TENSUM: Two-dimensional entropy stable unstructred mesh solver

Created by: Deep Ray, TIFR-CAM, Bangalore

Webpage: deepray.github.io

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TENSUM is a parallelized finite volume solver for compressible flows on unstructured triangular grids. It is based on the <u>TAXIS</u> solver developed by <u>Praveen Chandrashekar</u>. Details about the discretiziation and implementation of the various numerical schemes can be found in

- 1. <u>"Entropy stable schemes on two-dimensional unstructured grids for Euler equations"</u>, by D. Ray, P. Chandrashekar, U. Fjordholm and S. Mishra; Communications in Computational Physics, Vol. 19(5), pp. 1111-1140 (2016).
- 2. <u>"An entropy stable finite volume scheme for the two dimensional Navier–Stokes equations on triangular grids"</u>, by D. Ray, P. Chandrashekar; Applied Mathematics and Computation, Vol. 314, pp. 257-286 (2017).
- "Entropy-stable finite difference and finite volume schemes for compressible flows", doctoral thesis by D. Ray, 2017.

NOTE: If the math symbols do not display properly in README.md. have a look at README.pdf instead.

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Compiling the code

After cloning the git repository into your local system, you need to set the following paths/variables in your bashrc file

export TENSUM_HOME=<path to TENSUM directory>
PATH=\$PATH:\$TENSUM_HOME/py_wrap
PATH=\$PATH:\$TENSUM_HOME/grid_gen
PATH=\$PATH:\$TENSUM_HOME/src

The following primary exectuable files need to be generated:

- 1. grid_part in the directory grid_gen. This is used to read the mesh file and create paritioned mesh components, which are required by the main solver.
- 2. tensum in the directory src. This executes the main finite volume solver.

To generate the above executables at once, use the make command from the TENSUM home folder. Alternatively, you can go to the individual sub-directories and use make. To clear the executables and object files, use make clean.

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Using the code

If the various paths have been correctly added to the .bashrc file, then the solver can be used from anywhere in the system. Some important test cases have given in the **examples** sub-directory. It is recommended that all future test cases be run from the examples folder.

To run a particular problem, two parameter files are required. The first one is called <code>input.param</code> by default, and is needed by the python wrapper that initiates different parts of the code. The second parameter file is called <code>param.in</code> by default, and is needed by the executable <code>tensum</code>.

To run the code, go to the folder containing the input.param file and run

tensum_run.py input.param

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Description of input.param

The basic structure of the python parameter file is as follows:

```
# Basic paths/parameters
mesh_file_name = mymesh.geo
                 = 2
mesh_parts
mesh\_dimension = 2
partition_dir_loc = .
solver_param_file = param.in
# Flags for main operations
gen_mesh_and_part = yes
initiate solver = no
# Flags for solver
use_solver
                 = yes
read_from_restart = no
print_cells
               = yes
print_bounds
                = no
verbose
                 = yes
# Number of processors to be used in the solver.
                 = 2
nprocs
```

WARNING!! Do not use TABS in this parameter file, or else the python wrapper will not be able to read it correctly.

- mesh_file_name specifies the Gmsh geometry file that is used to generate the mesh. Currently, grid_part is only capable of handling Gmsh files. Furthermore, one can either specify the gmsh geometry file (with the file extension .geo) or the mesh file (with the file extension .msh)
- mesh parts specifies the number of partitions partitions the mesh is broken into.
- mesh_dimension species the spatial dimension of the mesh. This must always be set to be 2.
- partition_dir_loc specifies the path (relative to input.param) where the folder **PARTITION** containing the partitioned mesh files will be created, or is available. In the above example, the value . signifies that PARTITION is created/available in the same directory as the parameter file.
- solver_param_file specifies the name and location (relative to input.param) of the parameter file needed by tensum. In the above example, the file is name param.in and is located in the same folder.
- The mesh is generated and partitioned using the executable <code>grid_part</code> if <code>gen_mesh_and_part</code> is set to <code>yes</code>. The partitioned data is saved in the folder PARTITION. If this is not desired, then this flag must be set to <code>no</code>.
- The main solver is run, i.e., the executable tensum, if intiate_solver is set to yes. If this is not desired, then this flag must be set to no. The solver needs the specification of a few additional flags:
 - If use_solver is set to no, only the pre-processor part of the solver is run. This includes

reading the partitioned mesh data in PARTITION, and creating the various grid data structures needed by the solver. This flag should be used to check whether the mesh has been correctly partitioned, and to print out the primal and dual grids (if the print_cells flag is switched on). Set use_solver to yes to run the full solver.

