NAG Library Function Document

nag_pde_parab_1d_euler_exact (d03pxc)

1 Purpose

nag_pde_parab_1d_euler_exact (d03pxc) calculates a numerical flux function using an Exact Riemann Solver for the Euler equations in conservative form. It is designed primarily for use with the upwind discretization schemes nag_pde_parab_1d_cd (d03pfc), nag_pde_parab_1d_cd_ode (d03plc) or nag_pde_parab_1d_cd_ode_remesh (d03psc), but may also be applicable to other conservative upwind schemes requiring numerical flux functions.

2 Specification

```
#include <nag.h>
#include <nagd03.h>
```

```
void nag_pde_parab_1d_euler_exact (const double uleft[],
     const double uright[], double gamma, double tol, Integer niter,
     double flux[], Nag_D03_Save *saved, NagError *fail)
```

3 Description

nag_pde_parab_1d_euler_exact (d03pxc) calculates a numerical flux function at a single spatial point using an Exact Riemann Solver (see Toro (1996) and Toro (1989)) for the Euler equations (for a perfect gas) in conservative form. You must supply the *left* and *right* solution values at the point where the numerical flux is required, i.e., the initial left and right states of the Riemann problem defined below. In nag_pde_parab_1d_cd (d03pfc), nag_pde_parab_1d_cd_ode (d03plc) and nag_pde_parab_1d_cd_ode_remesh (d03psc), the left and right solution values are derived automatically from the solution values at adjacent spatial points and supplied to the function argument **numflx** from which you may call nag_pde_parab_1d_euler_exact (d03pxc).

The Euler equations for a perfect gas in conservative form are:

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial x}=0, \tag{1}$$

with

$$U=\begin{bmatrix}\rho\\ m\\ e\end{bmatrix} \quad\text{and}\quad F=\begin{bmatrix}m\\ \frac{m^2}{\rho}+(\gamma-1)\left(e-\frac{m^2}{2\rho}\right)\\ \frac{me}{\rho}+\frac{m}{\rho}(\gamma-1)\left(e-\frac{m^2}{2\rho}\right)\end{bmatrix}, \tag{2}$$

where ρ is the density, m is the momentum, e is the specific total energy and γ is the (constant) ratio of specific heats. The pressure p is given by

$$p=(\gamma-1)\left(e-\frac{\rho u^2}{2}\right), \tag{3}$$

where $u=m/\rho$ is the velocity.

The function calculates the numerical flux function $F(U_L,U_R)=F(U^*(U_L,U_R))$, where $U=U_L$ and $U=U_R$ are the left and right solution values, and $U^*(U_L,U_R)$ is the intermediate state $\omega(0)$ arising from the similarity solution $U(y,t)=\omega(y/t)$ of the Riemann problem defined by

$$\frac{\partial U}{\partial t}+\frac{\partial F}{\partial y}=0, \tag{4}$$

with U and F as in (2), and initial piecewise constant values $U=U_L$ for $y<0$ and $U=U_R$ for $y>0$. The spatial domain is $-\infty<y<\infty$, where $y=0$ is the point at which the numerical flux is required.

The algorithm is termed an Exact Riemann Solver although it does in fact calculate an approximate solution to a true Riemann problem, as opposed to an Approximate Riemann Solver which involves some form of alternative modelling of the Riemann problem. The approximation part of the Exact Riemann Solver is a Newton–Raphson iterative procedure to calculate the pressure, and you must supply a tolerance **tol** and a maximum number of iterations **niter**. Default values for these arguments can be chosen.

A solution cannot be found by this function if there is a vacuum state in the Riemann problem (loosely characterised by zero density), or if such a state is generated by the interaction of two non-vacuum data states. In this case a Riemann solver which can handle vacuum states has to be used (see Toro (1996)).

4 References

Toro E F (1989) A weighted average flux method for hyperbolic conservation laws *Proc. Roy. Soc. Lond.* **A423** 401–418

Toro E F (1996) *Riemann Solvers and Upwind Methods for Fluid Dynamics* Springer–Verlag

5 Arguments

1: **uleft**[**3**] – const double *Input*

On entry: **uleft**$[i-1]$ must contain the left value of the component U_i, for $i = 1, 2, 3$. That is, **uleft**[0] must contain the left value of ρ, **uleft**[1] must contain the left value of m and **uleft**[2] must contain the left value of e.

