

Homework #1 - Solutions

The system considered in this problem can be interpreted physically as the Euler equations of solid-body motion with additional linear damping and driving by a stochastic force. In this interpretation, \tilde{X}_i corresponds to the angular momentum \tilde{M}_i around the i -axis

and

$$A_i = \frac{(I_j - I_k)}{I_j I_k} \quad i, j, k \text{ cyclic permutations of } 1, 2, 3$$

in terms of the moments of inertia I_1, I_2, I_3 of the solid body. In this interpretation the "energy" $\frac{1}{2}(\tilde{X}_1^2 + \tilde{X}_2^2 + \tilde{X}_3^2)$ is actually one-half of the total angular momentum.

This system has been studied in the past as a testing ground for closure ideas. For example, see

R. H. Kraichnan, "Direct-interaction approximation for a system of several interacting simple shear waves," Phys. Fluids 6 1603-1609 (1963)

(a) The direct ensemble results are shown in the following plots. The run time was 4499.57 secs or just about 1 hour and 15 minutes.

(b) The backward operator $\hat{\mathcal{L}}^*$ for the 3-mode system is

$$\hat{\mathcal{L}}^* = \sum_{(ijk)} A_i X_j X_k \frac{\partial}{\partial X_i} - \sum_i \nu_i X_i \frac{\partial}{\partial X_i} + \sum_i \kappa_i \frac{\partial^2}{\partial X_i^2}$$

where $(ijk) = (123), (231), (312)$. We thus see that

$$\hat{\mathcal{L}}^* (X_i^2) = 2A_i \underbrace{X_i X_j X_k}_{X_1 X_2 X_3} - 2\nu_i X_i^2 + 2\kappa_i, \quad i=1,2,3$$

and

$$\hat{\mathcal{L}}^* (X_1 X_2 X_3) = \sum_{(ijk)} A_i X_j^2 X_k^2 - (\nu_1 + \nu_2 + \nu_3) X_1 X_2 X_3.$$

Using the definitions $M_i = \langle \tilde{X}_i^2 \rangle$ and $T = \langle \tilde{X}_1 \tilde{X}_2 \tilde{X}_3 \rangle$, we get that

$$\frac{dM_i}{dt} = \langle \hat{\mathcal{L}}^* (\tilde{X}_i^2) \rangle = 2A_i T - 2\nu_i M_i + 2\kappa_i$$

$$\frac{dT}{dt} = \sum_{(ijk)} A_i \langle X_j^2 X_k^2 \rangle - (\nu_1 + \nu_2 + \nu_3) T.$$

If we make the cumulant expansion, then

$$\begin{aligned} \langle X_j^2 X_k^2 \rangle &= \langle X_j^2 \rangle \langle X_k^2 \rangle + 2(\langle X_j X_k \rangle)^2 \\ &+ C_{jjkk} = M_j M_k + 2(\langle X_j X_k \rangle)^2 + C_{jjkk} \end{aligned}$$

where C_{jjkk} is the 4th-order cumulant of the random vector \tilde{X} .

In the $\mathcal{Q}N$ -closure at 3rd-order, one drops the 4th-order cumulants C_{jjkk} . We shall now show furthermore by symmetry arguments that

$$\langle X_j X_k \rangle = 0, \quad j \neq k.$$

Note that the original stochastic equations are invariant under three stochastic reflection symmetries:

$$\begin{aligned} (\tilde{X}_1, \tilde{X}_2, \tilde{X}_3) &\rightarrow (\hat{X}_1, -\hat{X}_2, \hat{X}_3) \\ (\tilde{X}_1, \tilde{X}_2, \tilde{X}_3) &\rightarrow (-\tilde{X}_1, \tilde{X}_2, -\tilde{X}_3) \\ (\tilde{X}_1, \tilde{X}_2, \tilde{X}_3) &\rightarrow (-\tilde{X}_1, -\tilde{X}_2, \tilde{X}_3). \end{aligned}$$

Let us show just the first. Since

$$\dot{\tilde{X}}_1 = A_1 \tilde{X}_2 \tilde{X}_3 - \nu_1 \tilde{X}_1 + \tilde{F}_1(t) = A_1 (-\hat{X}_2) (-\hat{X}_3) - \nu_1 \hat{X}_1 + \tilde{F}_1(t)$$

the equation for \tilde{X}_1 is invariant under this transformation. The equation for \tilde{X}_2 when multiplied by -1 becomes

$$(-\dot{\tilde{X}}_2) = A_2 \tilde{X}_1 (-\tilde{X}_3) - \nu_2 (-\tilde{X}_2) + \underbrace{(-\tilde{F}_2(t))}_{\tilde{F}'_2(t)}$$

Note that $\tilde{F}'_2(t) = -\tilde{F}_2(t)$ is a Gaussian white-noise which is statistically identical to $\tilde{F}_2(t)$. Thus, the equation for \hat{X}_2 is invariant under the transformation. The discussion of the equation for \tilde{X}_3 is identical to that for \hat{X}_2 .