- If read_from_restart is set to yes, then the solver recovers the solution from a set of
 restart files (if available). This is useful if the simulation was stopped abruptly, and can be
 resumed from the last set of restart files saved. If no restart file is available, then the solver starts
 from scratch.
- If print_cells is set to yes, then the primal and dual grids are saved in a file, which can be visualized using an additional scripts.
- If print_bounds is set to yes, then the solution bounds at each time step is saved in the file **bounds.dat**.
- If verbose is set to yes, then addition solver data will be printed on screen. This flag is useful for debugging purposes.
- The number of processors to be used by the solver is set using <code>nprocs</code> . **NOTE:** This must be a positive multiple of <code>mesh parts</code> .

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Partitioned file format

The unstructured meshes are generated using <u>Gmsh</u>, which is an open-source finite element grid generator with a built-in CAD engine, and equipped with several important post-processing tools. An important tool implemented inside Gmsh is METIS, which is a package used for graph partitioning. We use the information provided by METIS to partition the mesh based on the cell-graph. As an example, the mesh around a NACA-0012 airfoil is partitioned into 10 sub-meshes, as shown in Figure 1, with each partition depicted by a different colour.

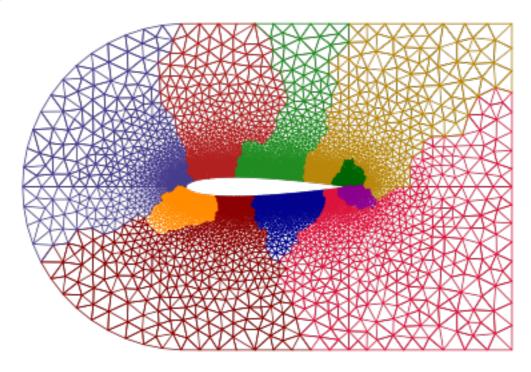


Fig. 1: Paritioned NACA-0012 mesh

The partitioning algorithm should ensure

- 1. Each sub-mesh has approximately the same number of cells, which is also termed as load balancing.
- 2. The amount of communication between processors is minimum, which depends on the length of the boundary between sub-meshes and the number of neighbouring sub-meshes.

The TENSUM solver can read in a Gmsh mesh file, and partition it into mesh_parts number of submesh files, which is stored in the PARTITION folder. The cells and vertices part of a given partition are termed as active elements. In addition, each partition file also contains information about those cells with at least one (but not all) vertex active in that partition. Such cells are termed as **ghost cells**, and their non-active vertices are termed as **ghost vertices**. The format of each partition file is as follows

In the above partition file

- <num_parts> is the number of mesh partitions. The paritions are indexed from 0 to
 <num_parts> 1, with the index number appearing in partition file name.
- <num_loc_nodes> is the number of vertices in the parition (including ghost vertices), while <num_total_nodes> is the total number of vertices in the full mesh.
- Assuming a global numbering of all vertices in the full mesh (starting from 0), the following data is available for each vertex associated with a partition:

- <g id> is the global index of the vertex
- x coord>
 ,
 y coord>
 and
 z coord>
 is the (x,y,z) spatial coordinates of the vertex
- o <num shared> is the number of mesh partitions in which the given vertex is active.
- <shared_id> is the list of indices of all paritions (including the current one) actively sharing
 the given vertex.
- <on boundary> is set to 1 if the vertex is on the domain boundary. Else it is set to 0.
- If the vertex is a ghost vertex, then <num_shared> is set to 1 and <shared_id> is the index of the current paritition.
- If the mesh has periodic boundaries, then additional information on periodic vertices is also mentioned in the file. The various periodic boundary vertices of the mesh are grouped into sets, with all vertices within a set being periodic to each other. These sets are indexed globally (starting from 0). A partition is said to be **associated** with a given periodic set, if at least one of the vertices in the set is an active vertex in the partition. For each partition, <num_periodic_sets> is the number of periodic sets the given parition is associated with. For each such periodic set P_i associated to the partition, the following information is given in the partition file.
 - \circ <Pi tag> is the index of the periodic set P_i .
 - \circ <Pij> is the subset of the periodic set P_i , listing those vertices which are active in the current partition. <num Pij> is the size of <Pij>.
 - \circ is the list of all partitions associated with the periodic set P_i , with <num_Li> being the size of this list.
- The boundary face of the mesh are also paritioned, with <num_loc_bfaces> being the number of boundary faces in the given partition, while <num_total_bfaces> being the total number of boundary face in the mesh. (NOTE: Boundary faces listed in the partition file are always belong to active elements). Each boundary face of a partition has the following information associated with it
 - <ftag> is the physical boundary tag of the boundary of which the face is a part of. These tags are defined by the user in the Gmsh geometry file of the mesh, and used to distinguish between different boundary types.
 - <face vertex list> is the list of global indices of vertices forming the face.
 - If the face has a periodic partner, then <periodic> is set to 1. Else this flag is set to 0.
- Finally, the cells in the mesh paritions are listed at the end of the file. <num_loc_cells> is the number of cells in the parition (including ghost cells), while <num_total_cells> is the total number of cells in the full mesh. For each cell in the partition, the following information is available
 - <cell vertex list> is the list of global indices of vertices forming the cell.
 - If the cell is a ghost cell, then <ghost> is set to 1. Else it is set to 0.