2: **uright**[**3**] – const double *Input*

On entry: **uright**$[i-1]$ must contain the right value of the component U_i, for $i = 1, 2, 3$. That is, **uright**[0] must contain the right value of ρ, **uright**[1] must contain the right value of m and **uright**[2] must contain the right value of e.

3: **gamma** – double *Input*

On entry: the ratio of specific heats, γ.

Constraint: **gamma** > 0.0.

4: **tol** – double *Input*

On entry: the tolerance to be used in the Newton–Raphson procedure to calculate the pressure. If **tol** is set to zero then the default value of 1.0×10^{-6} is used.

Constraint: **tol** ≥ 0.0.

5: **niter** – Integer *Input*

On entry: the maximum number of Newton–Raphson iterations allowed. If **niter** is set to zero then the default value of 20 is used.

Constraint: **niter** ≥ 0.

6: **flux**[**3**] – double *Output*

On exit: **flux**$[i-1]$ contains the numerical flux component $\hat{F}_i$, for $i = 1, 2, 3$.

7: **saved** – Nag_D03_Save * *Communication Structure*

saved may contain data concerning the computation required by nag_pde_parab_1d_euler_exact (d03pxc) as passed through to **numflx** from one of the integrator functions nag_pde_parab_1d_cd (d03pfc), nag_pde_parab_1d_cd_ode (d03plc) or nag_pde_parab_1d_cd_ode_remesh (d03psc). You should not change the components of **saved**.

8: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

NE_BAD_PARAM

On entry, argument $\langle\mathit{value}\rangle$ had an illegal value.

NE_INT

On entry, **niter** $= \langle\mathit{value}\rangle$.
Constraint: **niter** ≥ 0.

NE_INTERNAL_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

NE_ITER_FAIL_CONV

Newton–Raphson iteration failed to converge.

NE_REAL

Left pressure value $pl < 0.0$: $pl = \langle\mathit{value}\rangle$.

On entry, **gamma** $= \langle\mathit{value}\rangle$.
Constraint: **gamma** > 0.0.

On entry, **tol** $= \langle\mathit{value}\rangle$.
Constraint: **tol** ≥ 0.0.

On entry, **uleft**$[0] < 0.0$: **uleft**$[0] = \langle\mathit{value}\rangle$.

On entry, **uright**$[0] < 0.0$: **uright**$[0] = \langle\mathit{value}\rangle$.

Right pressure value $pr < 0.0$: $pr = \langle\mathit{value}\rangle$.

NE_VACUUM

A vacuum condition has been detected.

7 Accuracy

The algorithm is exact apart from the calculation of the pressure which uses a Newton–Raphson iterative procedure, the accuracy of which is controlled by the argument **tol**. In some cases the initial guess for the Newton–Raphson procedure is exact and no further iterations are required.

8 Parallelism and Performance

Not applicable.

9 Further Comments

nag_pde_parab_1d_euler_exact (d03pxc) must only be used to calculate the numerical flux for the Euler equations in exactly the form given by (2), with **uleft**$[i-1]$ and **uright**$[i-1]$ containing the left and right values of ρ, m and e, for $i = 1, 2, 3$, respectively.

For some problems the function may fail or be highly inefficient in comparison with an Approximate Riemann Solver (e.g., nag_pde_parab_1d_euler_roe (d03puc), nag_pde_parab_1d_euler_osher (d03pvc) or nag_pde_parab_1d_euler_hll (d03pwc)). Hence it is advisable to try more than one Riemann solver and to compare the performance and the results.

The time taken by the function is independent of all input arguments other than **tol**.

