

Advanced Transport Phenomena

Practical session 9

Solution of Population Balance Equations (PBEs) using the Discrete Sectional Method (DSM) and the Quadrature Method of Moments (QMOM)

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Population Balance Equations: Discrete Sectional Method (DSM)

Diffusion controlled growth (for spherical particles with initial radius $r_0 < 1\mu m$)

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r} (\dot{R}f) = 0$$

initial conditions: $f(r, t=0) = f^0(r)$

boundary conditions: $\dot{R}f(r=0, t) = 0, \dot{R}f(r=+\infty, t) = 0$

Initial solution

$$f^0(r) = ar^2 \exp(-br)$$

Analytical Solution

$$f(r, t) = \frac{r}{\sqrt{r^2 - 2k_G t}} f^0 \left(\sqrt{r^2 - 2k_G t} \right)$$

Growth rate

$$\dot{R} = \frac{dr}{dt} = \frac{k_G}{r}$$

Parameters

$$\begin{aligned} a &= 0.108 \mu m^{-1} cm^{-3} \\ b &= 0.60 \mu m^{-1} \\ k_G &= 0.78 \mu m^2 s^{-1} \end{aligned}$$

```
% a and b: distribution parameters
a = 0.108; % (1/mum/cm3)
b = 0.60; % (1/mum)

% Growth rate: dr/dt
kG = 0.78; % growth rate constant (mum2/s)
```

Numerical Solution (Discrete Sectional Method)

```
% Domain of integration
rMax = 30; % maximum radius (mum)
M = 100; % number of sections
tf = 20; % maximum time (s)

% Initial distribution (#/cm3/mum)
r = 0:rMax/M:rMax;
fIn = fInitial(r, a, b);
```

Discrete sections

$$N_i = f_{i+1} (r_{i+1} - r_i) \quad i = 1, \dots, M$$

```
% Number of particles (per unit of volume) in each interval (#/cm3)
NIn = zeros(M,1);
for i=1:M
    NIn(i) = fIn(i+1)*(r(i+1)-r(i));
end
```

Discretized equations

$$\frac{dN_1}{dt} = -f_2 \dot{R}_2$$

$$\frac{dN_i}{dt} = -f_{i+1} \dot{R}_{i+1} + f_i \dot{R}_i \quad i = 2, \dots, M-1$$

$$\frac{dN_M}{dt} = f_M \dot{R}_M$$

```
% Solution of discrete section equations
[t, N] = ode15s(@ODESystem, 0:1:tf, NIn, [], r, kG);
ntimes = length(t);
```

