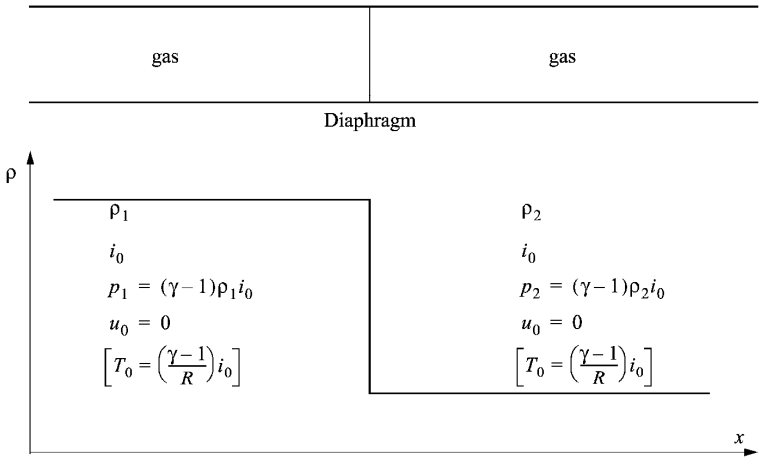
Exercise 1 – Shock tube

- Initial conditions:



- Equation of state (polytropic gas): $p = (\gamma - 1)\rho i$

$\gamma \doteq c_P / c_V$ $c_P \doteq$ specific heat at constant pressure
$c_V \doteq$ specific heat at constant volume

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Geometric data:

The calculation is 2-D plane strain. The tube is 50 units long and 0.5 units wide (this dimension is irrelevant).

Materials

The fluids are perfect gases. The assumed initial conditions are:

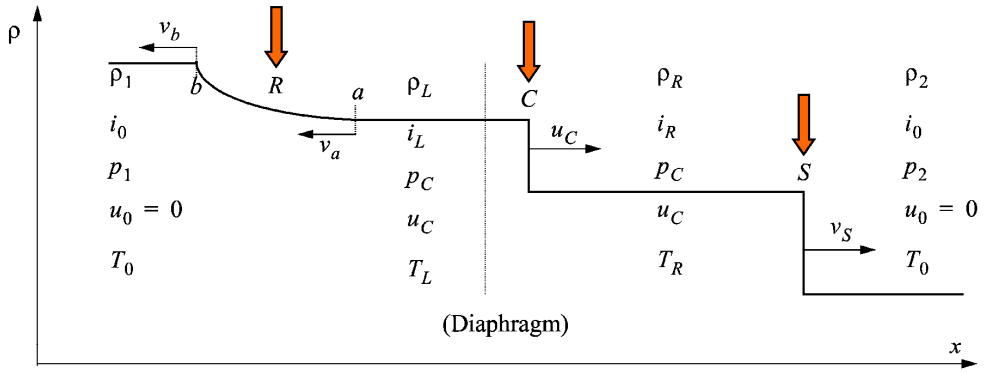
ρ_1	1.22
ρ_2	0.1237
γ	1.269
p_1	1.0×10^6
p_2	1.013×10^5
$i_1 = i_2$	3.046×10^6

The tube is rigid and does not need to be modelled.

Analytical solution (see e.g. Harlow & Amsden)

Shock tube (2)

- Analytical solution (self-similar):



- Shock S moves to the right at speed v_S
- Contact discontinuity C (particle initially at diaphragm) moves to the right at speed u_C
- Rarefaction wave $R(a,b)$ moves to the left at speeds v_a, v_b

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For the assumed initial values the solution is:

λ	9.863	u_C	925.4
P	2.888	v_S	1672.
p_C	2.927×10^5	v_a	30.12
ρ_R	0.2771	v_b	–1020.
ρ_L	0.4635	c_0	1020.
i_R	3.928×10^6	c_a	895.2
i_L	2.348×10^6	c_b	1020.

(with: $\lambda \doteq \rho_1 / \rho_2 = p_1 / p_2$ and $P \doteq p_C / p_2$).

Numerical solutions

First, we study the influence of pseudo-viscosity on Eulerian solutions:

$$q' = \begin{cases} \rho[C_Q l^2 (\nabla \cdot \underset{\sim}{v})^2 - C_L l a (\nabla \cdot \underset{\sim}{v})] & \text{for } \nabla \cdot \underset{\sim}{v} < 0 \\ 0 & \text{for } \nabla \cdot \underset{\sim}{v} \geq 0 \end{cases}$$