Description of param.in

The basic structure of the solver parameter file is as follows:

```
grid
{
   cell voronoi
}
numeric
{
   time_mode
               unsteady
   time_scheme ssprk3
   time_step
               0.0
   cfl
               0.8
   max_iter 5000
   final_time
               0.2
   min_residue 1.0e-6
   reconstruct
               minmod
     method
   }
   bc_scheme
               weak
   liou_fix
               no
   sample_list
     groups
            1 5
      }
     free_list
      {
     }
   rnd_file_loc rnd_nos.dat
   rnd_per_sample 5
}
material
{
              1.4
   gamma
   gas_const 1.0
              euler
   model
   viscosity
     model
              constant
     mu_ref
```

```
}
   prandtl
               1.0
   flux
               kepes_tecno_roe
   flux_par
   {
      alpha
                 0
                 0
      beta
   }
   balance
   {
      switch_active no
      ND
                    yes
      HEAT
                    yes
      VISC
                    yes
   }
}
constants
{
         0.3
   ХC
         1.0
   Τl
   Tr
         0.8
         0.75
   ul
         0.0
   ur
         1.0
   pl
         0.1
   pr
}
initial_condition
{
   temperature (x<xc)*Tl + (x>=xc)*Tr
   xvelocity (x<xc)*ul + (x>=xc)*ur
   yvelocity
               0.0
   zvelocity 0.0
   pressure (x<xc)*pl + (x>=xc)*pr
}
boundary
{
   100001 // inlet boundary
      type
                   inlet
      temperature Tl
                  ul
      xvelocity
      yvelocity
                   0.0
      zvelocity
                   0.0
      pressure
                   pl
   }
```

```
100002 // outlet boundary
   {
                 outlet
      type
   }
   100003
   100004
   {
              slip
      type
   }
}
exact_soln
{
   available
                no
}
integrals
{
}
output
{
   format
                         vtk
                         100
   frequency
   time_stamps
                         1
   use_online_stat_tool no
   variables
   {
      mach
      density
   }
   surfaces
   {
   }
   restart
                         yes
   restart_frequency
                         100
   log_output
                         yes
   soln_output
                         yes
   save_global
                         yes
   save_mesh_Pe
                         no
   find_error
                         no
}
```

NOTE: All the parameters must be specified in the above **fixed** order.

• Section grid :

- cell:
 - median for medial dual cells
 - voronoi for Voronoi dual cells
- Section numeric:
 - o time_mode :
 - steady for steady state problems. Local time step is used.
 - unsteady for unsteady flow problems. A global time-step is used based on the cfl
 number or prescribed uniform time step.
 - o time scheme :
 - heuns for second-order Heun's method. Useful when boundary conditions depend on time
 - ssprk3 for strong stability preserving RK3
 - rk4 for classical RK4
 - time_step : Set a non-negative numerical global uniform time-step.
 - cfl: Set a non-zero CFL to determine the local time-step. NOTE: Only one of time_step
 and cfl can (and must) be zero.
 - max_iter: Must be a positive integer. This sets the maximum number of time-iterations for steady flows. This number has no effect on the termination of unsteady flows.
 - final_time: Must a positive number, and sets the final time for unsteady simulations. For steady flows the solver automatically overides this value, replacing it with 1.0e20.
 - min_residue: Must be a non-negative values. The simulation terminates if the total flux residual drops to this value. It is meaningful to use this to terminate steady flows once the solution has converged. It is advisable to set this value to 0.0 when solving for unsteady flows.
 - reconstruct: Reconstruction method used to obtain a higher-order diffusion term (for TeCNO schemes)
 - For a first-order scheme, set the following options

```
{
  method first
}
```