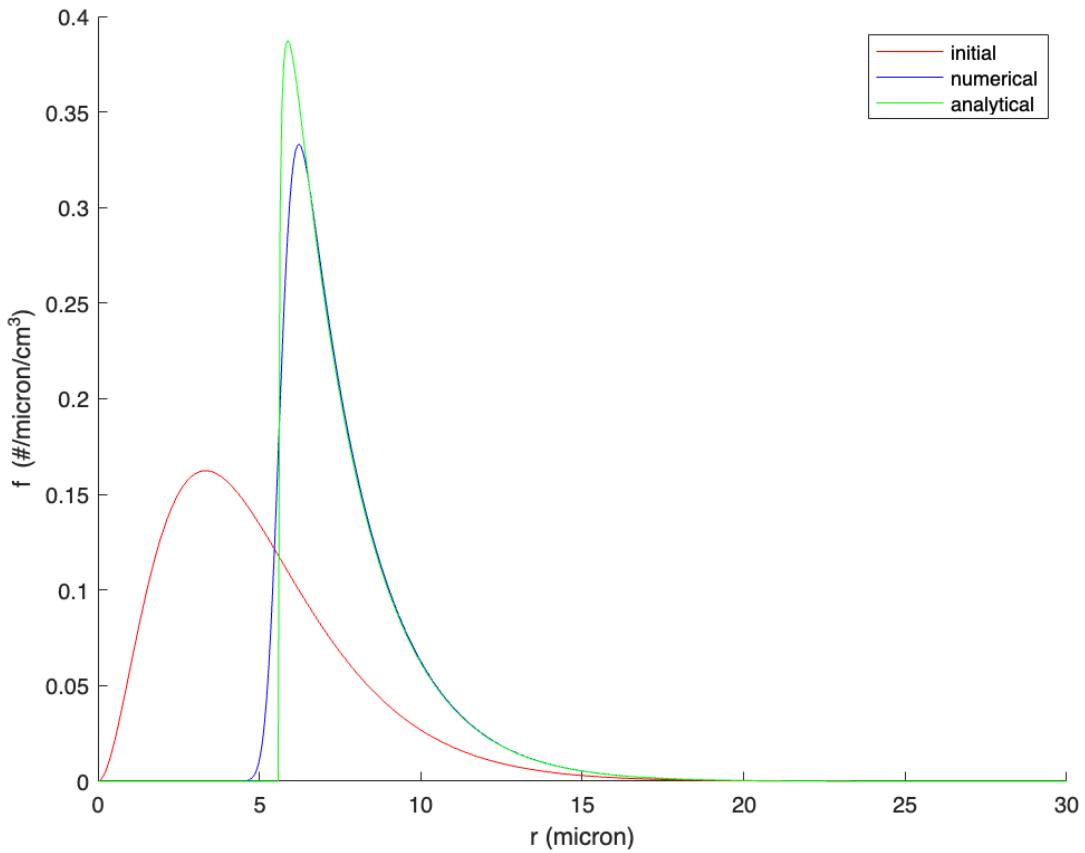
Reconstruct the density function

$$f_{i+1} = \frac{N_i}{r_{i+1} - r_i} \quad i = 1, \dots, M$$

```
% Reconstruction of density function (#/cm3/mum3)
f = zeros(ntimes, M+1);
for i=1:ntimes
    f(i, 2:end) = N(i,:)./(r(2:end)-r(1:end-1));
end
```

Plot solution at t=tf

```
figure; hold on;
plot(r, fIn, 'r');
plot(r, f(end,:), 'b');
plot(r, fAnalytical(r, tf, kG, a, b), 'g');
xlabel('r (micron)');
ylabel('f (#/micron/cm^3)');
legend('initial', 'numerical', 'analytical');
hold off;
```



Calculation of moments

```
% Calculation of moments (initial and final)
m0(1) = Moment(r, fIn, 0);
m0(2) = Moment(r, fIn, 1);
mf(1) = Moment(r, f(end,:), 0);
mf(2) = Moment(r, f(end,:), 1);

fprintf('Time=0 s: Ntot(#/cm3)=%f Rm(micron)=%f\n', m0(1), m0(2));
```

Time=0 s: Ntot(#/cm3)=0.999997 Rm(micron)=4.999912

```
fprintf('Time=20 s: Ntot(#/cm3)=%f Rm(micron)=%f\n', mf(1), mf(2));
```