SHOC01

Eulerian, “average” pseudo-viscosity ($C_L = 0.5$, $C_Q = 2.56$), $\alpha_0 = \beta_0 = 1$ (full donor)
The input file is:

```
SHOC01 = SHOCK-2D 03 EULERIAN CL=0.5 CQ=2.56 ALF0=BET0=1
*--------------------------------------------------------------------------
ECHO
*CONV win
*-------------------------------------------------------------Problem type
DPLA NONL EULE
*-------------------------------------------------------------Dimensioning
DIME
  PT2L 202 FL24 100
  NALE 1 ELVC 201
  MTPO 101
TERM
*--------------------------------------------------------------------Geometry
GEOM LIBR POIN 202 FL24 100 TERM
 0.00000E+00 0.00000E+00 5.00000E-01 0.00000E+00 1.00000E+00 0.00000E+00
 1.50000E+00 0.00000E+00 2.00000E+00 0.00000E+00 2.50000E+00 0.00000E+00
 3.00000E+00 0.00000E+00 3.50000E+00 0.00000E+00 4.00000E+00 0.00000E+00
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 2.90000E+01 5.00000E-01 2.95000E+01 5.00000E-01 3.00000E+01 5.00000E-01
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 3.20000E+01 5.00000E-01 3.25000E+01 5.00000E-01 3.30000E+01 5.00000E-01
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 5.00000E+01 5.00000E-01
   1   2 103 102   2   3 104 103   3   4 105 104   4   5 106 105
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  97  98 199 198  98  99 200 199  99 100 201 200 100 101 202 201
*-----------------------------------------------------------Material data
MATE FLUT RO 1.22 EINT 3.046E6 GAMM 1.269 PB 0 ITER 1 ALF0 1
          BET0 1 KINT 0 AHGF 0 CL 0.5 CQ 2.56 PMIN 0 NUM 1
          LECT 1 PAS 1 50 TERM
     FLUT RO 0.1237 EINT 3.046E6 GAMM 1.269 PB 0 ITER 1 ALF0 1
          BET0 1 KINT 0 AHGF 0 CL 0.5 CQ 2.56 PMIN 0 NUM 1
          LECT 51 PAS 1 100 TERM
*-----------------------------------------------------Boundary conditions
LINK COUP
     BLOQ 2 TOUS
     BLOQ 1 LECT 1 101 102 202 TERM
*-------------------------------------------------------------------Outputs
ECRI VITE ECRO TFRE 10.E-3
     FICH ALIC TFRE 10.E-3
     FICH ALIC TEMP FREQ 1
               POIN LECT 25 50 75 TERM
               ELEM LECT 25 50 75 TERM
     FICH XPLO DESC 'SHOC01' TFRE 10.E-3
               POIN LECT 1 PAS 1 101 TERM
*-----------------------------------------------------------------Options
OPTI NOTE
     CSTA 0.5
*-------------------------------------------------Transient calculation
CALCUL TINI 0. TEND 20.E-3
*=========================================================POST-TREATMENT
SUIT
Post-treatment
ECHO
RESU ALIC TEMP GARD PSCR
SORT GRAP
AXTE 1.0 'Time [s]'
*-----------------------------------------------------Curve definitions
COUR 1 'vx_a'     VITE COMP 1 NOEU LECT 25 TERM
COUR 2 'vx_b'     VITE COMP 1 NOEU LECT 50 TERM
COUR 3 'vx_c'     VITE COMP 1 NOEU LECT 75 TERM
COUR 4 'pr_a'     ECRO COMP 1 ELEM LECT 25 TERM
COUR 5 'pr_b'     ECRO COMP 1 ELEM LECT 50 TERM
COUR 6 'pr_c'     ECRO COMP 1 ELEM LECT 75 TERM
```

```
COUR 7 'ro_a'     ECRO COMP 2 ELEM LECT 25  TERM
COUR 8 'ro_b'     ECRO COMP 2 ELEM LECT 50  TERM
COUR 9 'ro_c'     ECRO COMP 2 ELEM LECT 75  TERM
*-----------------------------------------------------------------Plots
trac 1 2 3 axes 1.0 'VELOC. [M/S]'
trac 4 5 6 axes 1.0 'PRESS. [PA]'
trac 7 8 9 axes 1.0 'DENS. [KG/M3]'
*-------------------------------------------------Results qualification
QUAL ECRO COMP 2 LECT 25 TERM REFE 8.59884E-01  TOLE 1.E-2
     ECRO COMP 2 LECT 50 TERM REFE 5.23010E-01  TOLE 1.E-2
     ECRO COMP 2 LECT 75 TERM REFE 4.61656E-01  TOLE 1.E-2
*=========================================================POST-TREATMENT 2
SUIT
Post-treatment
ECHO
RESU ALIC GARD PSCR
SORT GRAP
AXTE 1.0 'Time [s]'
*-----------------------------------------------------Curve definitions
SCOU 1 'ro_01' NSTO 2 SAXE 1.0 'current_abscissa' LECT 1 PAS 1 101 TERM
                      ECRO COMP 2
*-----------------------------------------------------------------Plots
trac 1 axes 1.0 'DENS. [KG/M3]'
list 1 axes 1.0 'DENS. [KG/M3]'
*-------------------------------------------------Results qualification
QUAL ECRO COMP 2 LECT 25 TERM REFE 8.59884E-01  TOLE 1.E-2
     ECRO COMP 2 LECT 50 TERM REFE 5.23010E-01  TOLE 1.E-2
     ECRO COMP 2 LECT 75 TERM REFE 4.61656E-01  TOLE 1.E-2
*=======================================================================
FIN
```

SHOC03

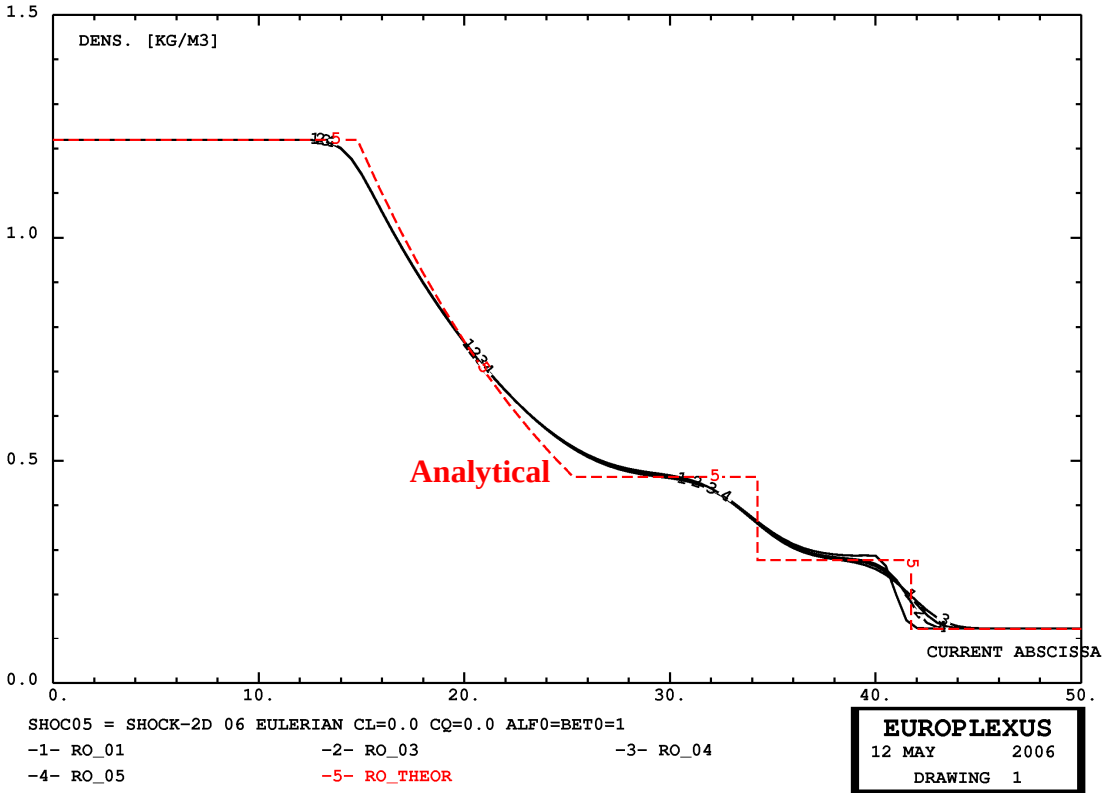
Same as SHOC01 but lower pseudo-viscosity ($C_L = 0.5$, $C_Q = 0$).