• For a second-order (unlimited) scheme, set

```
{
  method second
}
```

For a second-order scheme with minmod limiter, set the following options

```
{
  method minmod
}
```

• For a second-order scheme with TVB minmod limiter, set the following options

```
{
  method tvb_minmod
  M_value <M>
}
```

where <M> must be a positive number.

• For a second-order ENO reconstruction, set the following options

```
{
  method eno2
}
```

For a second-order scheme with Van-Albada limiter, set the following options

```
{
  method van_albada
}
```

- bc scheme : Determines how the boundary condition is implemented.
 - weak implements the boundary conditions weakly via the numerical flux
 - strong (not recommended) implements the boundary conditions in a strong manner by explicitly setting the solution values at the boundary vertices based on the type of boundary.
- liou_fix: Implements Liou's eigen-value fix to handle shock-instabilities. Set to yes to activate it. Else set it to no.
- sample_list: This is used to list the sample IDs for Monte-Carlo simulations. This can be
 done in two ways. groups can be used to list a range of samples, while free_list can be
 used to list single/isolated sample numbers. For instance

```
groups
{
    1 5
    11 12
}
free_list
{
    7
    9
    36
}
```

will lead to the list of sample IDs given by the set $\{1, 2, 3, 4, 5, 7, 9, 11, 12, 36\}$. If no sample IDs are specified, then a default sample ID = 0 is set.

• rnd_file_loc: The relative path of a file with random parameter inputs needed for Monte-Carlo simulations. The file should have the following format

```
<NSAMPLES>
<sample_id_1> <param_1^1> ... <param_1^NRAND>
<sample_id_2> <param_2^1> ... <param_2^NRAND>
...
<sample_id_NSAMPLES> <param_^1> ... <param_1^NRAND>
```

where <NSAMPLES> is the total number samples listed in the file, <sample_id_j> is the sample ID of the j-th sample and <param_j^1> ... <param_j^NRAND> are the NRAND random predefined paramaters for the j-th ID. The sample IDs need not be listed in a contiguous manner or in order. Furthermore, the code takes care of any repititions.

- rnd_per_sample: The number of random parameters per sample available for each sample ID. This corresponds to NRAND.
- Section material:
 - gamma: Ratio of specific heats. Must be > 1.
 - o gas const : Ideal gas constant. Must be positive.
 - viscosity : The viscosity model to be used for Navier-Stokes equations. The following options are available
 - Constant viscosity:

```
{
    model constant
    mu_ref <mu_val>
}
```

where <mu_val> must be a non-negative number.

• Sutherland model: $\mu(T) = \mu_{ref} \frac{T^{3/2}}{T + T_{ref}}$

```
{
    model sutherland
    mu_ref <mu_val>
    T_ref <T_val>
}
```

where <mu val> and <T val> are positive numbers.

■ Power law: $\mu(T) = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{\omega}$

```
{
    model sutherland
    mu_ref <mu_val>
    T_ref <T_val>
    omega <o_val>
}
```

where $|\langle mu_val \rangle|$, $|\langle T_val \rangle|$ and $|\langle o_val \rangle|$ are positive numbers.

- prandt1: Prandtl number. Must be positive.
- model: Set as euler for the inviscid Euler equations, and ns for Navier-Stokes.
- flux: Set the invisicid numerical flux to be used
 - simple avg : Arithmetic average flux
 - kep : Jameson's kinetic energy preserving scheme
 - roe ec : Entropy conservative flux by Ismail and Roe
 - <u>kepec</u>: Kinetic energy preserving and entropy conservative flux by Chandrashekar
 - kepes tecno roe : TeCNO scheme with KEPEC flux and Roe type dissipation
 - kepes tecno rusanov : TeCNO scheme with KEPEC flux and Rusanov type dissipation
- flux_par: Use to set the parameters proposed by Ismail and Roe to correct the dissipation operator and ensure the scheme is entropy consistent. alpha and beta must be non-

negative numbers. Set both these parameters to 0 to disable the correction.

