

# SAFETY COMPUTATIONAL FLUID DYNAMICS

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## INTRODUCTION

We consider the solution of the fundamental equations of continuum mechanics, particularly where a pressure wave propagates in a medium. The fundamental equations describe the conservation of mass, the conservation of linear momentum, the conservation of energy and are associated with an equation of state. The equations form a set of coupled first order nonlinear partial differential time dependent equations.

We consider a pressure wave propagating in the medium. A wave is a time dependent process that transfers energy from one point to another in a medium. The wave propagates through the medium because of a feedback loop that exists between the various physical properties of the medium that are changed by the energy deposition in the medium.

## EQUATIONS OF CONTINUUM MECHANICS

Four basic relations define continuum mechanics. For an arbitrary control volume  $V$ , a continuity conservation, momentum conservation, energy conservation equations and an equation of state define the problem. These are first order partial nonlinear coupled equations which are usually solved using analytical methods only in idealized situation. Numerical finite difference methods are used to solve them for more realistic situations.

The continuity equation or mass conservation equation over a control volume  $V$  can be expressed as:

$$\left\{ \begin{array}{l} \text{Rate} \\ \text{of creation} \\ \text{of mass} \end{array} \right\} \triangleq \left\{ \begin{array}{l} \text{Mass} \\ \text{outflow} \\ \text{rate} \end{array} \right\} - \left\{ \begin{array}{l} \text{Mass} \\ \text{inflow} \\ \text{rate} \end{array} \right\} + \left\{ \begin{array}{l} \text{Mass} \\ \text{storage} \\ \text{rate} \end{array} \right\} \quad (1)$$

The conservation of momentum equation or equation of motion is:

$$\left\{ \begin{array}{l} \text{Rate} \\ \text{of creation} \\ \text{of momentum} \end{array} \right\} \triangleq \left\{ \begin{array}{l} \text{Momentum} \\ \text{outflow} \\ \text{rate} \end{array} \right\} - \left\{ \begin{array}{l} \text{Momentum} \\ \text{inflow} \\ \text{rate} \end{array} \right\} + \left\{ \begin{array}{l} \text{Momentum} \\ \text{storage} \\ \text{rate} \end{array} \right\} \quad (2)$$
$$= \left\{ \begin{array}{l} \text{Sum of forces} \\ \text{acting on} \\ \text{control volume} \end{array} \right\}$$

The first law of thermodynamics suggests that energy can neither be created nor

destroyed, leading to the energy conservation equation:

$$\left\{ \begin{array}{l} \text{Rate} \\ \text{of creation} \\ \text{of energy} \end{array} \right\} \triangleq \left\{ \begin{array}{l} \text{Energy} \\ \text{outflow} \\ \text{rate} \end{array} \right\} - \left\{ \begin{array}{l} \text{Energy} \\ \text{inflow} \\ \text{rate} \end{array} \right\} + \left\{ \begin{array}{l} \text{Energy} \\ \text{storage} \\ \text{rate} \end{array} \right\} \quad (3)$$

To complete the formulation, an equation of state is needed.

## DISCRETIZATION OF THE CONTINUUM MECHANICS EQUATIONS

We consider a basic model of a one dimensional Lagrangian structure of a medium which could be gaseous fluid or solid. In this case the finite mesh is embedded in the material and moves with it. The medium is divided into slabs in the x coordinate. The pressure that is a function of x only moves with the slabs.

The conservation of mass or continuity equation is satisfied by defining a mass per unit area for each slab as a constant at all times since mass is conserved requiring no time superscript as:

$$(\Delta m)_j = \frac{(\Delta m)_{j+\frac{1}{2}} + (\Delta m)_{j-\frac{1}{2}}}{2} \quad (4)$$

Each slab is divided in half, and each neighboring halves are combined into slabs with mass:

$$(\Delta m)_j$$

The half integer subscripted variables are more naturally defined at the interfaces of secondary slabs which are positioned around the centers of the original slabs.

In the same way, the velocities are better defined at times  $t^{n+1/2}$  half way between the primary times  $t^n$  and  $t^{n+1}$ .

The computational cycle requires the computation the following discrete variables for all values of j:

$$\begin{aligned}
x_j^n &\equiv \text{position} && [cm] \\
V_{j-\frac{1}{2}}^n &\equiv \text{specific volume} && [\frac{cm^3}{gm}] \\
E_{j-\frac{1}{2}}^n &\equiv \text{specific internal energy} && [\frac{erg}{gm}] \\
p_{j-\frac{1}{2}}^n &\equiv \text{pressure} && [\frac{dyne}{cm^2}] \\
u_j^{n+\frac{1}{2}} &\equiv \text{velocity} && [\frac{cm}{sec}]
\end{aligned} \tag{5}$$

The computational cycle uses the beginning of time cycle values and integrates them to deduce the end of time cycle values:

$$\begin{array}{ccc}
\text{Beginning of time cycle} & & \text{End of time cycle} \\
x_j^{n-1} & \rightarrow & x_j^n \\
V_{j-\frac{1}{2}}^{n-1} & \rightarrow & V_{j-\frac{1}{2}}^n \\
E_{j-\frac{1}{2}}^{n-1} & \rightarrow & E_{j-\frac{1}{2}}^n \\
p_{j-\frac{1}{2}}^{n-1} & \rightarrow & p_{j-\frac{1}{2}}^n \\
u_j^{n-\frac{1}{2}} & \rightarrow & u_j^{n+\frac{1}{2}}
\end{array} \tag{6}$$

Let us define the computational time step:

$$(\Delta t)^{n-\frac{1}{2}} \equiv t^n - t^{n-1} \tag{7}$$

To advance the interface position we use the difference approximation for the velocities:

$$\begin{aligned}
u &\simeq \frac{\Delta x}{\Delta t} \\
u_j^{n-\frac{1}{2}} &= \frac{x_j^n - x_j^{n-1}}{t^n - t_j^{n-1}} \\
u_j^{n-\frac{1}{2}} &= \frac{x_j^n - x_j^{n-1}}{(\Delta t)_j^{n-\frac{1}{2}}}
\end{aligned} \tag{8}$$

By integration, the new interface positions become:

$$x_j^n = x_j^{n-1} + u_j^{n-\frac{1}{2}} (\Delta t)_j^{n-\frac{1}{2}} \quad (9)$$

New values for the specific volumes can be computed from the approximation:

$$V \simeq \frac{\Delta x \cdot \Delta A}{\Delta m} \simeq \frac{\Delta x}{\Delta m}, \quad \text{for } \Delta A = 1, \text{ a unit area.}$$

$$V_{j-\frac{1}{2}}^n = \frac{x_j^n - x_j^{n-1}}{(\Delta m)_{j-\frac{1}{2}}}, \quad \forall j. \quad (10)$$

The specific internal energy can be calculated based on the work done on the slab assuring conservation of energy through the thermodynamic relation:

$$dE = -p dV$$

$$\Delta E \simeq -p \Delta V$$

$$E_{j-\frac{1}{2}}^n - E_{j-\frac{1}{2}}^{n-1} = -p_{j-\frac{1}{2}}^{n-\frac{1}{2}} (V_{j+\frac{1}{2}}^n - V_{j-\frac{1}{2}}^{n-1}) \quad (11)$$

$$E_{j-\frac{1}{2}}^n = E_{j-\frac{1}{2}}^{n-1} - p_{j-\frac{1}{2}}^{n-\frac{1}{2}} (V_{j+\frac{1}{2}}^n - V_{j-\frac{1}{2}}^{n-1})$$

The pressure term  $p$  in Eqn. 11 can be calculated at an intermediate time  $t^{n-\frac{1}{2}}$  provided we knew its value:  $p_{j-\frac{1}{2}}^{n-\frac{1}{2}}$ . However, at this stage we only know the previous time step value of the pressure:  $p_{j-\frac{1}{2}}^{n-1}$ , so we extrapolate and use:

$$\frac{p_{j-\frac{1}{2}}^{n-\frac{1}{2}} - p_{j-\frac{1}{2}}^{n-1}}{p_{j-\frac{1}{2}}^{n-1} - p_{j-\frac{1}{2}}^{n-2}} = \frac{(t^n - t^{n-1})}{t^{n-1} - t^{n-2}} = \frac{1}{2} \frac{(\Delta t)^{n-\frac{1}{2}}}{(\Delta t)^{n-\frac{3}{2}}} \quad (12)$$

$$p_{j-\frac{1}{2}}^{n-\frac{1}{2}} = p_{j-\frac{1}{2}}^{n-1} + \frac{1}{2} (p_{j-\frac{1}{2}}^{n-1} - p_{j-\frac{1}{2}}^{n-2}) \frac{(\Delta t)^{n-\frac{1}{2}}}{(\Delta t)^{n-\frac{3}{2}}}$$

With the new updated values of  $p_{j-\frac{1}{2}}^{n-\frac{1}{2}}$ ,  $V_{j-\frac{1}{2}}^n$  and  $E_{j-\frac{1}{2}}^n$  we can determine a new value of the pressure  $p_{j-\frac{1}{2}}^n$  through an equation of state:

$$p_{j-\frac{1}{2}}^n = f(V_{j-\frac{1}{2}}^n, E_{j-\frac{1}{2}}^n) \quad (13)$$

As an example of an equation of state we can consider the gamma law gas:

$$p = (\gamma - 1) \frac{E}{V}, \text{ e.g. } \gamma = 1.4 \quad (14)$$

In general, the equation of state is defined in a table stored in the computer memory, and interpolation is used to pick the values of interest.

An updated velocity can now be calculated using the acceleration equation or the equation of motion:

$$\begin{aligned} \frac{du}{dt} &= -V \nabla p = -V \frac{\partial p}{\partial x} = -V \frac{\Delta p}{\Delta x} \\ \frac{u_j^{n+\frac{1}{2}} - u_j^{n-\frac{1}{2}}}{(\Delta t)^n} &= \frac{(x_{j+\frac{1}{2}}^n - x_{j-\frac{1}{2}}^n)}{(\Delta m)_j} \cdot \frac{(p_{j+\frac{1}{2}}^n - p_{j-\frac{1}{2}}^n)}{(x_{j+\frac{1}{2}}^n - x_{j-\frac{1}{2}}^n)} \\ u_j^{n+\frac{1}{2}} &= u_j^{n-\frac{1}{2}} + \frac{(p_{j+\frac{1}{2}}^n - p_{j-\frac{1}{2}}^n)}{(\Delta m)_j} \cdot (\Delta t)^n \end{aligned} \quad (15)$$

The derived difference equations are used for one computational cycle to update all the variables one time step. An artificial viscosity term is added to account for shock presence.

## NUMERICAL MODEL

The cycle involved in pressure wave propagation is shown in Fig. 1. Starting at the top of the loop with the applied pressure field, the equation of motion describing the conservation of momentum provides a functional relationship between the pressure field and the resulting acceleration of each point of the medium.

Accelerations when allowed to act over a small time increment  $dt$  produce new velocities. Velocities produce displacements, and displacements produce strains. Strains produce a new pressure field, and the cycle is repeated. The loop is the basis of numerical processes solving the equations of continuum mechanics for different geometries using the finite differences methods.

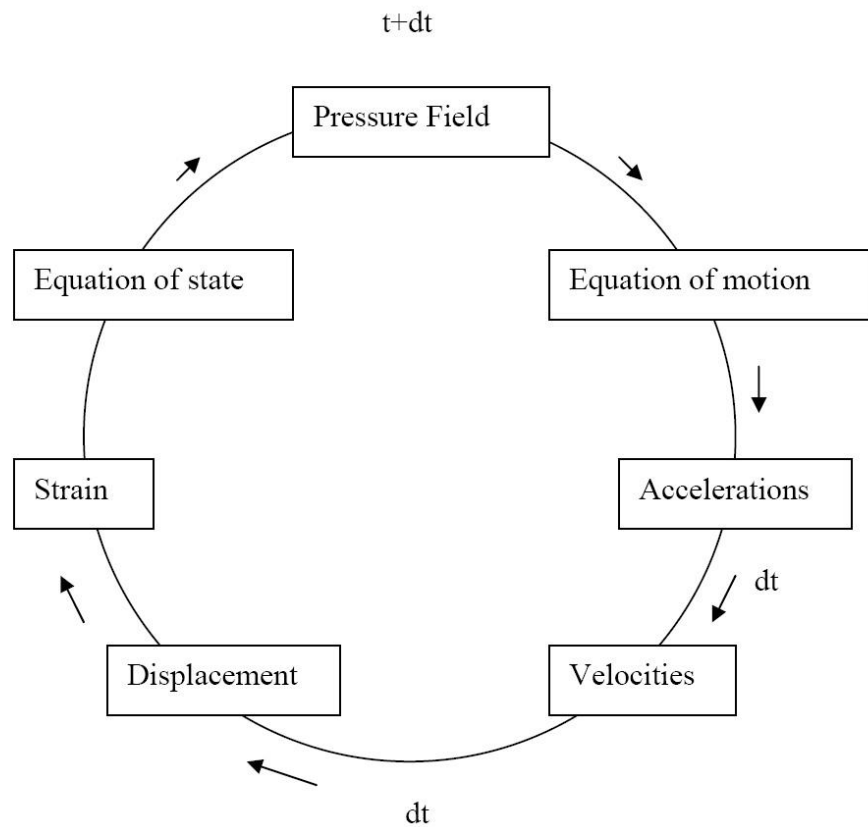


Figure 1. Pressure wave propagation in a medium.

## APPENDIX

### Computational Procedure

```

program computational_fluid_dynamics
!
! Simulating computational fluid dynamics in one dimension
! Lagrangian coordinates and a gas equation of state are used
! M. Ragheb, Univ. of Illinois at Urbana-Champaign
! Version 3.0
! Language: ANSI Fortran 94
!
      implicit none
!*****
! Hydrodynamic variables
! p(j,n)=pressure of j-1/2 th mass at at time update cycle n
! x(j,n)=position of j th mass at time update cycle n
  
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```

! v(j,n)=specific volume =1/density of j-1/2 th mass at time update cycle n
! e(j,n)=specific internal energy of j-1/2 th mass at time update cycle n
! u(j,n)=velocity of j-th mass at at time update cycle n
! n=1 is initial time cycle
! n=2 is new time cycle
!*****
! Arrays specification
! dimension(space,time)
      real p(100,2), x(100,2), v(100,2), e(100,2), u(100,2)
      real deltam,deltat,gamma
      integer max,j,n,timesteps

! constants initialization
! number of time steps in numerical simulation
      timesteps=100
! max=maximum number of spatial meshes of material
      max=10
! deltam=Lagrangian coordinates masses
      deltam=1.0
! deltat=time step
      deltat=0.01
! Equation of state's gas constant, p=(gamma-1)*(e/v)
      gamma=1.4

! Initial conditions of material

      do 11 j=1,max
          x(j,1)=j
! v=(dx.dA)/dm=dV/dm , dA=1=unit area
          v(j,1)=1.
          e(j,1)=2.0
          p(j,1)=(gamma-1.0)*(e(j,1)/v(j,1))
! du/dt = -v dp/dx = -(dx.dA/dm) dp/dx= -dp/dm , dA=unit area
          u(j,1)=0.
11      continue

! Boundary conditions
! initial speed pulse imparted to mass #5
      u(5,1)=10.

! Open output file
      open(9,file='cfd.out')

! loop over time steps
      do 99 n=1,timesteps

! integrating new time cycle variables
      write(*,*) 'Time step =', n
      write(*,*) 'x(j,1),x(j,2),v(j,1),v(j,2),e(j,1),e(j,2),p(j,1),p(j,2),u(j,1),u(j,2)'

! Updating positions
      do 77 j=1,max
          x(j,2)=x(j,1)+(u(j,1) * deltat)

! Updating specific volumes from conservation of energy equation
          if (j.eq.1) then

```

```

        v(j,2)= v(j,1)
    else
        v(j,2) = (x(j,2) - x(j-1,2))/deltam
    end if

! Updating specific internal energy (no pressure extrapolation)
    if(j.eq.1) then
        e(j,2)= e(j,1)
    else
        e(j,2)= e(j,1) -(p(j,1) * (v(j,2)-v(j-1,1)))
    end if

! Updating specific internal energy with pressure extrapolation

! if(j.le.2) then
! e(j,2)= e(j,1)
! else

! Extrapolated pressure
! p(j,1)=p(j-1,1)+(p(j-1,1)-p(j-2,1))/2.0

! e(j,2)= e(j,1) -(p(j,1) * (v(j,2)-v(j-1,1)))
! end if

! Updating pressure from equation of state
    p(j,2) = (gamma-1.0) * (e(j,2)/v(j,2))

! Updating velocities from conservation of momentum equation
    if (j.eq.1) then
        u(j,2) = u(j,1)
    else
        u(j,2) = u(j,1) - ((p(j,2)-p(j-1,2))*(deltat/deltam))
    end if

10    format(10(f6.1,1x))
20    format(10(e14.8,1x))

77    continue

! pause

! Moving updated values vector to initial values vector
    do 88 j=1,max
        x(j,1)=x(j,2)
        v(j,1)=v(j,2)
        e(j,1)=e(j,2)
        p(j,1)=p(j,2)
        u(j,1)=u(j,2)

! Write time step results on screen
        write(*,10) x(j,1),x(j,2),v(j,1),v(j,2),e(j,1),e(j,2), &
            & p(j,1),p(j,2),u(j,1),u(j,2)
! Write time step results on output file:'cfd.out'
        write(9,20) x(j,1),x(j,2),v(j,1),v(j,2),e(j,1),e(j,2), &
            & p(j,1),p(j,2),u(j,1),u(j,2)

```



**88**     **continue**

**pause**

**99**     **continue**

**close(99)**

**stop**

**end**

## **REFERENCES**

1. Joseph B. Keller, "Geometrical Acoustic. I. The Theory of Weak Shock Waves," Journal of Applied Physics, Vol. 25, No. 8, pp. 938-945, August 1958.
2. J. T. Cherry and F. L. Peterson, "Numerical Simulation of Stress Wave Propagation From Underground Nuclear Explosions," in "Peaceful Nuclear Explosions, Phenomenology and Status Report," Proceedings of a panel on the Peaceful Uses of Nuclear Explosions organized by the International Atomic Energy Agency, Vienna, 2-6 March, IAEA-PL-388/15, pp.241-325, 1970.