SHOC04

Same as SHOC01 but higher pseudo-viscosity ($C_L = 0.8$, $C_Q = 4.0$).

SHOC05

Same as SHOC01 but no pseudo-viscosity ($C_L = C_Q = 0$).



Conclusion: the pseudo-viscous pressure has a limited effect on results in Eulerian simulations. Solutions may be obtained even without any pseudo-viscosity.

Next, we investigate the effect of pseudo-viscosity on Lagrangian solutions:

SHOC08

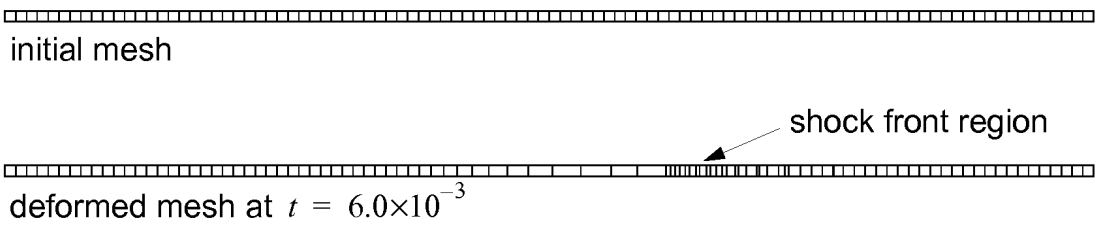
Lagrangian, no pseudo-viscosity ($C_L = C_Q = 0$). The solution is unstable.