Note that the initial distribution

$$\rho_0(x_1, x_2, x_3) = \frac{1}{\sqrt{(2\pi)^3 \sigma_1^2 \sigma_2^2 \sigma_3^2}} \exp\left[-\left(\frac{x_1^2}{2\sigma_1^2} + \frac{x_2^2}{2\sigma_2^2} + \frac{x_3^2}{2\sigma_3^2}\right)\right]$$

is also invariant under the symmetries, $\rho_0(x_1, -x_2, -x_3) = \rho_0(x_1, x_2, x_3)$, etc. Since the initial distribution and the dynamics are both invariant, so are all averages, at any time. In particular, using the symmetry $(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) \rightarrow (\tilde{x}_1, -\tilde{x}_2, -\tilde{x}_3)$

$$\langle \tilde{x}_1(t) \tilde{x}_2(t) \rangle = \langle \tilde{x}_1(t) (-\tilde{x}_2(t)) \rangle = -\langle \tilde{x}_1(t) \tilde{x}_2(t) \rangle$$

so that

$$\langle \tilde{x}_1(t) \tilde{x}_2(t) \rangle = 0$$

for all times t . The same argument applies for all $i \neq j$:

$$\langle \tilde{x}_i(t) \tilde{x}_j(t) \rangle = 0, \quad i \neq j.$$

Using this symmetry result together with the QN-closure thus gives

$$\langle x_j^2 x_k^2 \rangle \rightarrow M_j M_k$$

and the final equation for T becomes

$$\frac{dT}{dt} = A_1 M_2 M_3 + A_2 M_1 M_3 + A_3 M_1 M_2 - (\nu_1 + \nu_2 + \nu_3) T$$

Solving these equations for M_i , $i=1,2,3$ and T by direct numerical integration with the Euler scheme takes 4.862×10^{-3} secs. This is about a million times faster than the direct ensemble method applied in (a). The results initially are in very close agreement with the direct ensemble results. This is not a surprise. The direct ensemble calculation was initiated at time $t=0$ with Gaussian statistics, for which the quasi-normal closure is exact. As time proceeds we see that the QN closure gives qualitatively correct results, but begins to differ quantitatively. In particular, the QN closure overpredicts the triple moment T and thus overpredicts the transfer of energy from mode-1 into modes 2-3.

(c) For the surrogate variables we see that

$$\begin{aligned}
 \langle \tilde{Y}_i^2 \rangle &= \beta_i^2 \langle \tilde{N}_i^2 \rangle + 2\beta_i\beta_4 \langle \tilde{N}_i \tilde{N}_j' \tilde{N}_k' \rangle + \beta_4^2 \langle (\tilde{N}_j')^2 (\tilde{N}_k')^2 \rangle \\
 &= \beta_i^2 \langle \tilde{N}_i^2 \rangle + 2\beta_i\beta_4 \langle \tilde{N}_i \rangle \langle \tilde{N}_j' \rangle \langle \tilde{N}_k' \rangle \\
 &\quad + \beta_4^2 \langle (\tilde{N}_j')^2 \rangle \langle (\tilde{N}_k')^2 \rangle \\
 &= \beta_i^2 + \beta_4^2
 \end{aligned}$$

using the independence of the random variables and $\langle \tilde{N}_i^2 \rangle = \langle (\tilde{N}_i')^2 \rangle = 1$.