Time=20 s: Ntot(#/cm3)=0.999997 Rm(micron)=7.769062

Evolution of mean radius

```

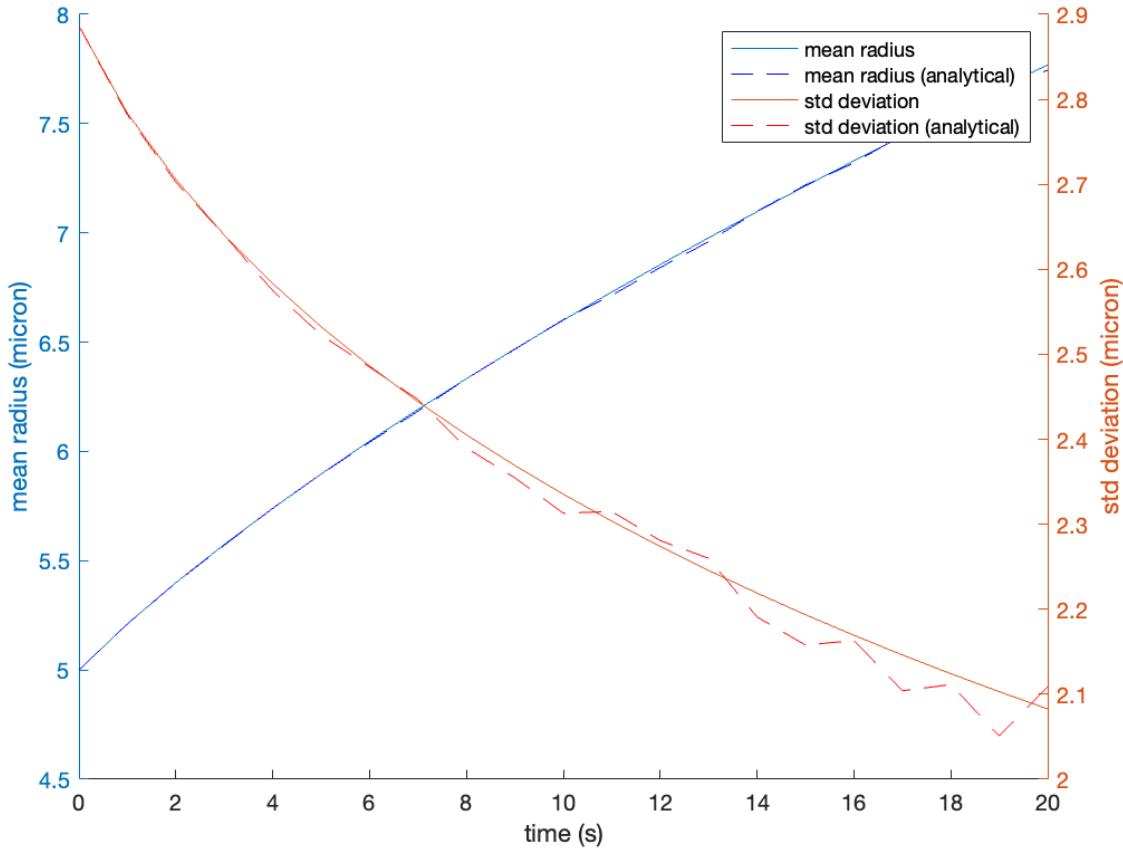
% Analytical results
muAnalytical1 = zeros(length(t),1);
muAnalytical2 = zeros(length(t),1);
for k=1:length(t)
    muAnalytical1(k) = AnalyticalMoments(1, r, t(k), kG, a, b);
    muAnalytical2(k) = AnalyticalMoments(2, r, t(k), kG, a, b);
end

% Numerical results
m1 = zeros(length(t),1);
m2 = zeros(length(t),1);
for i=1:length(t)
    m1(i) = Moment(r, f(i,:), 1);
    m2(i) = Moment(r, f(i,:), 2);

end

figure; hold on;
yyaxis left; ylabel('mean radius (micron)');
plot(t, m1);
plot(t, muAnalytical1, 'b--');
yyaxis right; ylabel('std deviation (micron)');
plot(t, sqrt(m2-m1.^2));
plot(t, sqrt(muAnalytical2-muAnalytical1.^2), 'r--');
xlabel('time (s)'); hold off;
legend('mean radius', 'mean radius (analytical)', 'std deviation', ...
    'std deviation (analytical)');

