NAG Library Function Document

nag_pde_parab_1d_euler_hll (d03pwc)

1 Purpose

nag_pde_parab_1d_euler_hll (d03pwc) calculates a numerical flux function using a modified HLL (Harten–Lax–van Leer) Approximate 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_hll (const double uleft[],
     const double uright[], double gamma, double flux[], Nag_D03_Save *saved,
     NagError *fail)
```

3 Description

nag_pde_parab_1d_euler_hll (d03pwc) calculates a numerical flux function at a single spatial point using a modified HLL (Harten–Lax–van Leer) Approximate Riemann Solver (see Toro (1992), Toro (1996) and Toro *et al.* (1994)) 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_hll (d03pwc).

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 an approximation to 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.

4 References

Toro E F (1992) The weighted average flux method applied to the Euler equations *Phil. Trans. R. Soc. Lond.* **A341** 499–530

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

Toro E F, Spruce M and Spears W (1994) Restoration of the contact surface in the HLL Riemann solver *J. Shock Waves* **4** 25–34

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.

Constraints:

uleft[0] ≥ 0.0;
Left pressure, $pl \geq 0.0$, where pl is calculated using (3).

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.

Constraints:

uright[0] ≥ 0.0;
Right pressure, $pr \geq 0.0$, where pr is calculated using (3).

3: **gamma** – double *Input*

On entry: the ratio of specific heats, γ.

Constraint: **gamma** > 0.0.

4: **flux**[**3**] – double *Output*

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

5: **saved** – Nag_D03_Save * *Communication Structure*

saved may contain data concerning the computation required by nag_pde_parab_1d_euler_hll (d03pwc) 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**.

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

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

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.
See Section 3.2.1.2 in the Essential Introduction for further information.

NE_BAD_PARAM

On entry, argument ⟨*value*⟩ had an illegal value.

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.

An unexpected error has been triggered by this function. Please contact NAG.
See Section 3.6.6 in the Essential Introduction for further information.

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.
See Section 3.6.5 in the Essential Introduction for further information.

NE_REAL

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

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

On entry, **uleft**$[0] = \langle value \rangle$.
Constraint: **uleft**$[0] \geq 0.0$.

On entry, **uright**$[0] = \langle value \rangle$.
Constraint: **uright**$[0] \geq 0.0$.

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

7 Accuracy

nag_pde_parab_1d_euler_hll (d03pwc) performs an exact calculation of the HLL (Harten–Lax–van Leer) numerical flux function, and so the result will be accurate to ***machine precision***.

8 Parallelism and Performance

Not applicable.

9 Further Comments

nag_pde_parab_1d_euler_hll (d03pwc) 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. The time taken is independent of the input arguments.

10 Example

This example uses nag_pde_parab_1d_cd_ode (d03plc) and nag_pde_parab_1d_euler_hll (d03pwc) 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

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

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_hll (d03pwc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

#include <stdio.h>
#include <string.h>
#include <math.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagd03.h>
#include <nagx01.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 UE(I, J) ue[npde*((J) -1)+(I) -1]
#define U(I, J)  u[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, i, ind, itask, itol, itrace, k;
  double        *algopt = 0, *atol = 0, *rtol = 0, *rsave = 0, *u = 0, *ue = 0;
  double        *x = 0, *xi = 0;
  Integer       *isave = 0;
  NagError      fail;
  Nag_Comm      comm;
  Nag_D03_Save  saved;
  struct user   data;

  INIT_FAIL(fail);

  exit_status = 0;

  /* 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;
    }

  printf(
         "nag_pde_parab_1d_euler_hll (d03pwc) Example Program Results\n");

  /* Skip heading in data file */

#ifdef _WIN32
  scanf_s("%*[^\n] ");
#else
  scanf("%*[^\n] ");
#endif

  /* 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)&data;

  /* 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)
    {
#ifdef _WIN32
      scanf_s("%lf", &UE(1, i));
#else
      scanf("%lf", &UE(1, i));
#endif
#ifdef _WIN32
      scanf_s("%lf", &UE(2, i));
#else
      scanf("%lf", &UE(2, i));
#endif
#ifdef _WIN32
      scanf_s("%lf", &UE(3, i));
#else
      scanf("%lf", &UE(3, i));
#endif
    }

  /* 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           = %6"NAG_IFMT"\n", isave[0]);
  printf(" Number of function evaluations = %6"NAG_IFMT"\n", isave[1]);
  printf(" Number of Jacobian evaluations = %6"NAG_IFMT"\n", isave[2]);
  printf(" Number of iterations           = %6"NAG_IFMT"\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;

  INIT_FAIL(fail);
  /* nag_pde_parab_1d_euler_hll (d03pwc).
   * Modified HLL 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_hll(uleft, uright, data->gamma, flux, saved, &fail);

  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_pde_parab_1d_euler_hll (d03pwc).\n%s\n",
```

```
              fail.message);
    }

  return;
}
```