We likewise see that

$$\begin{aligned}
 \langle \tilde{Y}_1 \tilde{Y}_2 \tilde{Y}_3 \rangle &= \langle (\beta_1 \tilde{N}_1 + \beta_4 \tilde{N}'_2 \tilde{N}'_3) (\beta_2 \tilde{N}_2 + \beta_4 \tilde{N}'_1 \tilde{N}'_3) (\beta_3 \tilde{N}_3 + \beta_4 \tilde{N}'_1 \tilde{N}'_2) \rangle \\
 &= \beta_4^3 \langle (\tilde{N}'_1)^2 (\tilde{N}'_2)^2 (\tilde{N}'_3)^2 \rangle \\
 &= \beta_4^3 \langle (\tilde{N}'_1)^2 \rangle \langle (\tilde{N}'_2)^2 \rangle \langle (\tilde{N}'_3)^2 \rangle = \beta_4^3
 \end{aligned}$$

since all the other seven terms, when factorized using statistical independence, contain at least one factor

$$\langle \tilde{N}_i \rangle = \langle \tilde{N}'_i \rangle = \langle \tilde{N}_i^3 \rangle = \langle (\tilde{N}'_i)^3 \rangle = 0$$

for $i=1,2,3$.

Finally,

$$\tilde{Y}_i^2 = \beta_i^2 \tilde{N}_i^2 + 2\beta_i \beta_4 \tilde{N}_i \tilde{N}'_j \tilde{N}'_k + \beta_4^2 (\tilde{N}'_j)^2 (\tilde{N}'_k)^2.$$

It is easy to check that the only non-vanishing contributions to $\langle \tilde{Y}_1^2 \tilde{Y}_2^2 \rangle$, for example, are

$$\begin{aligned}
 \langle \tilde{Y}_1^2 \tilde{Y}_2^2 \rangle &= \beta_1^2 \beta_2^2 \langle \tilde{N}_1^2 \rangle \langle \tilde{N}_2^2 \rangle + \beta_1^2 \beta_4^2 \langle \tilde{N}_1^2 \rangle \langle (\tilde{N}'_1)^2 \rangle \langle (\tilde{N}'_3)^2 \rangle \\
 &\quad + \beta_2^2 \beta_4^2 \langle \tilde{N}_2^2 \rangle \langle (\tilde{N}'_2)^2 \rangle \langle (\tilde{N}'_3)^2 \rangle \\
 &\quad + \beta_4^4 \langle (\tilde{N}'_1)^2 \rangle \langle (\tilde{N}'_2)^2 \rangle \langle (\tilde{N}'_3)^4 \rangle \\
 &= \beta_1^2 \beta_2^2 + \beta_1^2 \beta_4^2 + \beta_2^2 \beta_4^2 + 3\beta_4^4,
 \end{aligned}$$

(cont'd)

since

$$\langle \tilde{N}^2 \rangle = 1, \quad \langle \tilde{N}^4 \rangle = 3$$

for $\tilde{N} \sim N(0, 1)$. Thus,

$$\begin{aligned} \langle \tilde{Y}_1^2 \tilde{Y}_2^2 \rangle &= (\beta_1^2 + \beta_4^2)(\beta_2^2 + \beta_4^2) + 2\beta_4^4 \\ &= M_1 M_2 + 2\beta_4^4. \end{aligned}$$

The same argument works for all $\langle \tilde{Y}_i^2 \tilde{Y}_j^2 \rangle$, $i \neq j$.

Using the surrogates we get that

$$\begin{aligned} \Phi &= A_1 \langle \tilde{Y}_2^2 \tilde{Y}_3^2 \rangle + A_2 \langle \tilde{Y}_1^2 \tilde{Y}_3^2 \rangle + A_3 \langle \tilde{Y}_1^2 \tilde{Y}_2^2 \rangle \\ &= A_1 (M_2 M_3 + 2\beta_4^4) + A_2 (M_1 M_3 + 2\beta_4^4) + A_3 (M_1 M_2 + 2\beta_4^4) \\ &= A_1 M_2 M_3 + A_2 M_1 M_3 + A_3 M_1 M_2 \\ &\quad + 2(A_1 + A_2 + A_3) \beta_4^4 \end{aligned}$$

which the ΦN -closure result. Note that, in this statistical model,

$$\beta_i^2 = M_i - \beta_4^2 = M_i - |T|^{2/3}.$$

In order to have real-valued (i.e. non-imaginary) parameters, it is thus required that

$$|T|^{2/3} \leq M_i, \quad i=1, 2, 3.$$

When the QN-closure is implemented in the equation-free manner using this statistical model, a total run time of 716.78 secs. is required, or about 12 minutes. This is 6.28 times faster than the direct ensemble method. This makes sense, because the equation-free calculation uses 10 microscopic time-steps of size Δt at each of the 100 time-steps (separated by $\Delta t = 10^{-2}$) of the closure equations. This is a total of

$$10 \times 100 = 10^3$$

microscopic time-steps. The direct ensemble calculation with $\Delta t = 10^{-4}$ instead required 10^4 microscopic time-steps, which is about a factor of 10 larger.

