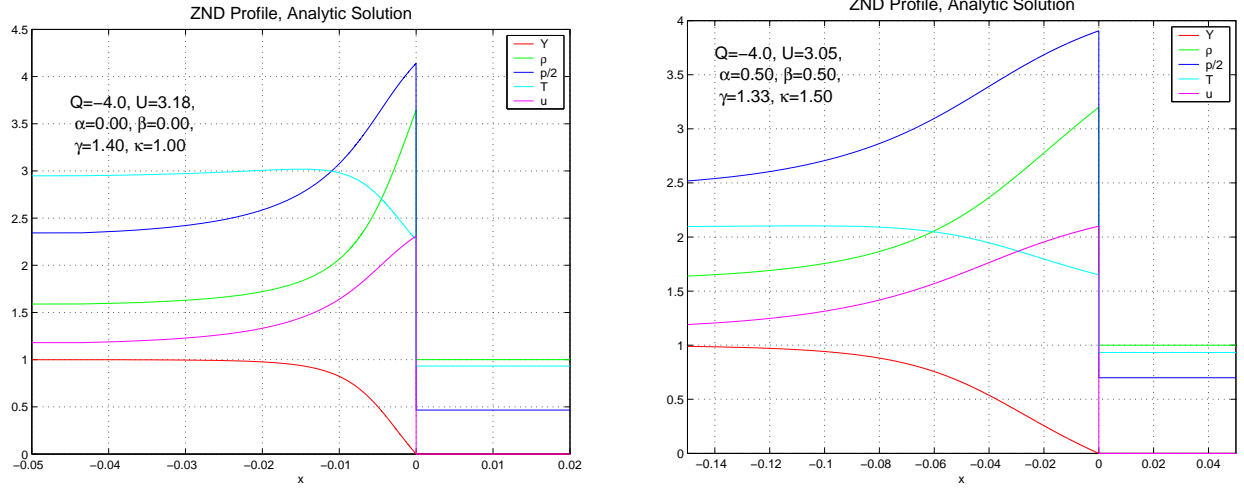


Figure 2: Profiles of a steady (Chapman-Jouget) detonation for an ideal gas (left) and the Mie-Gruneisen EOS (right).

This last equation relates the volume fraction of the final state,  $V_{CJ}$  to the initial values for  $p_0$ ,  $V_0$  and  $m$ . \*\*\*\*  
check this and finish \*\*\*\*

Figure 3 compares a computed solution with the analytic solution for the case of an ideal gas ( $\alpha = 0$ ,  $\beta = 0$ ).

Figure 4 compares a computed solution with the analytic solution for a different case with  $\kappa = 3/2$ .