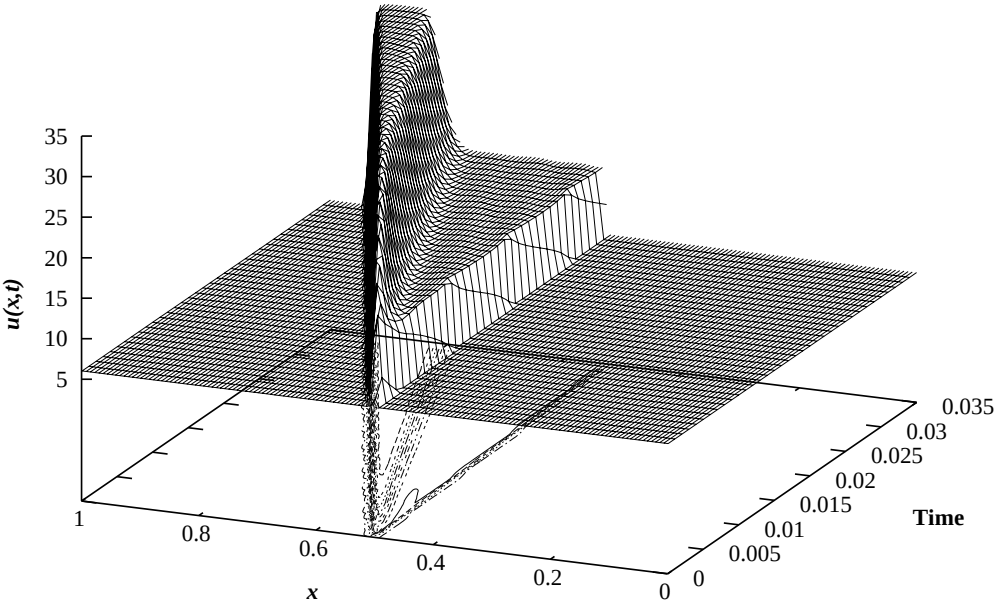
10.2 Program Data

```
nag_pde_parab_1d_euler_hll (d03pwc) 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
```