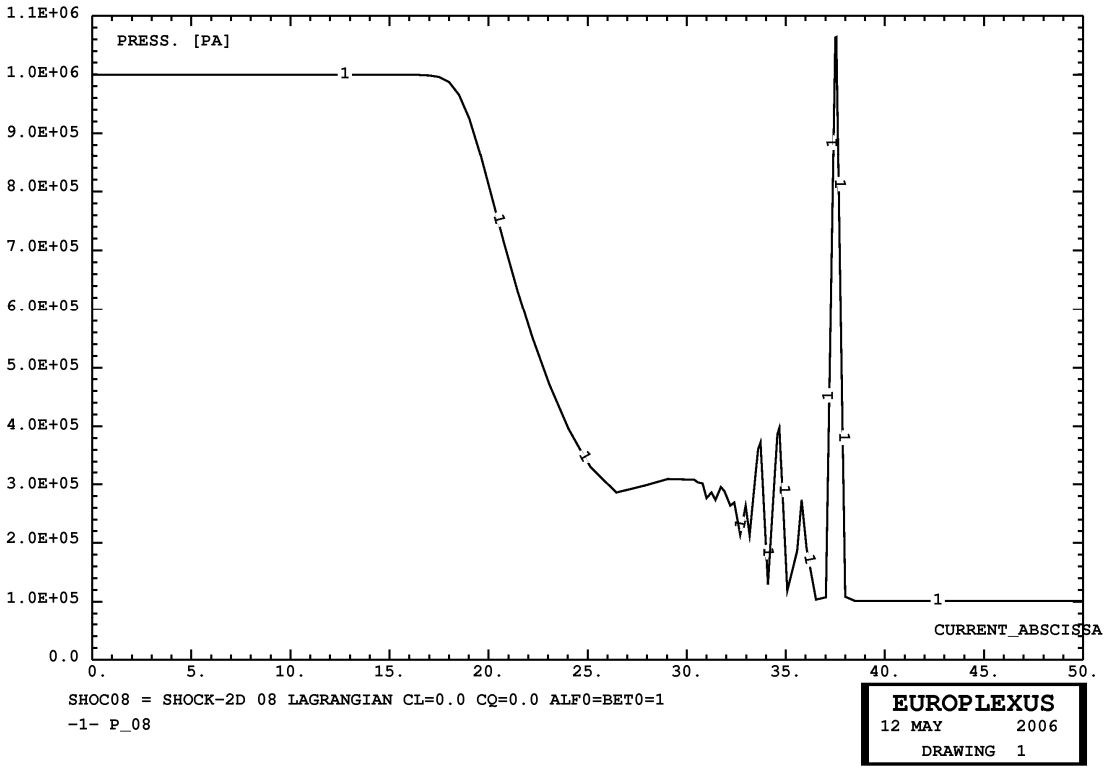
SHOC09

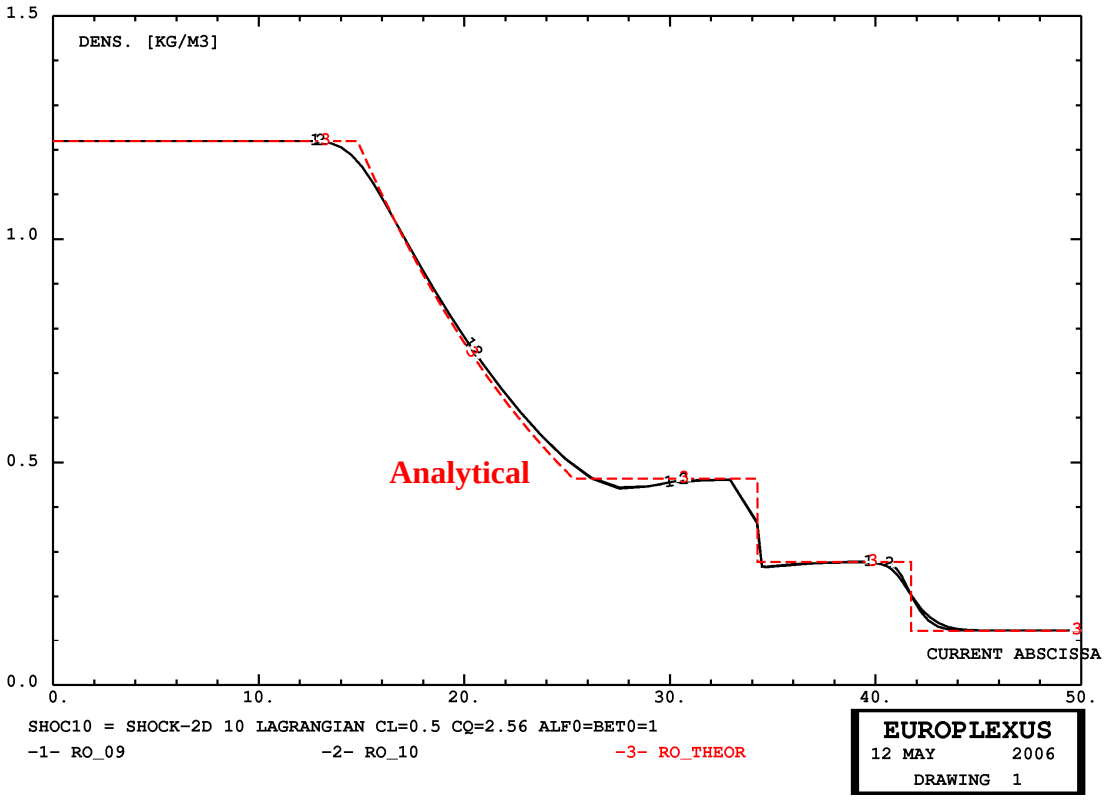
Same as SHOC08 but high pseudo-viscosity ($C_L = 0.8$, $C_Q = 4.0$).

SHOC10

Same as SHOC08 but "average" pseudo-viscosity ($C_L = 0.5$, $C_Q = 2.56$).





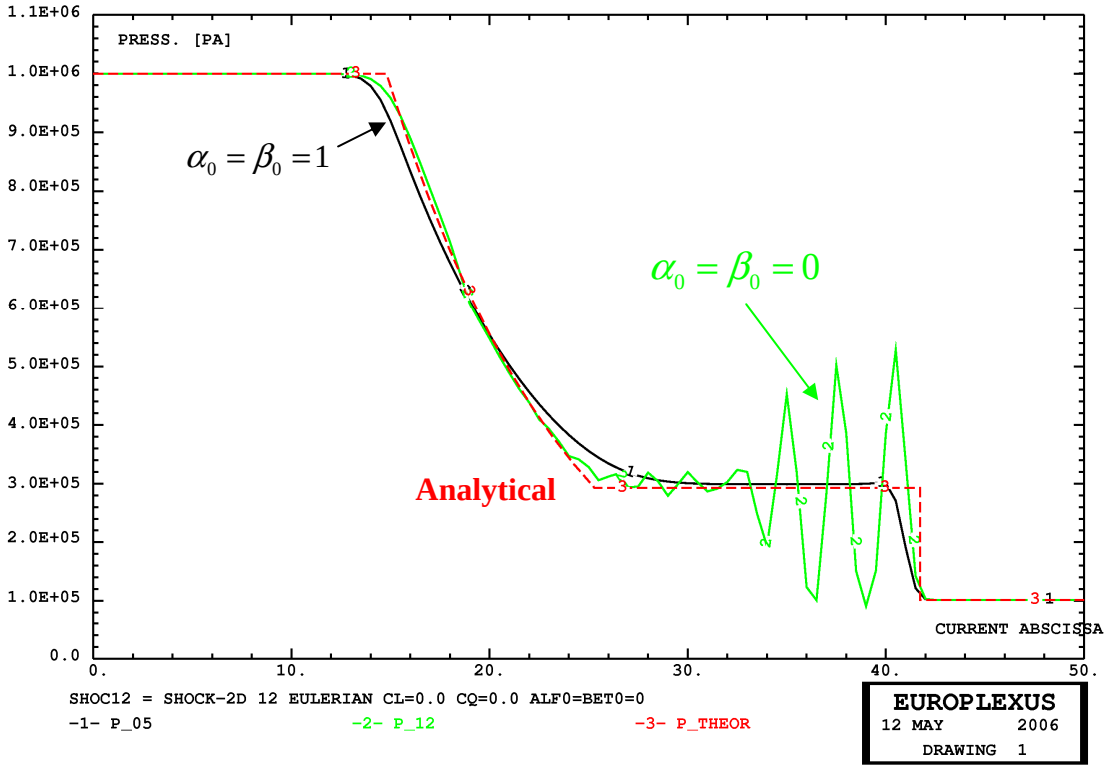


Conclusion: the pseudo-viscous pressure has a limited effect on results in Lagrangian simulations. Hovever, a small amout of pseudo-viscosity is needed otherwise the solution becomes unstable.

Finally, we investigate the effect of upwinding on Eulerian solutions:

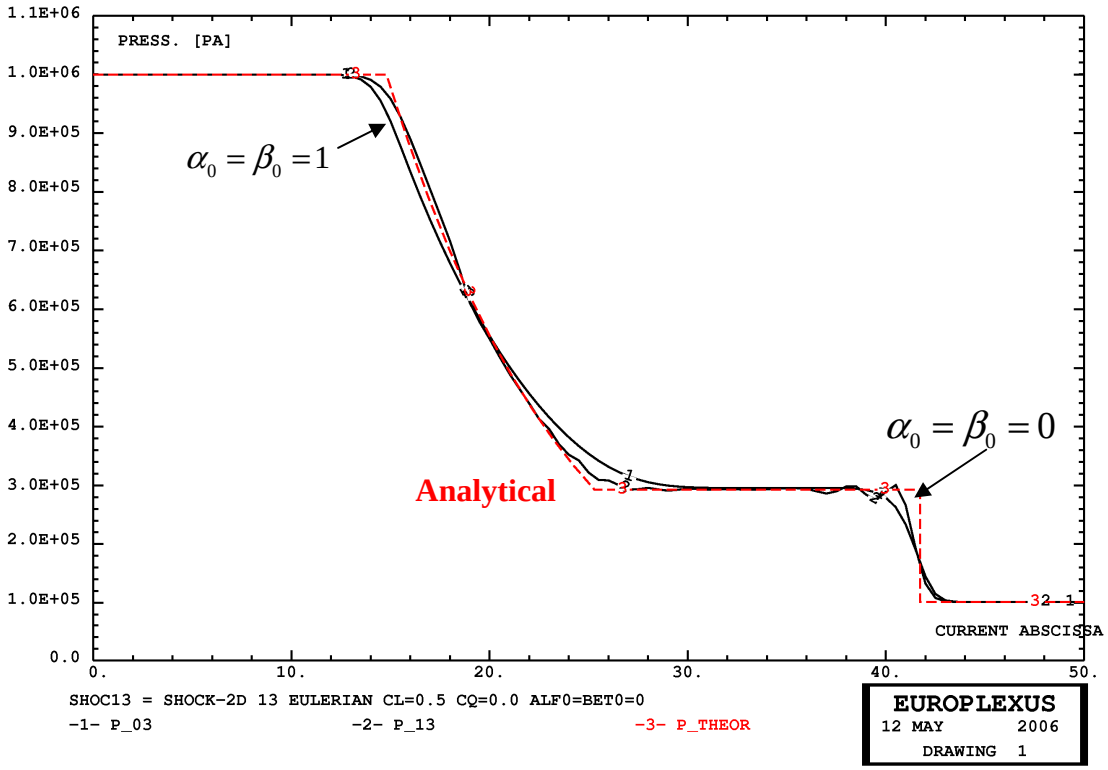
SHOC12

Eulerian, no pseudo-viscosity ($C_L = 0.0$, $C_Q = 0$), centred scheme ($\alpha_0 = \beta_0 = 0$). The solution presents strong oscillations but arrives to the final time.



SHOC13

Eulerian, very low pseudo-viscosity ($C_L = 0.5$, $C_Q = 0$), centred scheme ($\alpha_0 = \beta_0 = 0$). The solution presents some oscillations but is stable. Fronts are steeper than with the full-donor upwinding scheme.