```



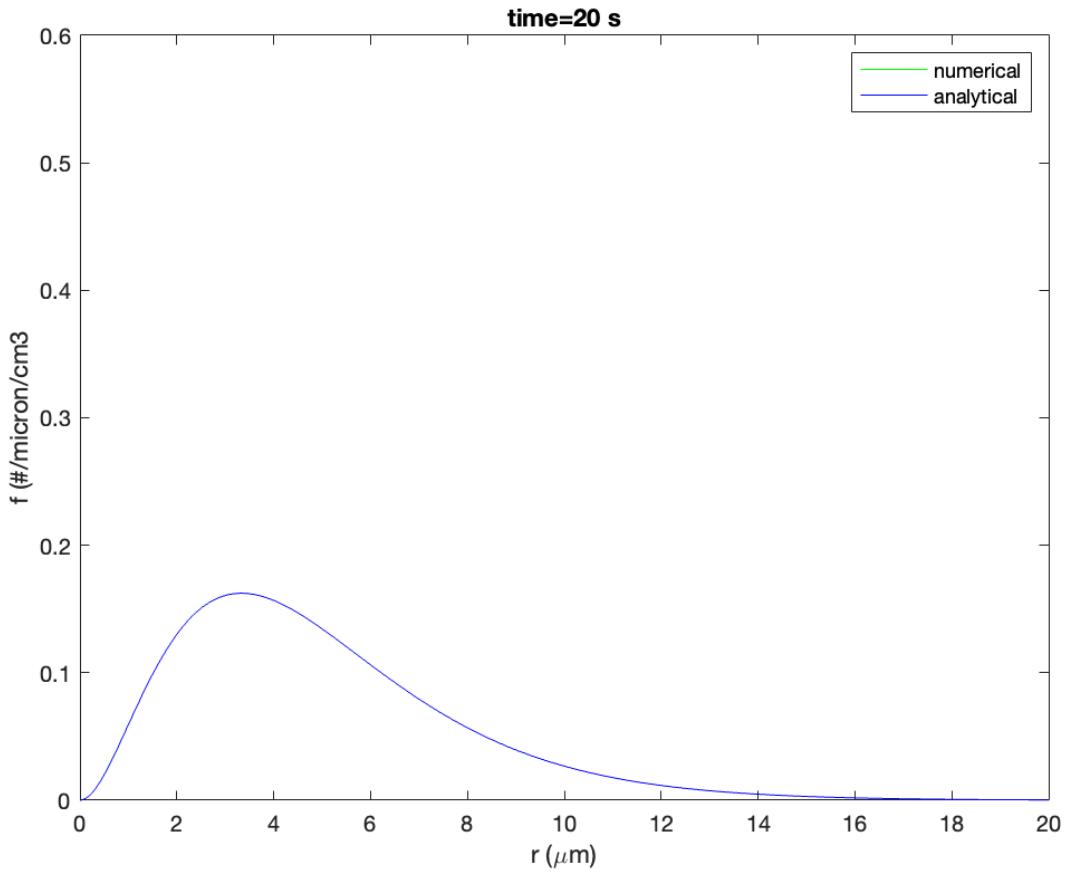
Dynamic evolution of density function

```

video_name = 'dsm.mp4';
videomp4 = VideoWriter(video_name, 'MPEG-4');
open(videomp4);

figure;
for k=1:length(t)
    hold off;
    plot(r, fAnalytical(r, t(k), kG, a, b), 'g');
    hold on;
    plot(r, f(k,:), 'b');
    hold on;
    xlabel('r (\mu m)'); ylabel('f (#/micron/cm^3)'); title('time=20 s');
    xlim([0 20]); ylim([0 0.6]);
    legend('numerical','analytical');
    frame = getframe(gcf);
    writeVideo(videomp4, frame);
end

```



```
close(videomp4);
```

Functions

```
function dN = ODESysteM(~, N, r, kG)

M = length(N);

f = zeros(M+1,1);
for i=1:M
    f(i+1) = N(i)/(r(i+1)-r(i));
end

dN = zeros(M,1);
dN(1) = -f(2)*Rdot(kG, r(2));
for i=2:M-1
    dN(i) = -f(i+1)*Rdot(kG, r(i+1)) + f(i)*Rdot(kG, r(i));
end
dN(M) = f(M)*Rdot(kG, r(M));

end
```

```

function drdt = Rdot(kG, r)
    drdt = kG/r;
end

```

```

function f = fAnalytical(r, t, kG, a, b)

f = zeros(length(r),1);
for i=1:length(r)
    arg = r(i)^2-2*kG*t;
    if (arg > 0)
        f(i) = r(i)/sqrt(arg).*fInitial(sqrt(arg), a, b);
    end
end

```

```

function m = Moment(r, f, order)

np = length(r);
m = 0;
for i=1:np-1
    deltar = r(i+1)-r(i);
    I = 0.50*(f(i+1)*r(i+1)^order+f(i)*r(i)^order);
    m = m + deltar*I;
end

```

```

function f = fInitial(r, a, b)

f = a*(r.^2).*exp(-b*r);

end

```

```

function muk = AnalyticalMoments(k, r, t, kG, a, b)

muk = 0.;
for j=1:length(r)-1
    deltar = r(j+1)-r(j);
    Ic = 0.50*(r(j+1)^(k)*fAnalytical(r(j+1), t, kG, a, ...
        b)+r(j)^(k)*fAnalytical(r(j), t, kG, a, b));
    muk = muk + Ic*deltar;
end

```

```
end
```

Population Balance Equations: Quadrature Method of Moments (QMoM)

Diffusion controlled growth (for spherical particles with initial radius $r_0 < 1\mu m$)

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r} (\dot{R}f) = 0$$

initial conditions: $f(r, t = 0) = f^0(r)$

boundary conditions: $\dot{R}f(r = 0, t) = 0, \dot{R}f(r = +\infty, t) = 0$

Initial solution

$$f^0(r) = ar^2 \exp(-br)$$

Analytical Solution

$$f(r, t) = \frac{r}{\sqrt{r^2 - 2k_G t}} f^0 \left(\sqrt{r^2 - 2k_G t} \right)$$