- balance: These flags are useful in studying the balancing effects of artificial viscosity in the inviscid flux, the physical dissiaption from the stress tensors and the heat flux. To activate these switches set switch_active to yes.
 - ND: Set as yes to enable artificial viscosity in the kepes_tecno fluxes. Setting this to no is equivalent to using kepec.
 - HEAT: Set as yes to enable the heat flux of Navier-Stokes. The heat flux is controlled by the coefficient of heat conductance κ . If the switch is set to no, then κ is taken to be null.
 - Navier-Stokes. This is controlled by the coefficient of viscosity μ . If the switch is set to no, then κ is taken to be null. **NOTE:** κ depends on μ . If HEAT is switched on and VISC is switched off, then κ is first determined from the non-zero value of μ , following which μ is set to 0.
- Section constant: Lists the various constants needed to describe the initial and boundary conditions. The value of π is already defined in the code, and can be called using the name MPI.
- Section <u>initial_condition</u>: Specifies the initial profiles for temperatue, velocity and pressure of the flow. These are prescribed (in order) as

```
temperature <temp_fun>
xvelocity <vx_fun>
yvelocity <vy_fun>
zvelocity <vz_fun>
pressure pre_fun>
```

where <temp_fun>, <vx_fun>, <vy_fun>, <vz_fun> and <pre_fun> are expression that are parsed. These expressions can be composed of any math function available in the library cmath.h, the constants (including M_PI) and the x, y spatial coordinates (TO DO: How to add library? How to use rnd numbers). For instance

```
xvelocity sin(2*M_PI*x) + sqrt(x*x + y*y)
```

Since the solver is at present restricted to 2D, set <vz fun> to 0.

• Section boundary: Prescribes the boundary conditions. This is done by first listing the physical boundary tags (described in the gmsh file), followed by the type of boundary conditions. If multiple boundaries (with different tags) have the identical boundary condition, then first list the tags and then prescribe the boundary condition. For instance, in the above sample parameter file, boundary faces with the tag 100003 and 100004 corrrespond to slip boundaries. The following boundary

conditions are available:

Periodic (need to apply this to an even number of face tags)

```
100001
100002
{
   type periodic
}
```

Slip

```
100001
{
   type slip
}
```

No-slip (for Navier-Stokes)

If the temperature is not specified, the wall is taken to be adiabatic.

Farfield

Inlet

```
100001
{
    type     inlet
    temperature <temp_fun>
    xvelocity <vx_fun>
    yvelocity <vy_fun>
    zvelocity <vz_fun>
    pressure pre_fun>
}
```

Outlet

```
100001
{
   type    outlet
}
```

Pressure conditions

The various variable expressions for boundary conditions can be build in a manner similar to the those appearing in <code>initial_condition</code>. In addition, the boundary conditions can depend on the time variable <code>t</code> . **NOTE:** Use Heun's method for time integration if the boundary conditions are time-dependent.

• Section exact: Used to prescribe the expression for the exact solution if available.

```
{
    available yes
    temperature <temp_fun>
    xvelocity <vx_fun>
    yvelocity <vy_fun>
    zvelocity <vz_fun>
    pressure pre_fun>
```

where the various expressions can be constructed in a manner similar to those used in the boundary conditions. If the exact solution is not available, set the flag available to no.

Section integrals: This is used to evaluate surface integrals along boundary faces. Currently, this
can only be used to evaluate surface forces due to pressure and the stress tensor (for viscous flows).
 For instance

```
integrals
{
    force
    {
        surf1
            100001
            100002
    }
}
```

where surf1 is a user-defined name to identify the force integral evaluated on the boundary faces with tags 100001 and 100002. Leave the integral section blank if no integrals are to be computed, as done in the sample parameter file.