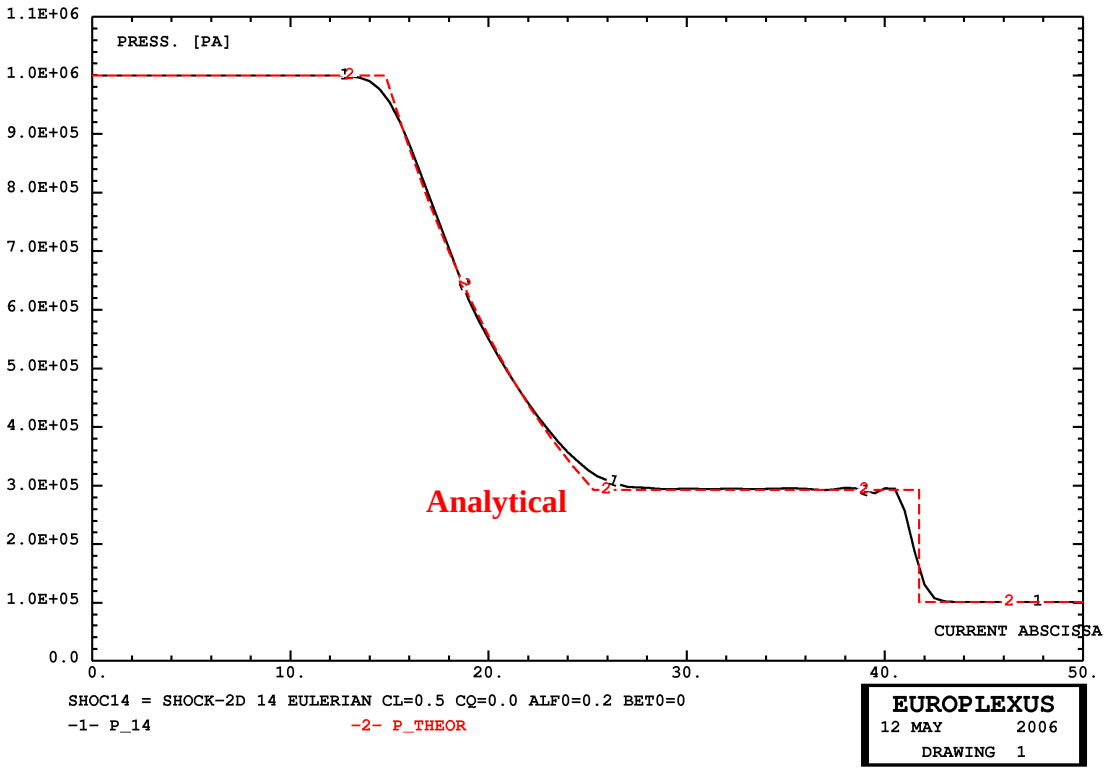


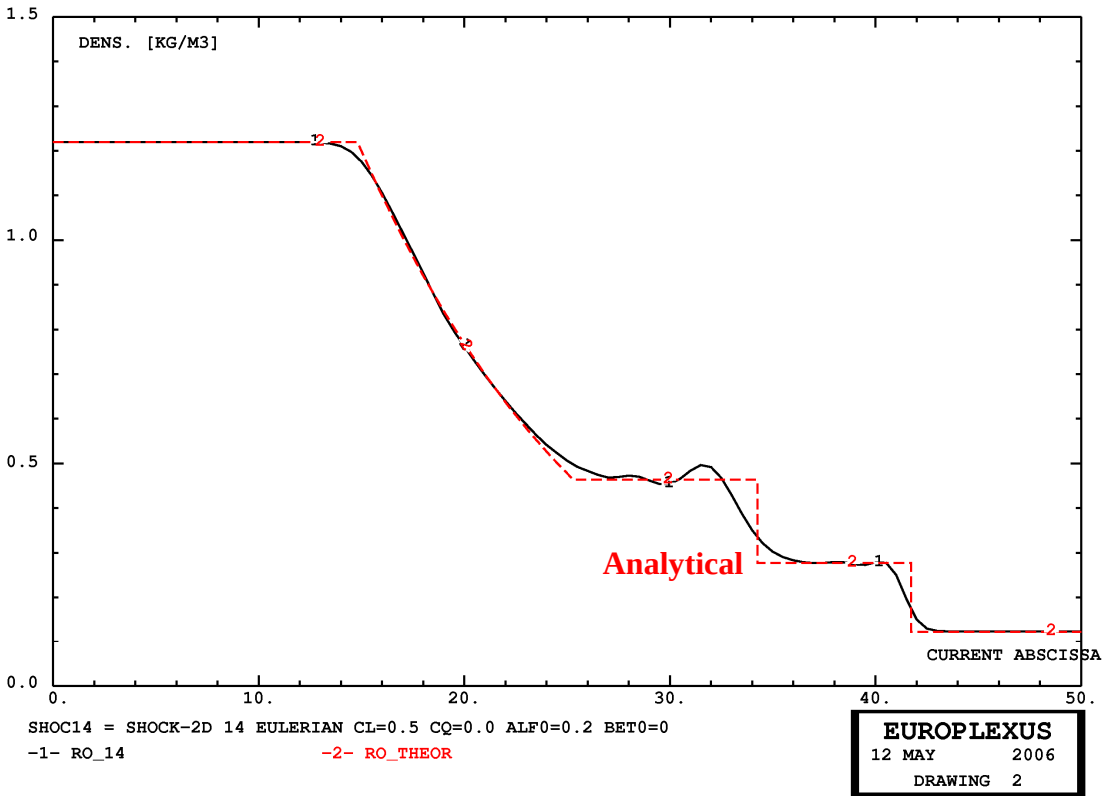
Conclusion: centred upwinding scheme produces steeper fronts than full-donor scheme. However, solutions present oscillations. A small amount of pseudo-viscosity is needed otherwise the solution becomes unstable.

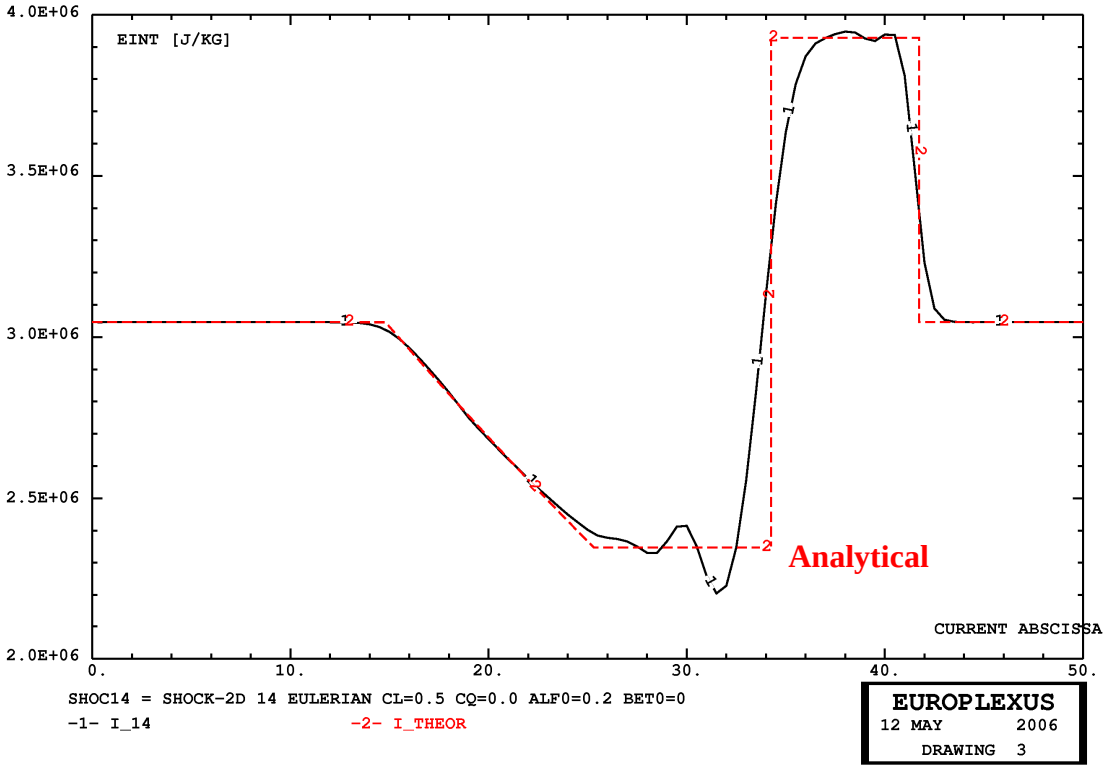
"Optimal" solution (for the present problem)

SHOC14

Eulerian, very low pseudo-viscosity ($C_L = 0.5$, $C_Q = 0$), intermediate upwinding for the mass equation ($\alpha_0 = 0.2$), centred scheme for the momentum equation ($\beta_0 = 0$).







General conclusions:

- Some pseudoviscosity is needed in Lagrangian solutions else they are unstable.
- Use as low pseudoviscosity as possible to obtain steep fronts.
- The full-donor scheme is somewhat over-diffusive, while the centred scheme yields sharper results.
- Use a slightly larger upwinding coefficient for the mass equation than for the momentum equation.

Shock tube problem solved with Finite Volumes

The same shock tube problems considered above with the FE technique may be solved by the alternative Finite Volume formulation available in the code.

To this end, besides the considerations on initial conditions, which in FE are associated with elements while in FV are associated with nodes, one has also to consider the fact that the two models assume quite different physical parameters for the input specification.

Hereafter, some guidelines are given on how to specify approximately equivalent initial material conditions with these two alternative models.

Initial conditions: FE vs. FV

The two fluid solvers have completely different ways to carry out the numerical discretization of the same governing equations (Euler equations); each of them has its specific formulation, its own set of variables and its own parameters, whose value has to be assigned in the input data (see Tab. 1).