Growth rate

$$\dot{R} = \frac{dr}{dt} = \frac{k_G}{r}$$

Parameters

$$\begin{aligned} a &= 0.108 \mu m^{-1} cm^{-3} \\ b &= 0.60 \mu m^{-1} \\ k_G &= 0.78 \mu m^2 s^{-1} \end{aligned}$$

```
% a and b: distribution parameters
a = 0.108; % (1/mum/cm3)
b = 0.60; % (1/mum)

% Growth rate: dr/dt
kG = 0.78; % growth rate constant (mum2/s)
```

Numerical Solution (Quadrature Method of Moments)

```
% Number of quadrature points
N = 3;

% Domain of integration
rMax = 30; % maximum radius (mm)
tf = 20; % maximum time (s)

% Initial distribution (#/cm3/mm)
r = 0:rMax/1000:rMax;
fIn = fInitial(r, a, b);
```

Initial moments and normalization

$$\mu_k = \int_0^{r_{\max}} r^k f^0(r) dr$$

$$\mu_k^{\text{norm}} = \frac{\mu_k}{\mu_0}$$

```
% Initial moments
Neq = 2*N; % number of moments/equations
muIn = zeros(Neq,1);
for k=0:Neq-1
    muIn(k+1) = AnalyticalMoments(k, r, 0, kG, a, b);
end

% Normalization
muNormIn = muIn/muIn(1);
```

Numerical solution of moment equations

$$\frac{d\mu_k}{dt} = k \sum_{i=1}^N \dot{R}_i r_i^{k-1} w_i$$

```
% Solution of moment equations
[t, muNorm] = ode15s(@ODESystem, 0:0.25:tf, muNormIn, [], kG);

% Denormalization
mu = muNorm*muIn(1);
```

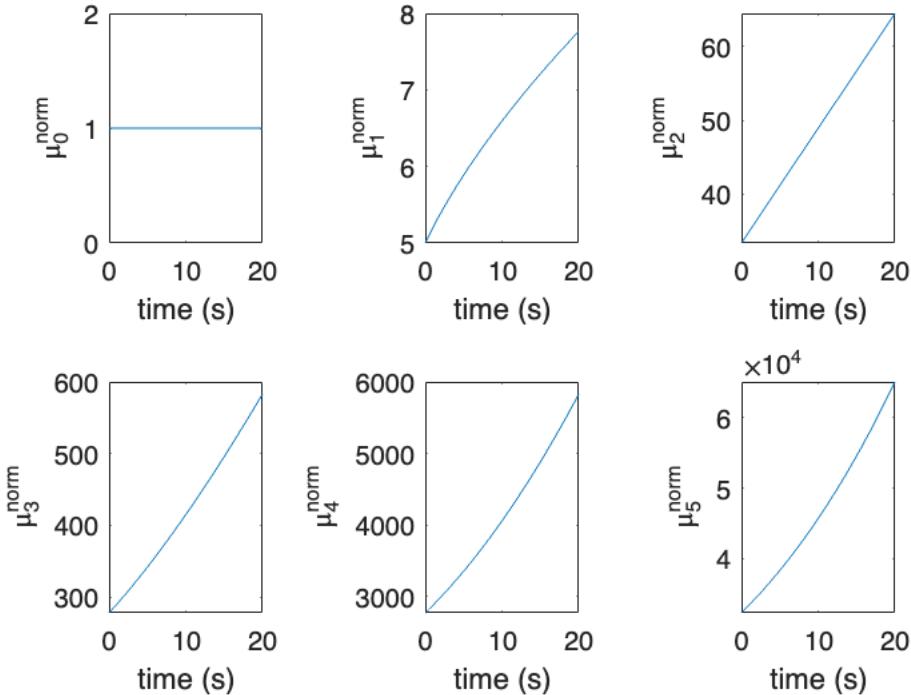
Plotting temporal evolution of moments

```
figure;
tiledlayout(2,3);
```

```

nexttile; plot(t, muNorm(:,1)); xlabel('time (s)'); ...
    ylabel('\mu_0^{norm}');
nexttile; plot(t, muNorm(:,2)); xlabel('time (s)'); ...
    ylabel('\mu_1^{norm}');
nexttile; plot(t, muNorm(:,3)); xlabel('time (s)'); ...
    ylabel('\mu_2^{norm}');
nexttile; plot(t, muNorm(:,4)); xlabel('time (s)'); ...
    ylabel('\mu_3^{norm}');
nexttile; plot(t, muNorm(:,5)); xlabel('time (s)'); ...
    ylabel('\mu_4^{norm}');
nexttile; plot(t, muNorm(:,6)); xlabel('time (s)'); ...
    ylabel('\mu_5^{norm}');