10 Example

This example uses nag_pde_parab_1d_cd_ode (d03plc) and nag_pde_parab_1d_euler_exact (d03pxc) to solve the Euler equations in the domain $0 \leq x \leq 1$ for $0 < t \leq 0.035$ with initial conditions for the primitive variables $\rho(x,t)$, $u(x,t)$ and $p(x,t)$ given by

$$\begin{aligned}
\rho(x,0) &= 5.99924, \quad u(x,0) = 19.5975, \quad p(x,0) = 460.894, \qquad \text{for } x < 0.5,\\
\rho(x,0) &= 5.99242, \quad u(x,0) = -6.19633, \quad p(x,0) = 46.095, \qquad \text{for } x > 0.5.
\end{aligned}$$

This test problem is taken from Toro (1996) and its solution represents the collision of two strong shocks travelling in opposite directions, consisting of a left facing shock (travelling slowly to the right), a right travelling contact discontinuity and a right travelling shock wave. There is an exact solution to this problem (see Toro (1996)) but the calculation is lengthy and has therefore been omitted.

10.1 Program Text

```
/* nag_pde_parab_1d_euler_exact (d03pxc) Example Program.
 *
 * Copyright 2001 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagd03.h>
#include <nagx01.h>
#include <math.h>

/* Structure to communicate with user-supplied function arguments */

struct user
{
  double elo, ero, rlo, rro, ulo, uro, gamma;
};

#ifdef __cplusplus
extern "C" {
#endif
static void NAG_CALL bndary(Integer, Integer, double, const double[],
                            const double[], Integer, const double[],
                            const double[], Integer, double[], Integer *,
                            Nag_Comm *);

static void NAG_CALL numflx(Integer, double, double, Integer, const double[],
                            const double[], const double[], double[],
                            Integer *, Nag_Comm *, Nag_D03_Save *);

#ifdef __cplusplus
}
#endif

#define U(I, J)  u[npde*((J) -1)+(I) -1]
#define UE(I, J) ue[npde*((J) -1)+(I) -1]


int main(void)
{
  const Integer npde = 3, npts = 141, ncode = 0, nxi = 0;
  const Integer neqn = npde*npts+ncode, lisave = neqn+24, intpts = 9;
  const Integer nwkres = npde*(2*npts+3*npde+32)+7*npts+4, lenode = 9*neqn+50;
  const Integer mlu = 3*npde-1, lrsave = (3*mlu+1)*neqn+nwkres+lenode;
  double        d, p, tout, ts, v;
  Integer       exit_status = 0, i, ind, itask, itol, itrace, k;
  double        *algopt = 0, *atol = 0, *rtol = 0, *u = 0, *ue = 0, *rsave = 0;
  double        *x = 0, *xi = 0;
  Integer       *isave = 0;
  NagError      fail;
  Nag_Comm      comm;
  Nag_D03_Save  saved;
  struct user   data;

  INIT_FAIL(fail);

  printf(
          "nag_pde_parab_1d_euler_exact (d03pxc) Example Program Results\n");


  /* Allocate memory */

  if (!(algopt = NAG_ALLOC(30, double)) ||
      !(atol = NAG_ALLOC(1, double)) ||
      !(rtol = NAG_ALLOC(1, double)) ||
      !(u = NAG_ALLOC(npde*npts, double)) ||
      !(ue = NAG_ALLOC(npde*intpts, double)) ||
      !(rsave = NAG_ALLOC(lrsave, double)) ||
      !(x = NAG_ALLOC(npts, double)) ||
      !(xi = NAG_ALLOC(1, double)) ||
      !(isave = NAG_ALLOC(lisave, Integer)))
    {
      printf("Allocation failure\n");
      exit_status = 1;
      goto END;
    }

  /* Skip heading in data file */
  scanf("%*[^\n] ");


  /* Problem parameters */

  data.gamma = 1.4;
  data.rlo = 5.99924;
  data.rro = 5.99242;
  data.ulo = 5.99924*19.5975;
  data.uro = -5.99242*6.19633;
  data.elo = 460.894/(data.gamma-1.0) + 0.5*data.rlo*19.5975*19.5975;
  data.ero = 46.095 /(data.gamma-1.0) + 0.5*data.rro*6.19633*6.19633;
  comm.p = (Pointer)

  /* Initialise mesh */

  for (i = 0; i < npts; ++i) x[i] = i/(npts-1.0);

  /* Initial values */

  for (i = 1; i <= npts; ++i)
    {
      if (x[i-1] < 0.5)
        {
          U(1, i) = data.rlo;
          U(2, i) = data.ulo;
          U(3, i) = data.elo;
        }
      else if (x[i-1] == 0.5)
        {
          U(1, i) = 0.5*(data.rlo + data.rro);
          U(2, i) = 0.5*(data.ulo + data.uro);
          U(3, i) = 0.5*(data.elo + data.ero);
        }
      else
        {
          U(1, i) = data.rro;