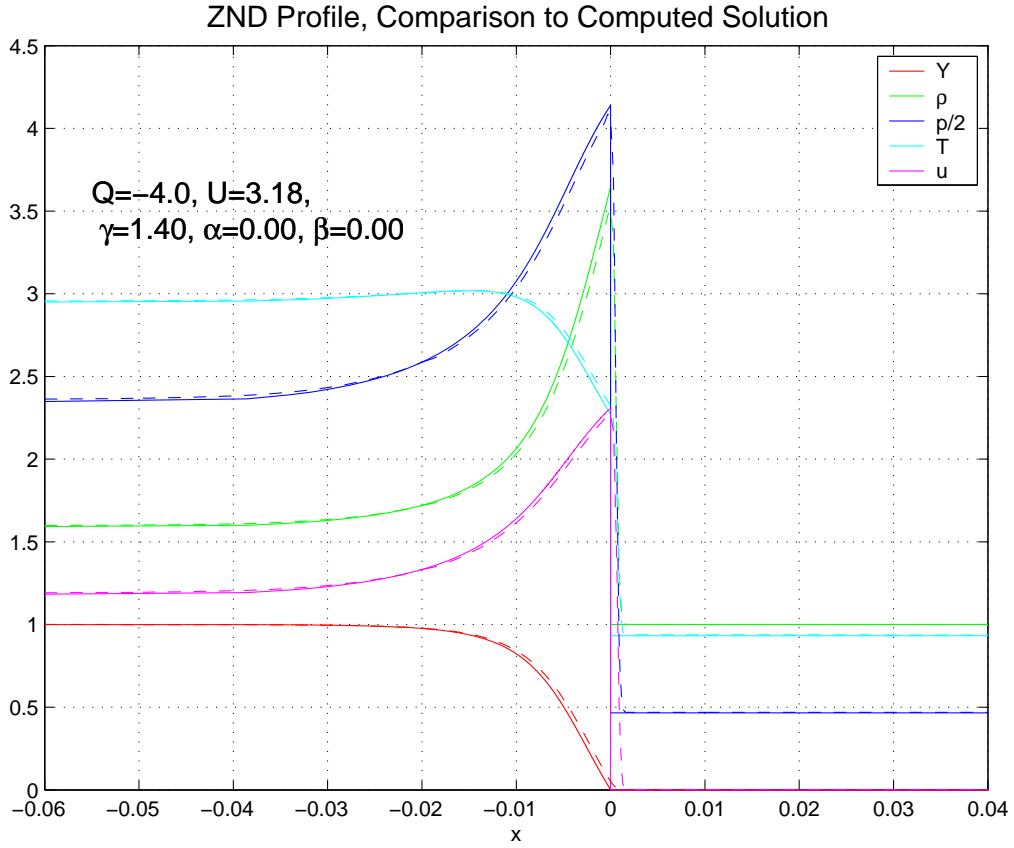
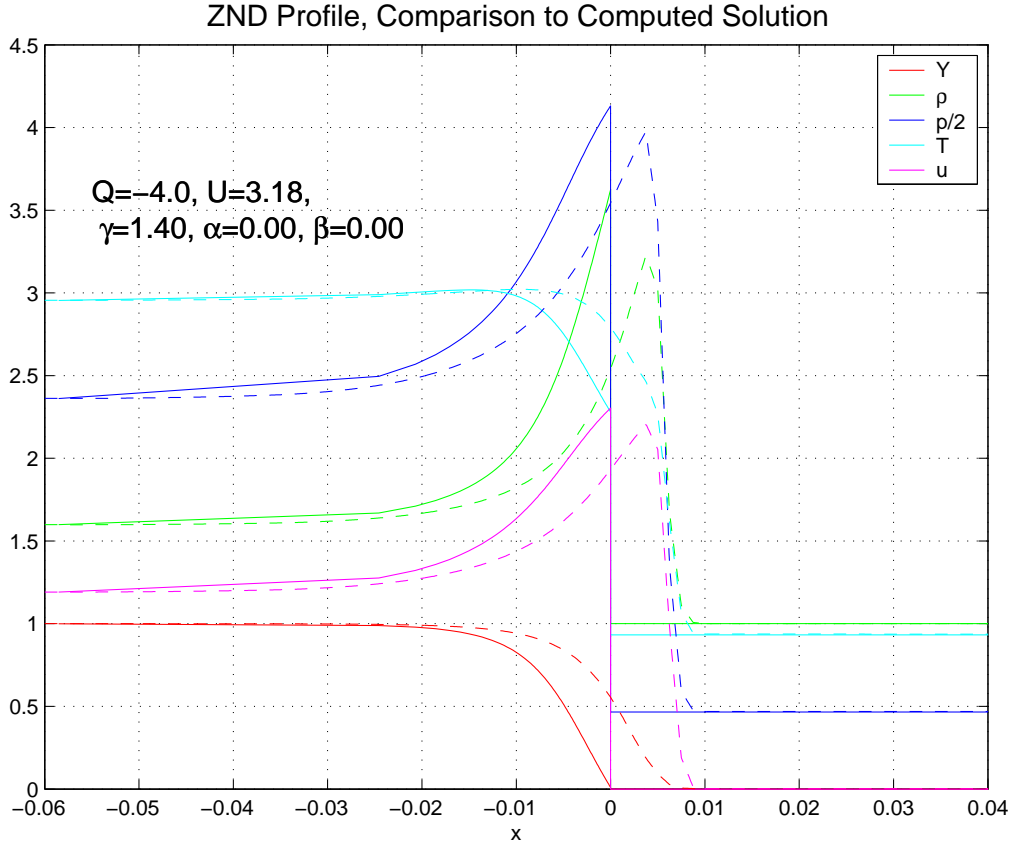


Figure 3: Comparison of the computed solution versus the analytic solution for a steady (Chapman-Jouget) detonation for an ideal gas. Left: 2-levels of AMR  $r = 4$ . Right: 3-levels of AMR.