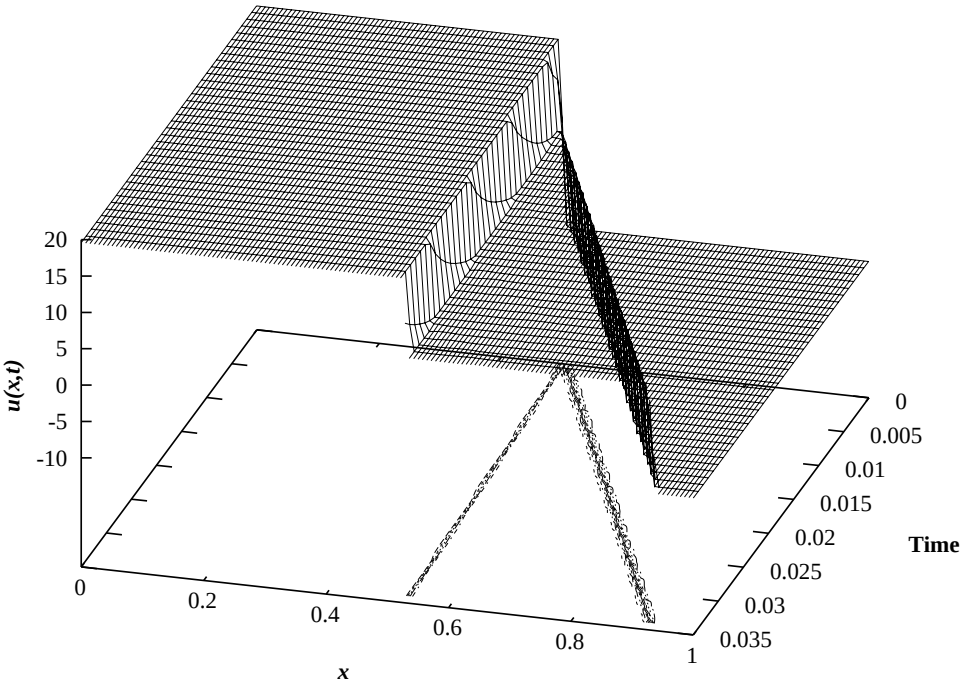
10.3 Program Results

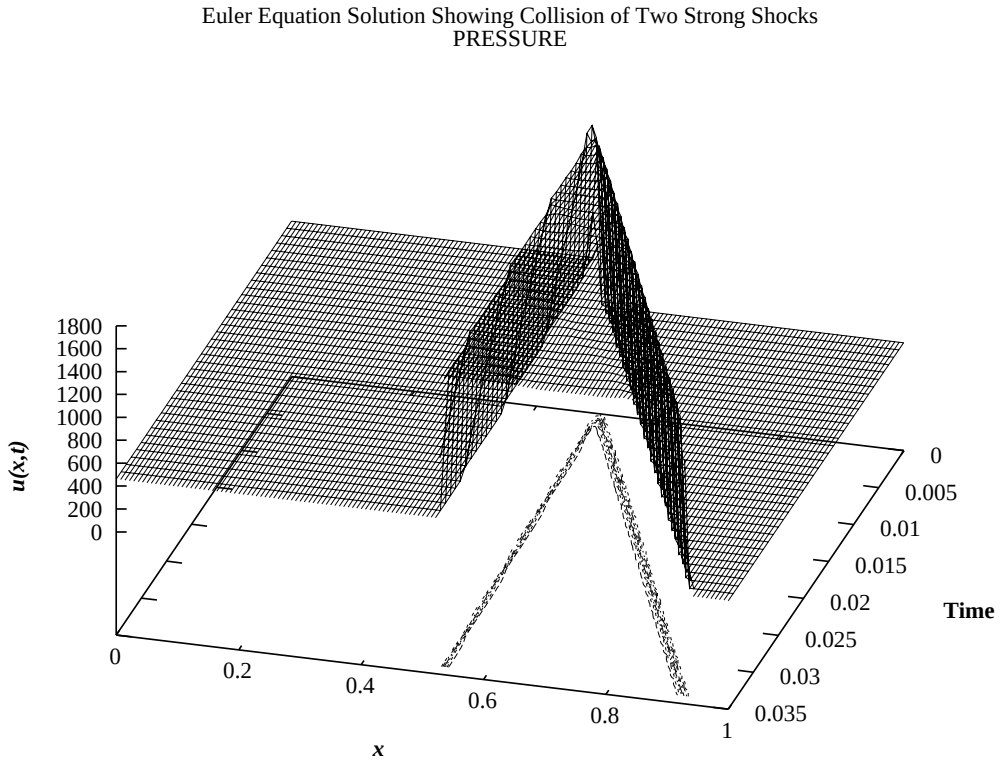
```
nag_pde_parab_1d_euler_hll (d03pwc) Example Program Results

 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  14.2215  14.2800   8.6581   8.6900   1.6872e+03   1.6920e+03
 0.7  14.2553  14.2800   8.6697   8.6900   1.6881e+03   1.6920e+03
 0.8  19.4441  14.2800   8.6783   8.6900   1.6905e+03   1.6920e+03
 0.9  31.0016  31.0400   8.6765   8.6900   1.6868e+03   1.6920e+03

 Number of time steps           =    699
 Number of function evaluations =   1714
 Number of Jacobian evaluations =      1
 Number of iterations           =      2
```

Example Program
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
u(x,t)
1800
1600
1400
1200
1000
800
600
400
200
0
0
0.2
0.4
0.6
0.8
1
x
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
Time