          U(2, i) = data.uro;
          U(3, i) = data.ero;
        }
    }

  itrace = 0;
  itol = 1;
  atol[0] = 0.005;
  rtol[0] = 5e-4;
  xi[0] = 0.0;
  ind = 0;
  itask = 1;
  for (i = 0; i < 30; ++i) algopt[i] = 0.0;

  /* Theta integration */

  algopt[0] = 2.0;
  algopt[5] = 2.0;
  algopt[6] = 2.0;

  /* Max. time step */

  algopt[12] = 0.005;

  ts = 0.0;
  tout = 0.035;

  /* nag_pde_parab_1d_cd_ode (d03plc).
   * General system of convection-diffusion PDEs with source
   * terms in conservative form, coupled DAEs, method of
   * lines, upwind scheme using numerical flux function based
   * on Riemann solver, one space variable
   */
  nag_pde_parab_1d_cd_ode(npde, &ts, tout, NULLFN, numflx, bndary, u, npts, x,
                          ncode, NULLFN, nxi, xi, neqn, rtol, atol, itol,
                          Nag_TwoNorm, Nag_LinAlgBand, algopt, rsave, lrsave,
                          isave, lisave, itask, itrace, 0, &ind, &comm, &saved,
                          &fail);

  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_pde_parab_1d_cd_ode (d03plc).\n%s\n",
              fail.message);
      exit_status = 1;
      goto END;
    }

  printf("\n t = %6.3f\n\n", ts);
  printf("%15s%18s%22s\n", "d", "v", "p");
  printf("%3s%10s%9s%9s%9s%11s%11s\n", "x", "Approx", "Exact",
          "Approx", "Exact", "Approx", "Exact");

  /* Read exact data at output points */

  for (i = 1; i <= intpts; ++i)
    {
      scanf("%lf", &UE(1, i));
      scanf("%lf", &UE(2, i));
      scanf("%lf", &UE(3, i));
    }

  /* Calculate density, velocity and pressure */

  k = 0;
  for (i = 15; i <= 127; i += 14)
    {
      ++k;
      d = U(1, i);
      v = U(2, i)/d;
      p = d*(data.gamma-1.0)*(U(3, i)/d - 0.5*v*v);
      printf("%4.1f", x[i-1]);
      printf("%9.4f", d);
      printf("%9.4f", UE(1, k));
      printf("%9.4f", v);
      printf("%9.4f", UE(2, k));
      printf("%13.4e", p);
      printf("%13.4e\n", UE(3, k));
    }

  printf("\n");
  printf(" Number of time steps           = %6ld\n", isave[0]);
  printf(" Number of function evaluations = %6ld\n", isave[1]);
  printf(" Number of Jacobian evaluations = %6ld\n", isave[2]);
  printf(" Number of iterations           = %6ld\n", isave[4]);

 END:

  NAG_FREE(algopt);
  NAG_FREE(atol);
  NAG_FREE(rtol);
  NAG_FREE(u);
  NAG_FREE(ue);
  NAG_FREE(rsave);
  NAG_FREE(x);
  NAG_FREE(xi);
  NAG_FREE(isave);

  return exit_status;
}


static void NAG_CALL bndary(Integer npde, Integer npts, double t,
                            const double x[], const double u[], Integer ncode,
                            const double v[], const double vdot[],
                            Integer ibnd, double g[], Integer *ires,
                            Nag_Comm *comm)
{
  struct user *data = (struct user *) comm->p;

  if (ibnd == 0)
    {
      g[0] = U(1, 1) - data->rlo;
      g[1] = U(2, 1) - data->ulo;
      g[2] = U(3, 1) - data->elo;
    }
  else
    {
      g[0] = U(1, npts) - data->rro;
      g[1] = U(2, npts) - data->uro;
      g[2] = U(3,
               npts) - data->ero;
    }
  return;
}

static void NAG_CALL numflx(Integer npde, double t, double x, Integer ncode,
                            const double v[], const double uleft[],
                            const double uright[], double flux[],
                            Integer *ires, Nag_Comm *comm, Nag_D03_Save *saved)
{
  struct user *data = (struct user *) comm->p;
  NagError    fail;
  Integer     niter = 0;
  double      tol = 0.0;

  INIT_FAIL(fail);

  /* nag_pde_parab_1d_euler_exact (d03pxc).
   * Exact Riemann Solver for Euler equations in conservative
   * form, for use with nag_pde_parab_1d_cd (d03pfc),
   * nag_pde_parab_1d_cd_ode (d03plc) and
   * nag_pde_parab_1d_cd_ode_remesh (d03psc)
   */
  nag_pde_parab_1d_euler_exact(uleft, uright, data->gamma, tol, niter, flux,
                               saved, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_pde_parab_1d_euler_exact (d03pxc).\n%s\n",
              fail.message);
    }

  return;
}
```