The results of the equation-free implementation of the QN closure are shown with the other results. They are quite close to the direct implementation of the QN closure in part (b). There are slight discrepancies due to the statistical fluctuations in the averaging to obtain the closure equations and the interpolation to smooth the output of the equation-free calculation.

```
%AA=[2;-1;-1];
%kk=[1;1e-3;1e-3];
%nu=[1e-3;1;1];
%
%T=1;

AA=[2;-1;-1];
kk=[5e-1;1e-1;1e-1];
nu=[1e-1;5e-1;5e-1];

M0=[0.8;0.6;0.6];
T=1;

N=1e4;

% MONTE CARLO

dt=T*1e-4;
S=T/dt;
Mmc=zeros(3,S+1);
Tmc=zeros(1,S+1);

tmc=0:dt:T;

tic
for i=1:N

x=sqrt(M0).*randn(3,1);
Mmc(:,1)=Mmc(:,1)+x.^2;
Tmc(1)=Tmc(1)+prod(x);

for j=1:S

NN=[x(2)*x(3);x(1)*x(3);x(1)*x(2)];
x = x+(AA.*NN-nu.*x)*dt + sqrt(2*dt*kk).*randn(3,1);

Mmc(:,j+1)=Mmc(:,j+1)+x.^2;
Tmc(j+1)=Tmc(j+1)+prod(x);

end
end
toc

Mmc=Mmc/N;
Tmc=Tmc/N;

figure
plot(tmc,Mmc,':')
xlabel('time t')
ylabel('2nd moments M')

figure
plot(tmc,Tmc,':')
xlabel('time t')
ylabel('3rd moment T')
```

```

pause

% QUASI-NORMAL CLOSURE

dt=T*1e-2;
S=T/dt;
Mqn=zeros(3,S+1);
Tqn=zeros(1,S+1);

tqn=0:dt:T;

tic
Mqn(:,1)=M0;
Tqn(1,1)=0;
for j=1:S
Mqn(:,j+1)=Mqn(:,j)+2*(AA*Tqn(1,j)-nu.*Mqn(:,j)+kk)*dt;
NN=[Mqn(2,j)*Mqn(3,j);Mqn(1,j)*Mqn(3,j);Mqn(1,j)*Mqn(2,j)];
Tqn(1,j+1)=Tqn(1,j)+sum(AA.*NN-nu*Tqn(1,j))*dt;
end
toc

figure
plot(tqn,Mqn,'-',tmc,Mmc,'--')
xlabel('time t')
ylabel('2nd moments M')

figure
plot(tqn,Tqn,'-',tmc,Tmc,'--')
xlabel('time t')
ylabel('3rd moment T')
pause

% EQUATION-FREE IMPLEMENTATION OF QN CLOSURE

dt=T*1e-2;
ddt=T*1e-4;
NS=10;

S=T/dt;
Mef=zeros(3,S+1);
Tef=zeros(1,S+1);

tef=0:dt:T;

tic
Mef(:,1)=M0;
Tef(1,1)=0;

for j=1:S
bb4=sign(Tef(j))*(abs(Tef(j)))^(1/3);
bb=sqrt(abs(Mef(:,j)-bb4^2));