More in detail, in the FE model the perfect gas state equation used to close the system of Euler equations has the form:

$$p = (\gamma - 1)\rho i ,$$

where p is the pressure (Pa), ρ is the density (Kg/m3), i is the internal energy per unit mass (J/Kg) and γ (-) is the ratio between the constant pressure and constant volume specific heats c_P (J /kmole K) and c_V (J /kmole K).

In the FV model the same state equation takes the form:

$$p = RT\frac{\rho}{w},$$

where R is the universal constant of gases (J /kmole K), T is the absolute temperature (K) and w is the molar weight (kg/kmole). Note that the state equation in the FV model could be more complex, taking into account a more general mixture of Joule gases. We consider here a single-component perfect gas for simplicity.

Finite Volumes	**Finite Elements**
Input parameters: p , T , R , c_V , w	Input parameters: ρ , i , γ
State equation: $p = RT\frac{\rho}{w}$	State equation: $p = (\gamma - 1)\rho i$
p = pressure (Pa)	
ρ = density (kg/m3),	
R = universal constant of gases (J /kmole K)	i = internal energy per unit mass i (J/kg)
w = molar weight (kg/kmole).	γ = ratio between c_P and c_V (-)
c_V = Specific heat at constant volume (J /kmole K)	N/a
T = temperature (K)	N/a

Tab. 1 – FE and FV models equations and parameters

Switching from FV to FE, an equivalent input can be obtained readily from the identities:

$$\gamma = \frac{R}{c_v} + 1 \ ; \qquad i = \frac{c_v}{w}T \ ; \qquad \rho = \frac{wp}{RT} .$$

The inverse path is not so straightforward. The switch from FE to FV is not univocally determined unless the molar weight w is known. Indeed the physics of the problem only depends on the internal energy i (see above), which is proportional to the ratio T/w by means of the value:

$$c_v = \frac{R}{\gamma - 1}$$

Then it is possible to choose any couple T and w so as to have the appropriate i, but values of temperature would in general *not* be correct during a calculation.

As an example, consider the following set of initial conditions, which have been chosen without actual physical relevance and have been rounded in order to easily check the equivalence of the several parameters values in the FE and FV representation. They are summarised in the following tables 2 and 3:

FE	ρ (kg/m3)	i (J/kg)	γ (-)
LP zone	2.0	1.E+05	1.5
HP zone	2.0	5.E+05	1.5

Tab. 2 - FE model initial conditions

FV	p (Pa)	T (K)	c_V (J /kmole K)	R (J /kmole K)	w (kg/kmole)
LP zone	1.E+05	100.0	2.E+04	1.E+04	20.0
HP zone	5.E+05	500.0	2.E+04	1.E+04	20.0

Tab. 3 - FV model initial conditions

Assume we want to simulate two perfect gases, one initially at high pressure and the other initially at low pressure. Let $\gamma = 1.5$ and $\rho = 2$ kg/m3 for both gases. If the HP-gas has an initial pressure of $p_H = 5.E5$ Pa, then we get from the equation of state in FE form: $i_H = p_H/(\gamma - 1)\rho = 5.E5$ J/kg. Similarly, for the LP-gas at, say, $p_L = 1.E5$ Pa we obtain $i_L = p_L/(\gamma - 1)\rho = 1.E5$ J/kg. These values completely define the FE material data.

To get an equivalent FV description, we must provide the constant of perfect gases, which in standard units is about $R = 1.E4$ J/kmole K, and we must choose a molar weight, say $w = 20$ kg/kmole for both gases. Then we obtain the specific heat at constant volume (same for both gases) from the relation $c_V = R/(\gamma - 1) = 2.E4$

Assuming for both gases the same initial density $\rho = 2$ kg/m3 as in the FE case, we may compute the temperature from the relation $T = wp/\rho R$. For the H-P gas ($p_H = 5.E5$ Pa) this gives $T = 500$ K, while for the L-P gas $p_L = 1.E5$ Pa) this gives $T = 100$ K.

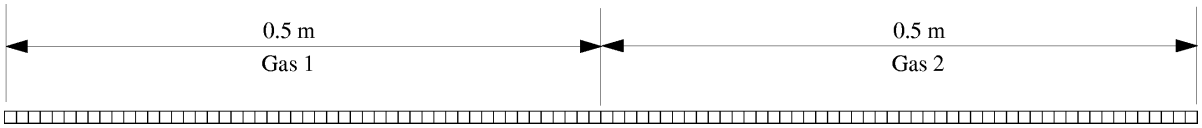
Example of shock tube problem solved by FV

The problem is similar but not identical to the ones considered previously.

LARR01

This numerical example concerns a shock tube with two components. The problem data have been taken from Larrouturou: a 1 m long, 1 cm wide shock tube is divided into two 0.5 m long zones, see Fig. 5, separated by a membrane that breaks at $t = 0$, thus initiating the transient. The left zone contains a pure perfect gas (A) with $\gamma_A = 1.4$, at a state defined by $p_A = 1$, $\rho_A = 1$, whereas the right zone contains another pure, perfect gas (B) with $\gamma_B = 1.2$ at a state defined by $p_B = 0.1$, $\rho_B = 0.125$. The test is a two-component version of the classical Sod problem.

A solution of this problem is obtained in two space dimensions using quadrilateral 'elements'. The 2D mesh consists of 100 quadrilateral elements, see sketch below.



Mesh for the Larrouturou test (2D quadrilaterals)

The general solution pattern is very similar to the one corresponding to the classical single-component Sod problem, although the three intermediate states separated by the characteristic waves are different, due to the different values for the two gases. The mass of gas A advances with the contact discontinuity and compresses gas B, where the typical shock wave develops.

The Figure below summarizes the results obtained at $t = 0.16$. As pointed out by Larrouturou, the modification in the Roe solver to perform the upwinding of the partial density fluxes is mandatory to preserve the positivity of the scheme.