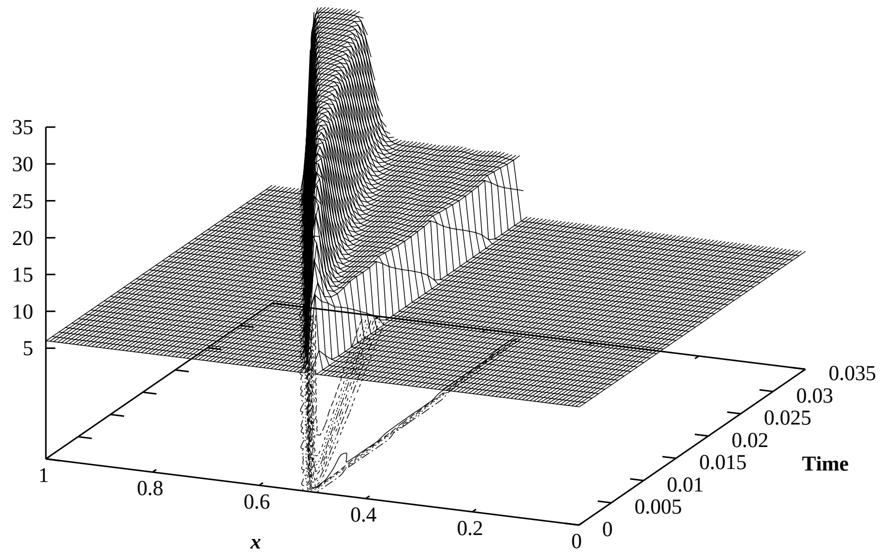
10.2 Program Data

```
nag_pde_parab_1d_euler_exact (d03pxc) Example Program Data
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.5999E+01   0.1960E+02   0.4609E+03
 0.1428E+02   0.8690E+01   0.1692E+04
 0.1428E+02   0.8690E+01   0.1692E+04
 0.1428E+02   0.8690E+01   0.1692E+04
 0.3104E+02   0.8690E+01   0.1692E+04
```