```

```

dMdt=zeros(3,1); dTdt(1,1)=0;
for i=1:N
NN=randn(3,1);NNp=randn(3,1);
NNNp=[ NNp(2)*NNp(3);NNp(1)*NNp(3);NNp(1)*NNp(2) ];
x0=bb.*NN+bb4*NNNp;

x=x0;
for k=1:NS
NN=[x(2)*x(3);x(1)*x(3);x(1)*x(2)];
x = x+(AA.*NN-nu.*x)*ddt + sqrt(2*ddt*kk).*randn(3,1);
end
dMdt=dMdt+(x.^2-x0.^2)/ddt/NS;
dTdt=dTdt+(prod(x)-prod(x0))/ddt/NS;

end
dMdt=dMdt/N;dTdt=dTdt/N;

Mef(:,j+1)=Mef(:,j)+dMdt*dt;
Tef(j+1)=Tef(j)+dTdt*dt;

end
toc

POLM1=polyfit(tef,Mef(1,:),4);M1efs=polyval(POLM1,tef);
POLM2=polyfit(tef,Mef(2,:),4);M2efs=polyval(POLM2,tef);
POLM3=polyfit(tef,Mef(3,:),4);M3efs=polyval(POLM3,tef);
Mefs=[M1efs;M2efs;M3efs];