- Section output: Sets various parameters controlling the output to screen and save files.
 - format : Sets the format for the solution save files. Currently only vtk is supported.
 - frequency: Must be a positive integer. Sets the number of iterations/time-steps after which a solution is saved. NOTE: This is only used for steady flows. Furthermore, only the initial and final solution files are saved, with the final solution file being re-written at the end of every frequency number of iterations or after a valid termination of simulation. This is also true for the ensemble statistics (point-wise mean and variance) when use_online_stat_tools set to yes.
 - time_stamps: Must be a positive integer. Sets the number of time stamps at which the solution is saved, excluding the initial solution. For instance, if final_time = 4 and time_stamps = 4, then the solutions are saved at times t = 0, 1, 2, 3, 4. This is also true for the ensemble statistics (point-wise mean and variance) when use_online_stat_tools set to yes. **NOTE:** This is only used for unsteady flows.
 - use_online_stat_tools : Set to yes if online statistics evaluation is needed. Else set to no . **NOTE:** The online statistics can be evaluated only if the number of requested samples is more than one.
 - \circ variables: Lists additional variables to save in the solution files. The currently supported variables are mach, density, entropy (i.e., $\log(p/\rho^{\gamma})$) and vorticity. If the Navier-Stokes model is used with mu_ref > 0, then the cell-wise mesh_Peclet number can also be saved to file.
 - surfaces: Physical boundary tags of faces at which the solution (and skin-friction) is evaluated and saved to file. For instance

```
surfaces
{
    100001
    100002
}
```

Leave this section empty if surface evaluations are not needed.

- restart: If this is set to yes, then restart files are save after every
 restart_frequency
 number of iterations. This is useful to restart simulations from checkpoints if the simulation ended abruptly.
- restart_frequency: Must be a positive integer.
- log_output : If set to yes then log files are written (WHAT FILES?)
- soln output: If set to yes, then solution files are written.
- save_global: If set to yes, then the time evolution of total kinetic energy and total (mathematical) entropy is written to file.
- find_error: If set to yes, the norms of the error with respect to the exact solution
 (exact_soln) at final time are written to file. NOTE: The error can be evaluated only if the exact solution is available.

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Example test cases

We now describe some of the default test cases available with the solver.

One-dimensional shocktube problem

We solve for a one-dimensional shocktube probem in 2D, with the initial data given by

$$(\rho, vel_x, vel_y, p)_L = (1, 0.75, 0, 1), \quad (\rho, vel_x, vel_y, p)_R = (0.125, 0, 0, 0.1)$$

with the initial discontinuity located at x = 0.3 in the domain $[0, 1] \times [0, 0.04]$. We use inlet boundary conditions on the left, outlet on the right, and periodic on the top and bottom boundaries.

Generate the mesh and run the solver using

```
$ tensum_run input.param
```

which will make use of the mesh geometry file shocktube.geo and the solver parameter file param.in. By default, no sample ID is specified, and thus the solution files are saved in directory SAMPLE 0.

To view the solution, you need to use a visualizer capable of reading partitioned VTK files. We recommend using <u>Vislt</u>. Open the file <u>master file.visit</u> in the folder <u>SAMPLE 0</u>.

To extract the data along the line y = 0.02, we use Vislt's command line interface (cli)

```
$ visit -cli -s line_extract SAMPLE_0
```

which will read the data in SAMPLE_0 and create the data files with the name line_data_k.dat , with $k = 0, \ldots, \text{time_stamps}$ (see param.in). In each file, the columns represent x, ρ, vel_x, p from left to right. NOTE: Make sure that density is listed in variables under the output section of param.in . The solution can be plotted and compared with the reference solution using the plot_soln.py script

```
./plot_soln SAMPLE_0/line_data_k.dat
```

where the value of k should be set equal to time_stamps. The script will generate and save the plots in pdf format.

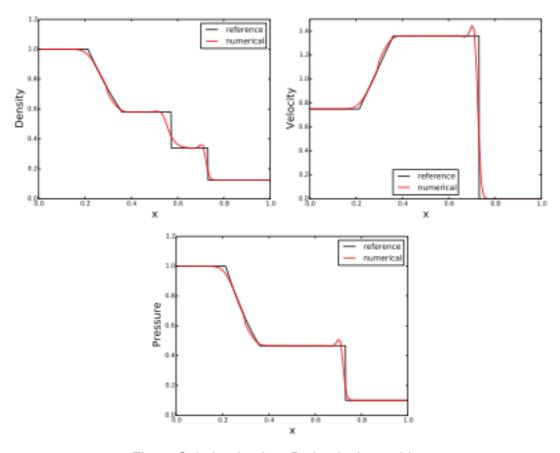


Fig. 2: Solution for the 1D shocktube problem

The second					- 6		100	
bac	k.	t∩ :	tan	ı	Ot.	CON	ten	tQ
Dao		·	uu		\mathbf{v}	OUL	will	ı

Isentropic vortex

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