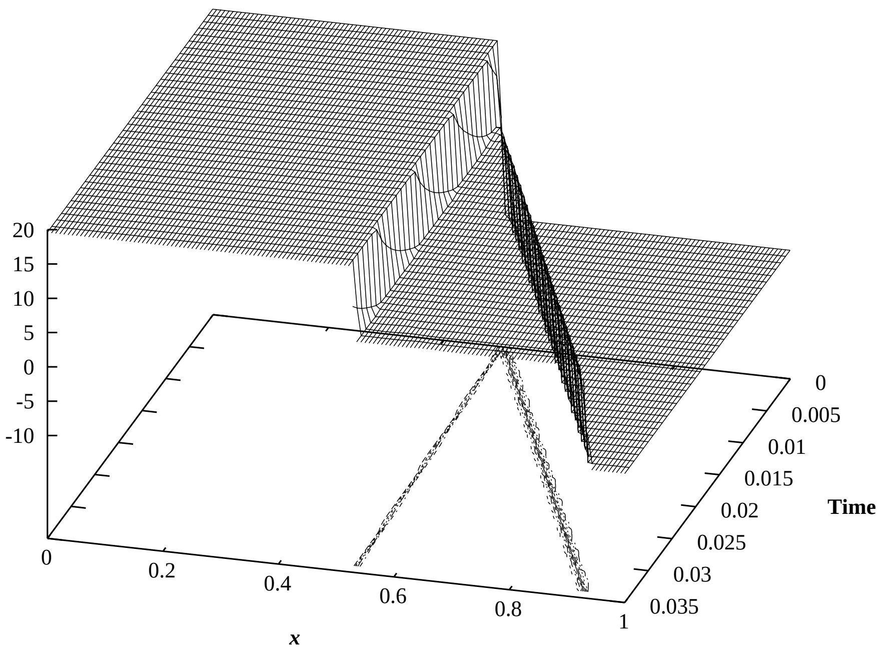
10.3 Program Results

```
nag_pde_parab_1d_euler_exact (d03pxc) Example Program Results

 t =  0.035

              d                  v                     p
  x    Approx    Exact   Approx    Exact     Approx      Exact
 0.1    5.9992    5.9990  19.5975  19.6000   4.6089e+02   4.6090e+02
 0.2    5.9992    5.9990  19.5975  19.6000   4.6089e+02   4.6090e+02
 0.3    5.9992    5.9990  19.5975  19.6000   4.6089e+02   4.6090e+02
 0.4    5.9992    5.9990  19.5975  19.6000   4.6089e+02   4.6090e+02
 0.5    5.9992    5.9990  19.5975  19.6000   4.6089e+02   4.6090e+02
 0.6   14.2268   14.2800   8.6600   8.6900   1.6878e+03   1.6920e+03
 0.7   14.2459   14.2800   8.6720   8.6900   1.6884e+03   1.6920e+03
 0.8   19.2143   14.2800   8.6742   8.6900   1.6892e+03   1.6920e+03
 0.9   30.9967   31.0400   8.6747   8.6900   1.6875e+03   1.6920e+03

 Number of time steps           =    697
 Number of function evaluations =   1708
 Number of Jacobian evaluations =      1
 Number of iterations           =      2
```

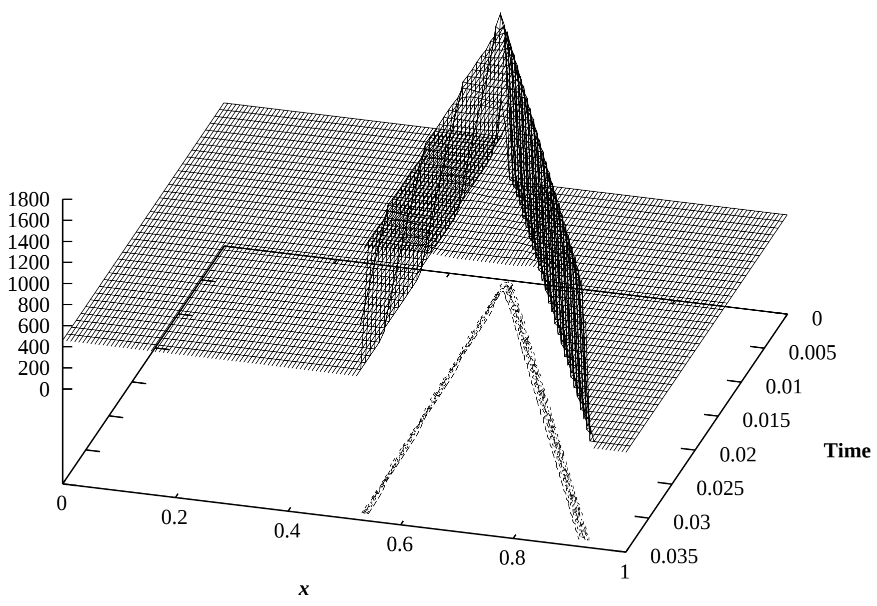
Example Program 1
Euler Equation Solution Showing Collision of Two Strong Shocks
DENSITY



Euler Equation Solution Showing Collision of Two Strong Shocks
VELOCITY



Euler Equation Solution Showing Collision of Two Strong Shocks
PRESSURE


x
Time