```



Evolution of mean radius

```

% Analytical results
for k=1:length(t)
    muAnalytical1(k) = AnalyticalMoments(1, r, t(k), kG, a, b);
    muAnalytical2(k) = AnalyticalMoments(2, r, t(k), kG, a, b);
end

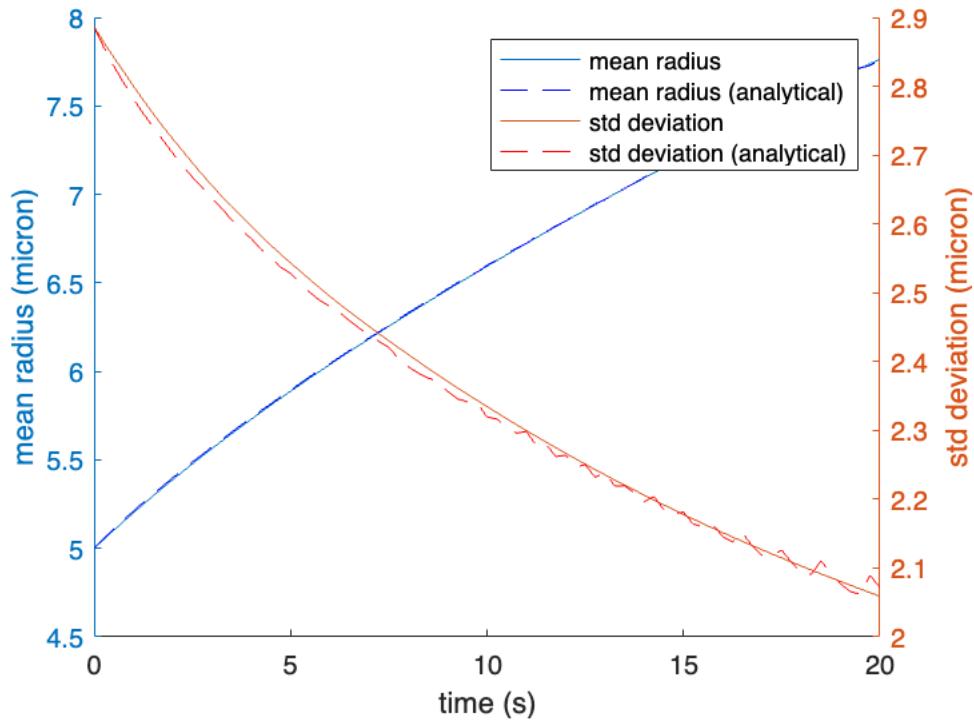
figure; hold on;
yyaxis left; ylabel('mean radius (micron)');
plot(t, muNorm(:,2));
plot(t, muAnalytical1/muIn(1), 'b--');
yyaxis right; ylabel('std deviation (micron)');

```

```

plot(t, sqrt(muNorm(:,3)-muNorm(:,2).^2));
plot(t, sqrt(muAnalytical2-muAnalytical1.^2), 'r--');
xlabel('time (s)'); hold off;
legend('mean radius', 'mean radius (analytical)', 'std deviation', ...
'std deviation (analytical)');