POLT=polyfit(tef,Tef,4);Tefs=polyval(POLT,tef);

figure
plot(tef,Mef,':',tef,Mefs,'-')
xlabel('time t')
ylabel('2nd moments M')

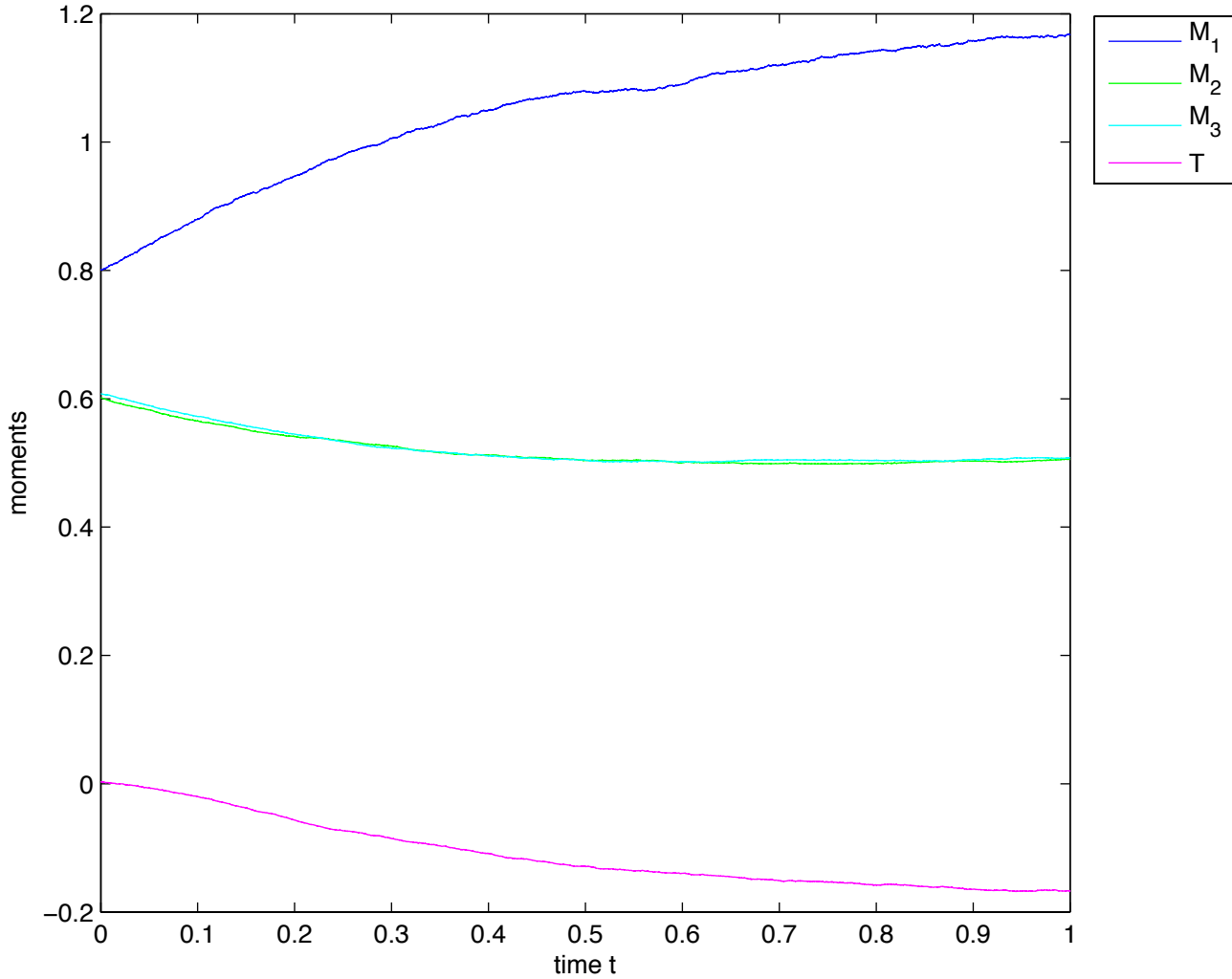
figure
plot(tef,Tef,':',tef,Mefs,'-')
xlabel('time t')
ylabel('3rd moment T')

figure
plot(tef,Mefs,'-',tmc,Mmc,'--')
xlabel('time t')
ylabel('2nd moments M')

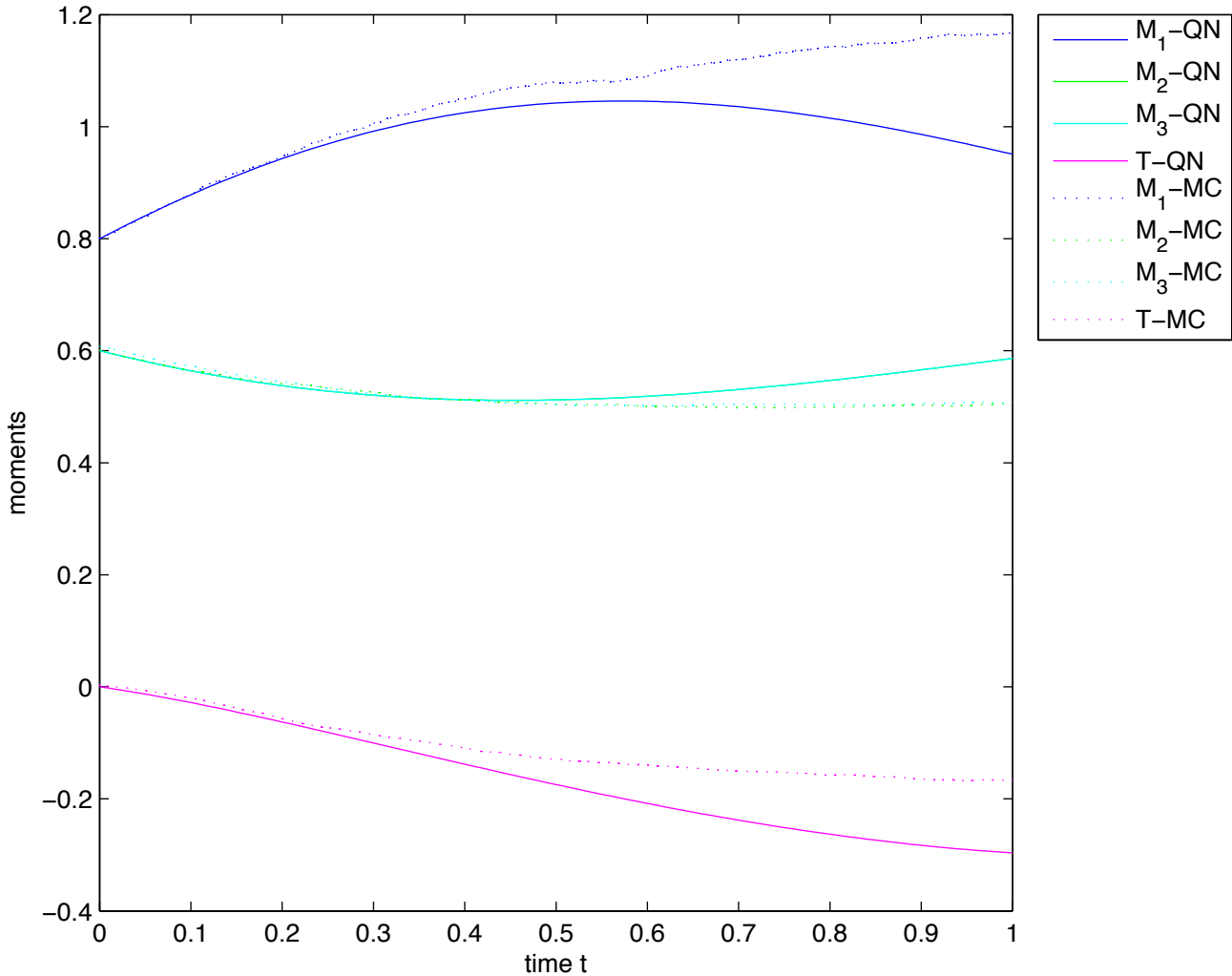
figure
plot(tef,Tefs,'-',tmc,Tmc,'--')
xlabel('time t')
ylabel('3rd moment T')

```

Direct Ensemble Method Results for Three-Mode Model



Quasi-Normal Closure Results for Three-Mode Model



Equation-Free Implementation of QN Closure for Three-Mode Model