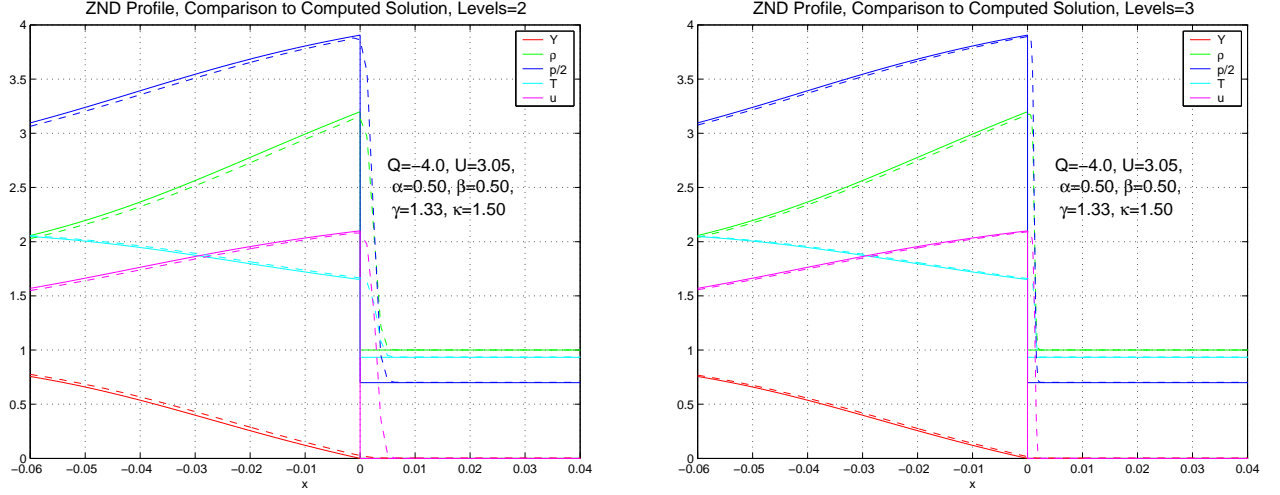


Figure 4: Comparison of the computed solution ( $t = 1$ ) versus the analytic solution for a steady (Chapman-Jouget) detonation for the Mie-Gruneisen EOS. Left: 2-levels of AMR  $r = 4$ . Right: 3-levels of AMR. The base grid has  $\Delta x = 5.e - 3$  before refinements were added.

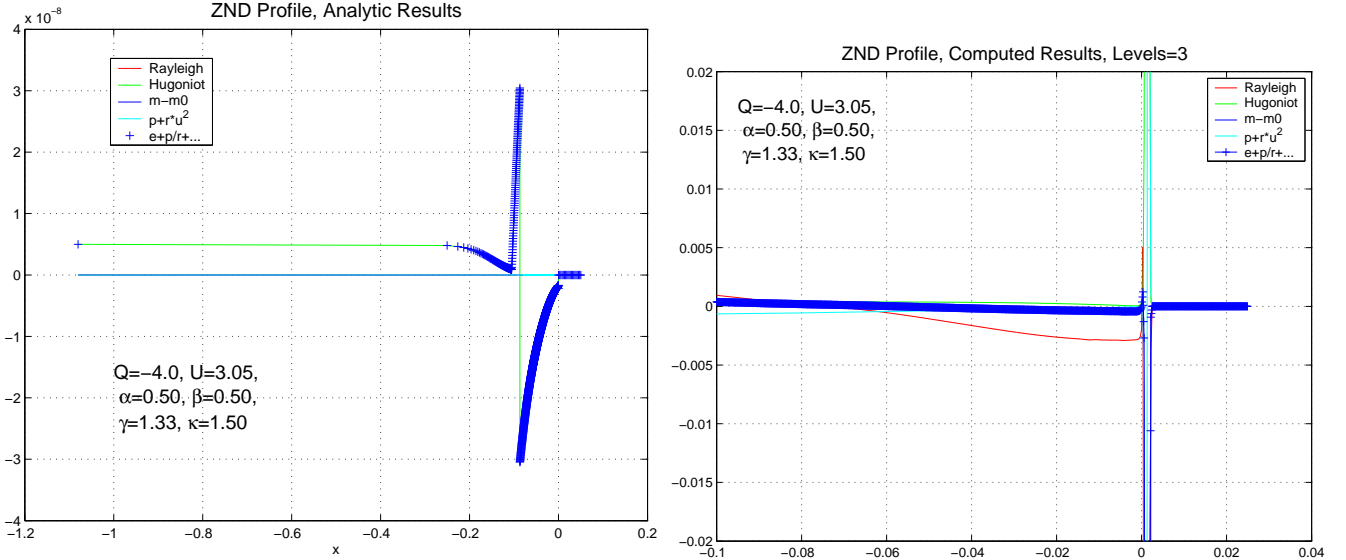


Figure 5: Diagnostics of the solution. The error in some conserved quantities is shown for the analytic solution (left, note scale) and the computed solution (right). The case was for a Mie-Gruneisen EOS (3-levels results shown in figure 4).

## 10 Convergence results

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