MONTE CARLO SIMULATION OF FLUID FLOW

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INTRODUCTION

We consider the situation of Free Molecular Collisionless and Reflective Flow. Collisionless flows occur in the field of rarefied gas dynamics. The molecules in this case can impinge on a surface and then be reflected to re-impinge on the surface several times before escape. These types of flow which involve multiple interactions occur in internal as well as external flows past bodies of complex geometry.

If we consider a surface exposed to a gas under free-molecule conditions, the number of molecules incident per unit time on a surface element dr at the location r directly from the external gas can be written as:

$$N_1(r)dr \tag{1}$$

The number of molecules per second that strikes dr at their second collision is:

$$N_2(r)dr = \int_r P(r',r)N_1(r')dr'dr \tag{2}$$

where P(r',r) is the probability that a molecule reflected from the element of surface dr' at the location r' strikes the new location r.

The number of particles striking dr at their third collision becomes:

$$N_3(r)dr = \int_r P(r',r)N_2(r')dr'dr \tag{3}$$

As described by G. Bird, the total number flux at a location r becomes the sum:

$$N(r) = N_1(r) + N_2(r) + N_3(r) + ... \tag{4}$$

Substituting from Eqs.1-3 into Eqn. 4 yields:

$$\begin{aligned} N(r) = N_1(r) + \\ \int_r P(r',r)[N_1(r') + N_2(r') + N_3(r') + ...]dr' \end{aligned} \tag{5}$$

This yields a Fredholm integral equation of the second kind:

$$N(r) = N_1(r) + \int_r P(r',r)N(r)dr' \tag{6}$$

This integral equation is analogous to other equations arising in the field of neutron transport, namely the description of a neutron beam impinging on a shield, or the slowing down of a neutron in a moderator. This means that the methods of analysis in both fields are similar.

PARTICLE TRACKING IN MONTE CARLO SIMULATIONS

The tracking of particles in complex geometries is an important aspect of Monte Carlo simulations. Complex geometries are described in particle transport codes in terms of different surfaces whose intersections and unions are in turn described in combinatorial geometries modules.

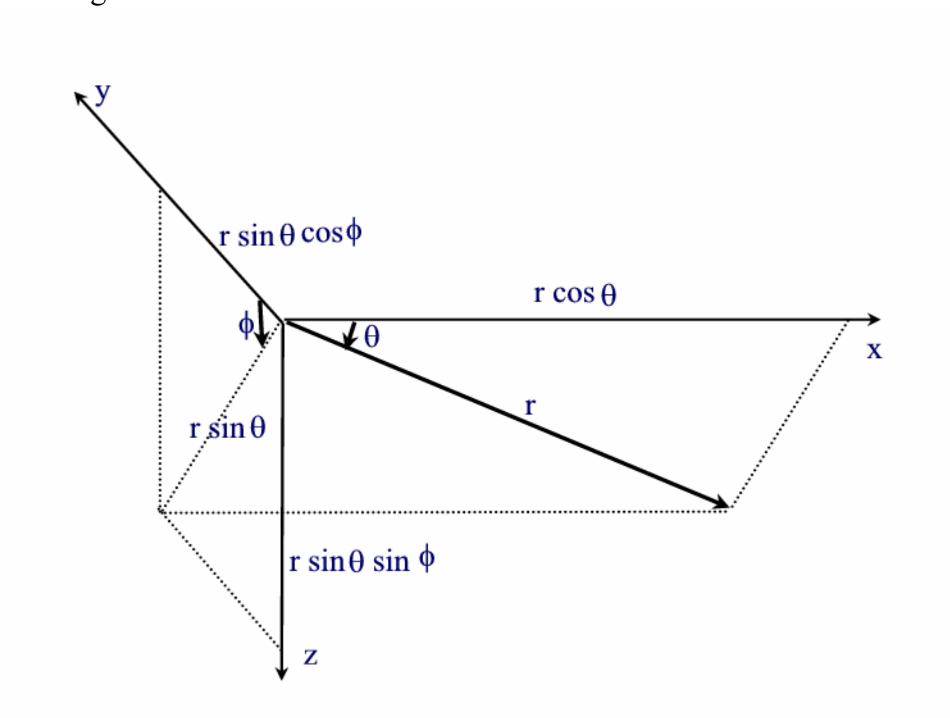

Fig. 1: Geometry for particle tracking and determination of direction cosines.

The intersection of particle trajectories with different surfaces can be obtained from three-dimensional coordinate geometry. Considering the x-axis as the direction of propagation, the direction cosines of a particle are given by:

$$
\begin{aligned}
u &= \frac{x}{r} = \cos\theta \\
v &= \frac{y}{r} = \sin\theta\cos\phi \\
w &= \frac{z}{r} = \sin\theta\sin\phi
\end{aligned}
\tag{7}
$$

A straight line trajectory can be described in terms of these u, v and w direction cosines and the initial point from which the line originates: (x_1, y_1, z_1). We consider the intersection of a line of length l described as:

$$\begin{aligned} x &= x_1 + u.l \\ y &= y_1 + v.l \\ z &= z_1 + w.l \end{aligned} \tag{8}$$

with a quadric surface given by:

$$\begin{aligned} S(x,y,z) = a_{11}x^2 + a_{22}y^2 + a_{33}z^2 + \\ 2a_{23}yz + 2a_{31}zx + 2a_{12}xy + \\ 2a_{14}x + 2a_{24}y + 2a_{34}z + \\ a_{44} = 0 \end{aligned} \tag{9}$$

Defining:

$$\begin{aligned} A_1 &= a_{11}u^2 + a_{22}v^2 + a_{33}w^2 + \\ &\quad 2a_{23}vw + 2a_{31}wu + 2a_{12}uv \\ A_2 &= u(a_{11}x_1 + a_{12}y_1 + a_{13}z_1 + a_{14}) + \\ &\quad v(a_{21}x_1 + a_{22}y_1 + a_{23}z_1 + a_{24}) + \\ &\quad w(a_{31}x_1 + a_{32}y_1 + a_{33}z_1 + a_{34}) \\ A_3 &= S(x_1, y_1, z_1) \end{aligned} \tag{10}$$

The positive real root of the quadratic equation gives the intersection point of the line and the quadratic surface:

$$A_1 l^2 + 2A_2 l + A_3 = 0 \tag{11}$$

The two real roots are:

$$\begin{aligned} l_{1,2} &= \frac{-2A_2 \pm \sqrt{4A_2^2 - 4A_1A_3}}{2A_1} \\ &= \frac{-A_2 \pm \sqrt{A_2^2 - A_1A_3}}{A_1} \end{aligned} \tag{12}$$

The real roots are substituted into the equation of the line to determine the two intersection points:

$$
\begin{aligned}
X_1 &= x_1 + u.l_1 \\
Y_1 &= y_1 + v.l_1 \\
Z_1 &= z_1 + w.l_1
\end{aligned}
\tag{13}
$$

and:

$$
\begin{aligned}
X_2 &= x_1 + u.l_2 \\
Y_2 &= y_1 + v.l_2 \\
Z_2 &= z_1 + w.l_2
\end{aligned}
\tag{14}
$$

The positive root is taken as the new point from which to start a new particle reflection and transport.

CYLINDRICAL TUBE FREE MOLECULAR FLOW

As an application we consider the free molecular gas flow through a cylindrical tube of radius r and length b as shown in Fig. 2. The gas impinges from the left side and flows through the tube through the process of effusion to the right side along the x-axis. The molecules passing through the tube are of two categories:

1. Those that pass directly through the tube,
2. Those that are reflected once or multiple times through the inner surface of the tube.

The total particle flux through the tube thus takes the form of Eqn. 6 as:

$$N_{total} = N_{direct} + \int_0^b N(x)P(x)dx \tag{15}$$

where P(x) is the probability that a particle reflected from the element of length dx at x passes through the tube.

This equation cannot be applied to unsteady flows since it does not contain the time explicitly. Its solution has been first been attempted by Clausing in 1926. The test-particle Monte Carlo method can be applied to its solution by considering a large number of molecular trajectories to calculate the values of N_{total} and N_{direct}.

The solution to the problem is dependent on the tube length to diameter ratio:

$$L = \frac{b}{r} \tag{16}$$

as shown in Fig. 2.

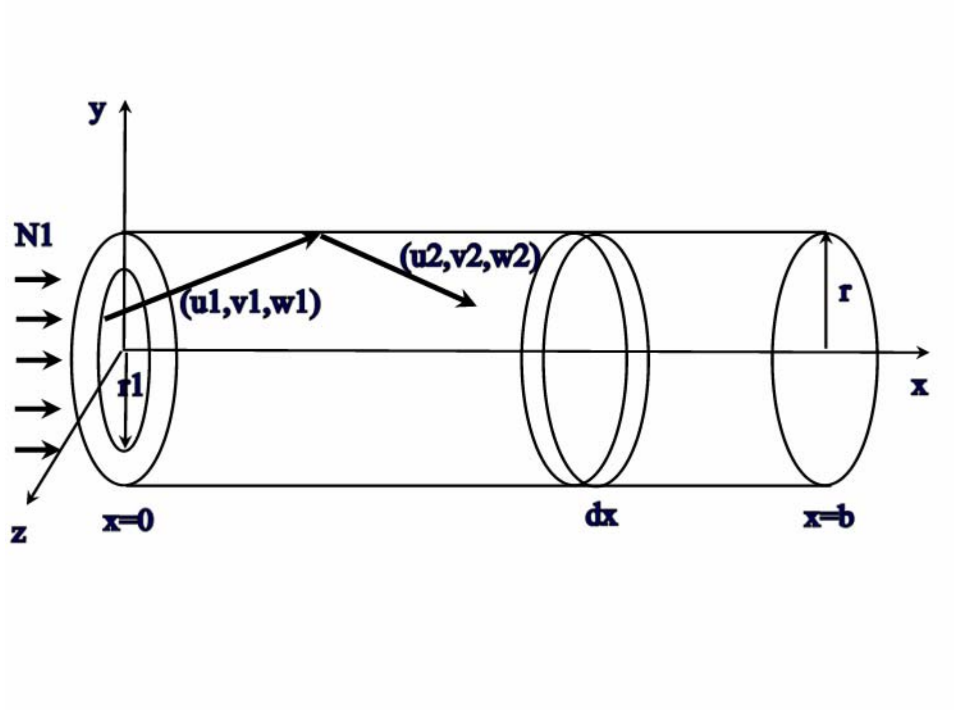

Fig. 2: Cylindrical Tube Flux problem geometry.

MONTE CARLO PROCEDURE

The first step in simulating the particle transport problem is to sample the radial position of the source particle on the left face of the tube. The appropriate probability density function for the radial position is:

$$p(r)dr = \frac{2\pi r dr}{\int_0^a 2\pi r dr} = \frac{2\pi r dr}{\pi a^2} \quad (17)$$

Its cumulative distribution function is equated to a pseudorandom number uniformly distributed over the unit interval as:

$$C(r) = \frac{\int_0^r 2\pi r dr}{\pi a^2} = \left(\frac{r}{a}\right)^2 = \rho_1 \quad (18)$$

Upon inversion this yields a sampled radius r given by:

$$r = a\rho_1^{1/2} \quad (19)$$

The impinging particles follow a cosine probability density function representing a source on a plane covering a 2π solid angle, with the polar angle varying over the interval 0 to π/2, given by:

$$p(\theta,\phi)d\theta d\phi = \frac{2\sin\theta\cos\theta d\theta d\phi}{2\pi} \tag{20}$$

which can be separated into the two probability density functions for the polar and the azimuthal angles:

$$\begin{aligned} &p(\theta,\phi)d\theta d\phi = p(\theta)d\theta . p(\phi)d\phi, \\ &p(\theta)d\theta = 2\sin\theta\cos\theta d\theta, \\ &p(\phi)d\phi = \frac{d\phi}{2\pi}. \end{aligned} \tag{21}$$

The cumulative distribution function for the azimuthal angle is given by:

$$C(\phi) = \frac{\int_0^\phi d\phi}{2\pi} = \frac{\phi}{2\pi} = \rho_2 \tag{22}$$

Upon inversion this yields the sampled azimuthal angle:

$$\phi = 2\pi\rho_2 \tag{23}$$

The cumulative distribution for the polar angle is given by:

$$\begin{aligned} C(\theta) &= 2\int_0^\theta \sin\theta\cos\theta d\theta = 2\int_\theta^0 \cos\theta d(\cos\theta) \\ &= \cos^2\theta\,|_\theta^0 = 1-\cos^2\theta = \rho_3 \end{aligned} \tag{24}$$

This yields for the sampled polar cosine of the polar angle:

$$\mu = \cos\theta = (1-\rho_3)^{1/2} \approx \rho_3^{1/2} \tag{25}$$

The direction cosines can then be calculated according to Eqn. 7:

$$
\begin{aligned}
u &= \frac{x}{r} = \mu \\
v &= \frac{y}{r} = (1-\mu^2)^{1/2}\cos\phi \\
w &= \frac{z}{r} = (1-\mu^2)^{1/2}\sin\phi
\end{aligned}
\tag{26}
$$

The particle tracking process then proceeds according to the procedure shown in Fig. 3.

```
!	Free_Molecular_Flow.for
!	Free collisionless molecular flow through a circular tube
!	Test Particle Monte Carlo Simulation
!	Magdi Ragheb, Univ. of Illinois at Urbana-Champaign
	program Free_Molecular_Flow
	real ltr,direct,fdirect,passing,fpassing,l1,m1,n1
	integer trials
	real :: radius=10.0
	real :: length=10.0
!	Length to radius ratio, ltr
	ltr=length/radius
	write(*,*) 'Length to radius ratio=',ltr
!	Total number of trials
	trials=1000000
	write(*,*) 'Total number of trials=',trials
!	Initialize counters
!	Number of particles passing directly through tube without
!	collisions: through
	direct=0.0
!	Total number passing through tube
	passing=0.0
!	Loop over total number of trials
	do i=1,trials
!	Sample a random radius at tube entry face
		call random(rr)
		r=radius*sqrt(rr)
!	Sample source direction cosines
		call source(l1,m1,n1)
!	Calculate position of source intersection with cylinder
		a=m1*m1
		b=n1*n1
		c=radius*radius
		d=r*r
		position=l1*(r*m1+sqrt(c*(a+b)-d*b))/(a+b)
!	Test for particle exiting cylinder
		if(position.gt.length) goto 777
!	Calculate diffuse direction cosines for reflection off the wall
!	Upon reflection, m1 reverses to l1 and m1 reverses to l1
111		call source(m1,l1,n1)
!	Determine next intersection point
		position=position+2.0*l1*radius*m1/(m1*m1+n1*n1)
!	Test if position less than zero
		if (position.lt.0.0) goto 999
!	Test for position larger than length of tube
```

```
                if (position.gt.length) goto 888
!         Let particle reflect off boundary
                go to 111
!         Score a particle directly passing through tube
777       direct=direct+1.0
!         Score a transmitted particle
888   passing=passing+1.0
!         Do not score, start new saource particle
999   continue
          end do

!         Generate output results
!         Fraction passing directly through tube without collisions
          fdirect=direct/trials
!         Total fraction of particles passing through tube
          fpassing=passing/trials
          write(*,*)'Fraction passing directly through=',fdirect
          write(*,*)'Total fraction passing=',fpassing

          end

          subroutine source(w,u,v)
          real u,v,w
!         Simulation of effusion or gas emission
          pi=3.14159
          call random(rr)
!         Direction cosine along direction of effusion or z-axis
!         w=cos(polar angle theta), takes values from zero to one
          costheta=sqrt(rr)
          sintheta=sqrt(1.0-w*w)
!         Sample azimuthal angle phi
          call random(rr)
          phi=2.0*pi*rr
!         Direction cosines
!         relative to x-axis
          u=sintheta*cos(phi)
!         relative to y-axis
          v=sintheta*sin(phi)
!         relative to z-axis
          w=costheta
          return
          end
```

Fig. 3: Monte Carlo procedure for the cylindrical Tube Flux Problem.

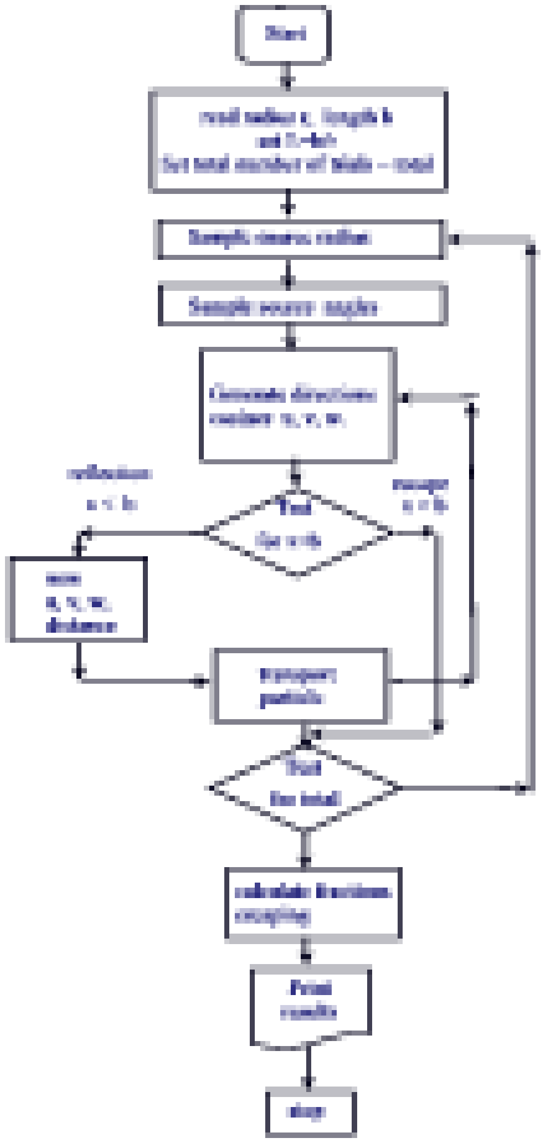

Fig. 4: Flow Chart for computational steps.

A special case of the quadratic surface of Eqn. 9 for the case of the cylinder is given with:

$$a_{22} = a_{33} = 1,$$
$$a_{44} = -r^2.$$

The initial coordinates take advantage of symmetry and and become:

$$z_0 = 0,$$
$$y_0 = -r_1,$$
$$x_0 = 0.$$

Thus one can deduce that the coordinates of the intersection of the particle's path with the cylinder, using symmetry is:

$$x_{\text{int}} = \frac{u\{r_1 v + [r^2(v^2 + w^2) - r_1^2 w^2\}^{1/2}]}{v^2 + w^2},$$
$$y_{\text{int}} = -r$$
$$z_{\text{int}} = 0.$$

The new x coordinate value of the next point of intersection with the cylindrical surface becomes:

$$x_{new} = x_{\text{int}} + \frac{2ru_{\text{int}} v_{\text{int}}}{v_{\text{int}}^2 + w_{\text{int}}^2}$$

A flow Chart for the computational steps is shown in Fig. 4.

DISCUSSION

The result of the Monte Carlo simulation for a tube with a length to radius ratio of unity is shown in Table 1. It is also compared to the same analytical result by Clausius for the same ratio.

It should be noticed that the methodology discussed here is useful for steady state flows. Howewver since it does not involve the time variable explicitly, if unsteady flow is under consideration, then an approach involving Direct Simulation Monte Carlo (DSMC) becomes the possible alternative.

Table 1: Comparison of Monte Carlo and Analytical results.

	Monte Carlo Simulation 10^6 particles	*Exact Analytical result Clausing (1932)*
Length to radius ratio	1	1
Fraction passing directly through	0.38919	-
Total fraction passing through tube	0.683983	0.672

EXERCISE

1. For the problem of free molecular flow through a tube, plot the fraction passing directly through and the total fraction passing as a function of the length to radius ratio of the tube.