```



Plot density functions

```

% Plot the distribution function
figure;
tiledlayout(1,2);

% Initial time
nexttile; hold on; xlabel('r (\mu m)'); ylabel('f (#/micron/cm^3)'); ...
title('time=0'); xlim([0 20]);
plot(r, fIn, 'r');
[w, L] = MomentInversion(muNorm(1, :));
for i=1:N
    line([L(i),L(i)], [0 w(i)*muIn(1)]);
end
legend('initial', 'numerical');
hold off;

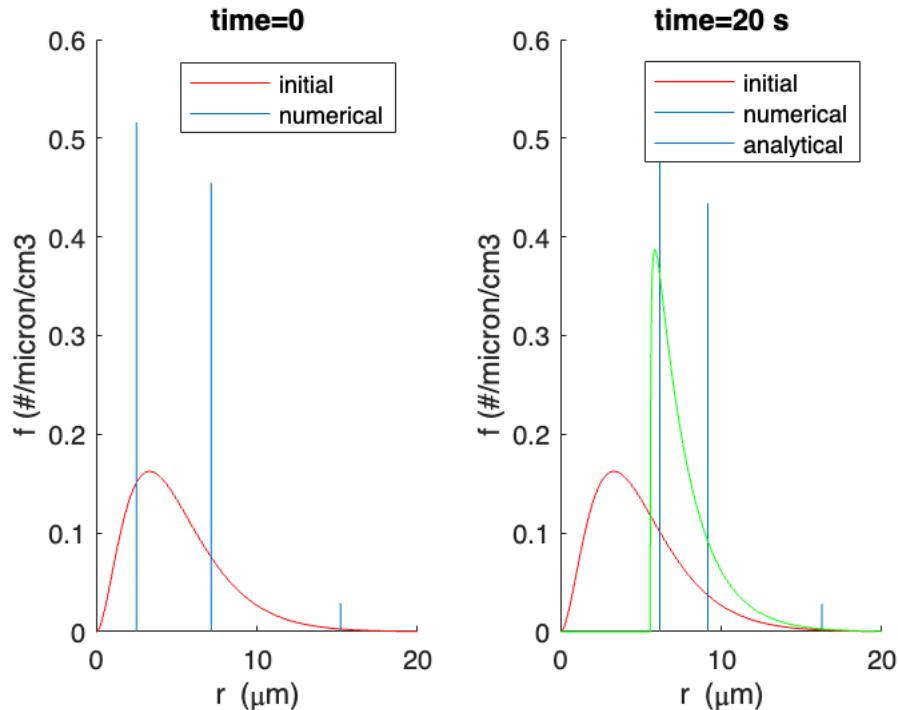
% Final time
nexttile; hold on; xlabel('r (\mu m)'); ylabel('f (#/micron/cm^3)'); ...
title('time=20 s'); xlim([0 20]);

```

```

plot(r, fIn, 'r');
[w, L] = MomentInversion(muNorm(end, :));
for i=1:N
    line([L(i),L(i)], [0 w(i)*muIn(1)]);
end
plot(r, fAnalytical(r, tf, kG, a, b), 'g');
legend('initial', 'numerical','analytical');
hold off;

```



```

[w, L] = MomentInversion(muNorm(1, :));
fprintf('Time=0 s: rm(micron)=%f sigma(micron)=%f\n', Lm(w,L), ...
StdDev(w,L));

```

Time=0 s: rm(micron)=4.999926 sigma(micron)=2.886409

```

[w, L] = MomentInversion(muNorm(end, :));
fprintf('Time=20 s: rm(micron)=%f sigma(micron)=%f\n', Lm(w,L), ...
StdDev(w,L));

```

Time=20 s: rm(micron)=7.764768 sigma(micron)=2.058881

Dynamic evolution of the density function

```

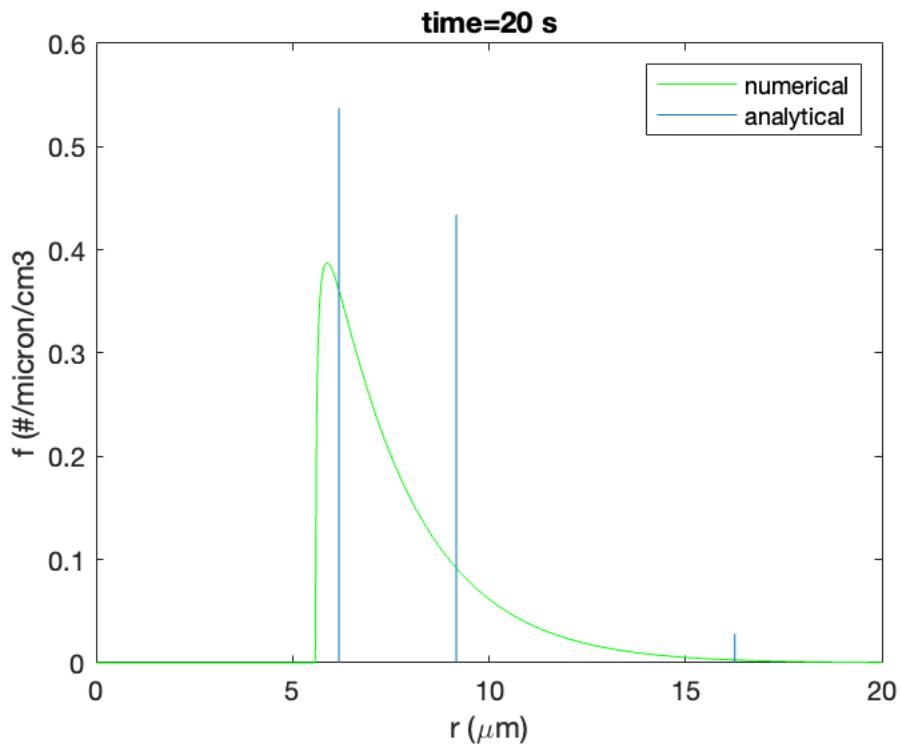
video_name = 'qmom.mp4';
videomp4 = VideoWriter(video_name, 'MPEG-4');
open(videomp4);

figure;
for k=1:length(t)

    [w, L] = MomentInversion(muNorm(k, :));

    hold off;
    plot(r, fAnalytical(r, t(k), kG, a, b), 'g');
    hold on;
    for i=1:N
        line([L(i),L(i)], [0 w(i)*muIn(1)]);
    end
    hold on;
    xlabel('r (\mu m)'); ylabel('f (#/micron/cm3)'); title('time=20 s');
    legend('numerical','analytical');
    xlim([0 20]); ylim([0 0.6]);
    frame = getframe(gcf);
    writeVideo(videomp4, frame);
end