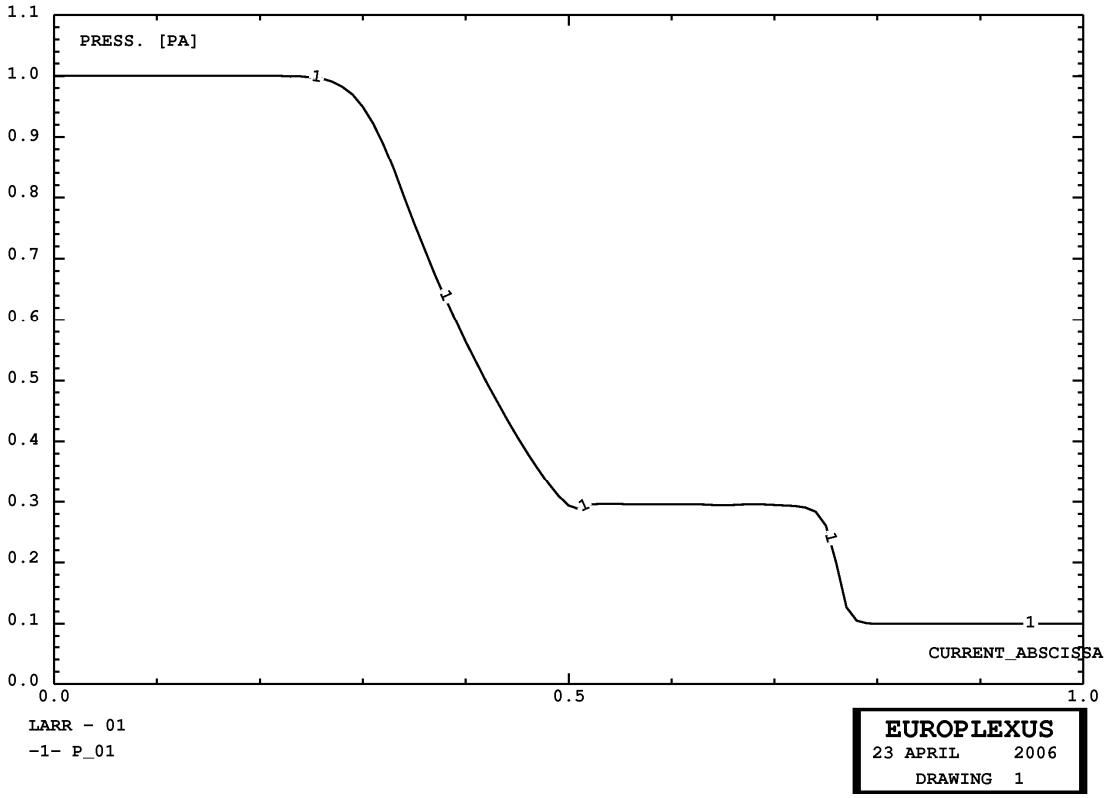
Altogether, pressure results exhibit a smaller dispersion than density and especially temperature results. Another expected result is that second-order solutions exhibit a substantially better spatial precision (steeper fronts) than first-order solutions.

The input files (mesh generation by K2000 plus input for EUROPLEXUS) read:

```
opti dime 2 echo 1 elem qua4;
opti titr 'LARR - 01';
*
p1=0 0;
p2=1 0;
 p3=0 0.01;
* p3=0 2.;
p4=0.5 0;
tol=0.001;
*
c1=p1 d 1 p3;
s1=c1 tran 50 p4;
p5=p4 'PLUS' p3;
c2=p4 d 1 p5;
s2=c2 tran 50 p4;
l1 = p1 d 100 p2;
flui=s1 et s2;
mesh=flui et l1;
elim mesh tol;
*
tass mesh;
*
opti sauv form 'larr01.msh';
sauv form mesh;
opti trac psc ftra 'larr01_mesh.ps';
trac qual mesh;
fin;
```

```
LARR - 01
$
 ECHO
$CONV WIN
CAST MESH
DPLA NONL EULE
$
DIME
 PT2L 202
 MC24 100 ZONE 1
 NDVC 804
 NALE 1
$ elvc only needed for xplot ...
 ELVC 500
 MTPO 101
TERM
$
GEOM
  MC24 FLUI
TERM
$
$ multicomponent material
$
MATE MCGP NCOM 2 R 1.00
          COMP 'A14' PM 2.5 CV1 2.5 CV2 0 CV3 0
          COMP 'B12' PM 2.5 CV1 5.0 CV2 0 CV3 0
          TOUS
$
INIT MCOM COMP 'A14'   MFRA 1.0 LECT S1 TERM
          COMP 'A14'   MFRA 0.0 LECT S2 TERM
          COMP 'B12'   MFRA 0.0 LECT S1 TERM
          COMP 'B12'   MFRA 1.0 LECT S2 TERM
          PRES 1.  LECT S1 TERM
          PRES 0.1 LECT S2 TERM
          TEMP 2.5 LECT S1 TERM
          TEMP 2.  LECT S2 TERM
          VEL1 0.0    TOUS
          VEL2 0.0    TOUS
          VEL3 0.0    TOUS
$
LINK COUP BLOQ 2 TOUS
          1 LECT 1 2 201 202 TERM
$
ECRI VITE ACCE FINT FEXT TFRE 0.08
     FICH K200 TFRE 0.01 POIN TOUS
     FICH ALIC TFRE 0.16
     FICH FORM XPLO TFRE 0.16 DESC 'LARR01'
               POIN LECT L1 TERM
     FICH FORM TPLO TFRE 0.0002 DESC 'LARR01'
               POIN LECT 17 15 13 11 9 7 5 3 1
TERM
$
OPTI NOTE CSTA 0.25
OPTI MC ORDR 2 NUFL ROE
 log 1
CALCUL TINI 0 TEND 0.16
SUIT
Post-treatment
ECHO
RESU ALIC GARD PSCR
SORT GRAP
AXTE 1.0 'Time [s]'
SCOU 1 'p_01'  NSTO 2 SAXE 1.0
       'current_abscissa' LECT L1 TERM MCPR
SCOU 2 'ro_01' NSTO 2 SAXE 1.0
       'current_abscissa' LECT L1 TERM MCRO
trac 1 axes 1.0 'PRESS. [PA]'
trac 2 axes 1.0 'DENS. [KG/M3]'
FIN
```

The pressure distribution at $t = 0.16$ is:



and the density: