POD 22

Taylor Dispersion via MC.

We can simulate convection and diffusion leading to dispersion by tracking the motion of tracers undergoing a random walk. At each time step they take a step w/ standard deviation

$$\Delta x = \text{randn} * (2 * D * dt)^{1/2}$$

We then follow them in space!

Effectively, we are integrating the Langevin equation in time and tracking the statistics.

The growth in the variance is just 2K!

For channel flow we have the velocity: $u_z = \frac{3}{2} U \left(1 - \frac{y^2}{b^2}\right)$

For a channel w/ side walls at $x = \pm b$ it is more complex! Using sep. of variables you find:

$$u_z^* = \frac{u_z}{U} = \frac{3}{2}(1 - y^{*2})$$
$$+ \sum_{n=1}^{\infty} \frac{6(-1)^n}{\sigma_n^3} \frac{\cosh \sigma_n x^*}{\cosh \sigma_n \frac{a}{b}} \cos \sigma_n y^*$$

where $\sigma_n = (n - \frac{1}{2})\pi$

and $y^* = y/b$, $x^* = \frac{x}{b}$

w/ side walls at $x^* = \pm a/b$

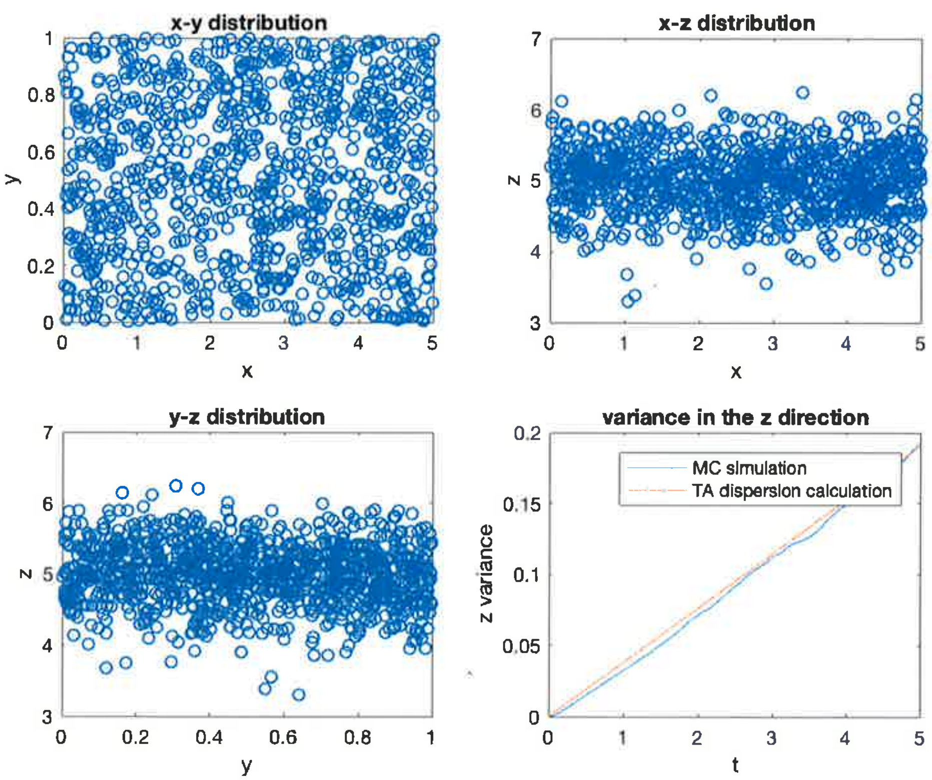
Integrating the correction, you find that the effect of the side wall is approximated by a stagnant region of width $\frac{5}{8}a$ on each side. It's easy to add this into our MC simulation.

POD 22: MC Simulation of Taylor Dispersion

We construct a simple Monte Carlo simulation of dispersion in a channel, first with no effect of the side walls, and then with the no-slip side walls causing a velocity reduction. The effect of the side walls is approximated by causing all tracers within 5/8 of the edges to have a velocity of zero. By symmetry, we shall only consider the top right quarter of the rectangular channel. It has a dimensionless half-height of 1 and a dimensionless half width of ab (e.g., a/b).

```
n= 1000;
ab = 5;

% We distribute them randomly.
x = ab*rand(n,1);
y = rand(n,1);
z = zeros(n,1);

dt = 0.00005; %Our time step
tquit = 5;
t = [dt:dt:tquit]'; %Our times

uz = @(y) 1.5*(1-y.^2); %our velocity

varz = zeros(1/dt,1); %we keep track of the variance.

for i=1:tquit/dt-1
    dz1 = uz(y);

%    k = find(x>ab-5/8); dz1(k)=0; %The side wall fix...

    x = x + randn(n,1)*(2*dt)^.5;
    x = abs(x); %We reflect in the x-direction at the center
    x = min(x, 2*ab-x); %We reflect in from the right side

    y = y + randn(n,1)*(2*dt)^.5;
    y = abs(y);
    y = min(y, 2-y); %We reflect in from the top

    dz2 = uz(y);

%    k = find(x>ab-5/8); dz2(k)=0; %The side wall again.

    z = z + (dz1+dz2)/2*dt; %We update the velocity

    varz(i) = var(z);

end

    figure(1)
    subplot(2,2,1),plot(x,y,'o')
    xlabel('x')
    ylabel('y')
    title('x-y distribution')
    drawnow

    subplot(2,2,2),plot(x,z,'o')
    xlabel('x')
    ylabel('z')
```

```
title('x-z distribution')
drawnow

subplot(2,2,3),plot(y,z,'o')
xlabel('y')
ylabel('z')
title('y-z distribution')
drawnow

subplot(2,2,4),plot(t(1:i),varz(1:i),t(1:i),4/105*t(1:i))
xlabel('t')
ylabel('z variance')
title('variance in the z direction')
legend('MC simulation','TA dispersion calculation')
drawnow
```



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Calc. of side Wall Correction

$$\mu \nabla^2 u = -G = \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$y^* = y/b \quad , \quad x^* = x/b \quad \therefore \text{ wall is at } x^* = a/b \gg 1$$

Take $u^* = \frac{3}{2}(1 - y^{*2}) + u_d(x^*, y^*)$

so $$\frac{\partial^2 u_d^*}{\partial x^{*2}} + \frac{\partial^2 u_d^*}{\partial y^{*2}} = 0$$

$$\left.\frac{\partial u_d^*}{\partial y^*}\right|_{y^*=0} = 0 \qquad \left.u_d^*\right|_{y^*=1} = 0$$

$$\left.u_d^*\right|_{x^* = \frac{a}{b}} = -\frac{3}{2}(1 - y^{*2})$$

so $$u_d^* = F(y^*)\, G(x^*)$$

$$\frac{G''}{G} = -\frac{F''}{F} = \sigma^2$$

$$F = \cancel{A}^{\,0} \sin \sigma y^* + B \cos \sigma y^*$$

$$\sigma_n = \left(n - \tfrac{1}{2}\right)\pi$$

so $\quad G = \underbrace{\cancel{A}}_{0}\sinh\sigma x^* + \underbrace{B}_{\text{want even f}^{\underline{n}}}\cosh\sigma x^*$

So $\quad u_d^* = \displaystyle\sum_{n=1}^{\infty} A_n \cosh\sigma_n x^* \cos\sigma_n y^*$

Now $\quad u_d^*\Big|_{x^* = \frac{a}{b}} = -\frac{3}{2}\left(1 - y^{*2}\right)$

$$= \sum_{n=1}^{\infty}\left[A_n \cosh\sigma_n \frac{a}{b}\right]\cos\sigma_n y^*$$

$$\therefore\ A_n \cosh\sigma_n \frac{a}{b} = 2\int_0^1 \frac{-3}{2}\left(1 - y^{*2}\right)\cos\sigma_n y^* \, dy^*$$

$$= \frac{48\,(-1)^n}{\pi^3(2n-1)^3} = \frac{6\cancel{8}\,(-1)^n}{\sigma_n^{\,3}}$$

$$\therefore\ A_n = \frac{6\cancel{8}\,(-1)^n}{\sigma_n^{\,3}}\ \frac{1}{\cosh\sigma_n \frac{a}{b}}$$

and $\quad u^* = \dfrac{3}{2}\left(1 - y^{*2}\right) + \displaystyle\sum_{n=1}^{\infty} \frac{6\cancel{8}(-1)^n}{\sigma_n^{\,3}}\ \frac{\cosh\sigma_n x^* \cos}{\cosh\sigma_n \frac{a}{b}}\cancel{\sin}\,\sigma_n y^*$

We can approximate the slow down at the side walls by a stagnant layer of thickness $\delta^* = \delta/a$

$$-\frac{\delta}{a} = \int_0^1 \int_0^{a/b} \sum_{n=1}^{\infty} \frac{6(-1)^n}{\sigma_n^3} \frac{\cosh \sigma_n x^*}{\cosh \sigma_n \frac{a}{b}} \cos \sigma_n y^* \, dx^* dy^*$$

$$= \int_0^1 \sum_{n=1}^{\infty} \frac{6(-1)^n}{\sigma_n^4} \underbrace{\left[\frac{\sinh \sigma_n \frac{a}{b}}{\cosh \sigma_n \frac{a}{b}}\right]}_{\approx 1} \cos \sigma_n y^* \, dy^*$$

$$= \sum_{n=1}^{\infty} +\frac{6(-1)^n}{\sigma_n^5} \sin \sigma_n y^* \Big|_0^1$$

$$= \sum_{n=1}^{\infty} +\frac{6(-1)^n}{\sigma_n^5} = \sum_{n=1}^{\infty} \frac{6(-1)^n}{\left(\left(n-\frac{1}{2}\right)\pi\right)^5}$$

$$= \frac{5}{8}$$

So for our simulation we just have a layer of width $5/8$ next to each side where $u=0$