```



```
close(videomp4);
```

Functions

```
function dmuNorm = ODESSystem(~, muNorm, kG)

Neq = length(muNorm);
N = Neq/2;

[w,L] = MomentInversion(muNorm);

dmuNorm = zeros(Neq, 1);

for i=1:Neq
    k = i-1;
    sum = 0;
    for j=1:N
        sum = sum + L(j)^(k-1)*Rdot(kG, L(j))*w(j);
    end
    dmuNorm(i) = k*sum;
end

end
```

```
%% Growth rate
function drdt = Rdot(kG, r)

drdt = kG/r;

end
```

```
%% Moment inversion function (PD algorithm, Gordon 1968)
function [w, L] = MomentInversion(muNorm)

N = length(muNorm)/2;

P = zeros(2*N+1, 2*N+1);
P(1,1) = 1;
P(1,2) = 1;
for i=2:2*N
    P(i,2) = (-1)^(i-1)*muNorm(i-1+1);
end

for j=3:2*N+1
    for i=1:2*N+2-j
        P(i,j) = P(1,j-1)*P(i+1,j-2)-P(1,j-2)*P(i+1,j-1);
    end
end

alpha = zeros(2*N,1);
alpha(1) = 0;
```

```

for i=2:2*N
    alpha(i) = P(1,i+1)/P(1,i)/P(1,i-1);
end

a = zeros(N,1);
for i=1:N
    a(i) = alpha(2*i)+alpha(2*i-1);
end

b = zeros(N-1,1);
for i=1:N-1
    b(i) = sqrt(alpha(2*i+1)*alpha(2*i));
end

A = diag(a);
for i=1:N-1
    A(i,i+1) = b(i);
    A(i+1,i) = b(i);
end

[V,csi] = eig(A);
L = diag(csi);

w = zeros(N,1);
for i=1:N
    w(i) = V(1,i)^2;
end

end

```

```

function f = fInitial(r, a, b)
    f = a*(r.^2).*exp(-b*r);
end

```

```

function f = fAnalytical(r, t, kG, a, b)
    f = zeros(length(r),1);
    for i=1:length(r)
        arg = r(i)^2-2*kG*t;
        if (arg > 0)
            f(i) = r(i)/sqrt(arg).*fInitial(sqrt(arg), a, b);
        end
    end
end

```

```

%% Mean value
function m = Lm(w,L)

m = dot(w,L);

end

```

```

%% Standard deviation
function sigma = StdDev(w,L)

m = Lm(w,L);
sigma = sqrt( dot(w, L.^2) - m.^2);

end

```

```

%% Moments of the analytical solution
function muk = AnalyticalMoments(k, r, t, kG, a, b)

muk = 0.;
for j=1:length(r)-1
    deltar = r(j+1)-r(j);
    Ic = 0.50*(r(j+1)^(k)*fAnalytical(r(j+1), t, kG, a, ...
        b)+r(j)^(k)*fAnalytical(r(j), t, kG, a, b));
    muk = muk + Ic*deltar;
end

end

```